I²CNER

International Institute for Carbon-Neutral Energy Research

2022 Annual Report

I²CNER

wpi World Premier International Research Center Initiative

KYUSHU UNIVERSITY

ILLINOIS

Table of Contents

World Premier International Research Center Initiative (WPI)

Background

An intensifying global demand for talented researchers is accelerating the need to circulate good brains among the world. This trend has prompted Japan to establish new research centers that attract top-notch researchers from around the world so as to be a hub within global brain circulation.

Program Summary

WPI provides concentrated support for projects to establish and operate research centers that have at their core a group of very high-level investigators. These centers are to create a research environment of a sufficiently high standard to give them a highly visible presence within the global scientific community—that is, to create a vibrant environment that will be of strong incentive to frontline researchers around the world to want to come and work at these centers.

Formulation of New Missions

In December 2020, new missions were formulated with the addition of "Values for the Future," and the enhancement of the four conventional missions: Science, Fusion, Globalization, and Reform.

New WPI Mission

World-Leading Scientific Excellence and Recognition

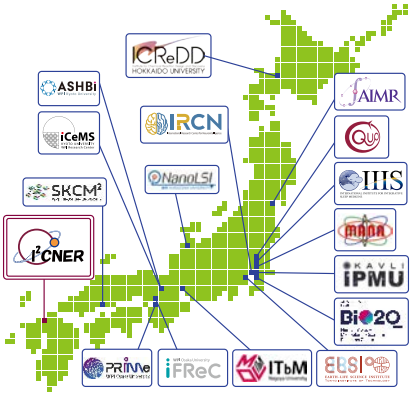
- The Highest Level of Research Impact
- Expanding Knowledge Frontiers through Interdisciplinarity and Diversity

Global Research Environment and System Reform

- Harnessing Talent and Potential through Global Brain Circulation
- Interdisciplinary and Inter-organizational Capacity Building
- Effective, Proactive and Agile Management

Values for the Future

- Societal Value of Basic Research
- Human Resource Building: Higher Education and Career Development
- Self-sufficient and Sustainable Center Development



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 (I²CNER) Kyushu University
Toward the realization of a low-carbon society, I²CNER 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.

Human Biology-Microbiome-Quantum Research Center (Bio2Q) Keio University
Bio2Q will develop novel research techniques to understand the interactions between multiple organs and the microbiome, and develop methods to apply quantum computing to human biology.

International Institute for Sustainability with Knotted Chiral Meta Matter(SKCM²) Hiroshima University
While introducing a new research paradigm of"knotted chiral meta matter,"SKCM2 aspires to create artificial materials with highly desirable material properties by design to help address challenging global problems, like the growing energy demand and climate change.

Premium Research Institute for Human Metaverse Medicine (PRIMe) Osaka University
PRIMe aims at creating digital twins of humans that will replicate biological phenomena and pathological processes in human organs in cyberspace and focuses on advanced integration of human organoid-based biomedical science and information and mathematical sciences.

WPI Academy Centers (other than I²CNER)

Message from the Director

Climate change issues such as global warming are becoming more serious recently, and the shift to a carbon-neutral society based on renewable energy has become important and urgent global issue. International Institute for Carbon-Neutral Energy Research (I²CNER) was established in 2010 as the WPI Institute, the only institute at that time bearing the name of Carbon-Neutral Energy, and joined the WPI Academy member in 2020. In the last 13 years, I²CNER has been working comprehensively to develop the innovative science and technology necessary to realize a carbon-neutral society.

There are still many difficult challenges exist for shifting from the current energy system that mainly uses fossil fuels to a society based on renewable energy and materials. However, for this, novel energy conversion technology as well as overall design of a social system which uses materials and energy linked each other is required. In this regard, under one roof, I²CNER is developing to create innovative energy conversion technologies that are interconnected.

Renewable energies such as solar and wind power are widely and evenly distributed energy without regional segregation, and are equally distributed to all people on earth. However, renewable energy has large fluctuations and low energy density, so it is required to develop an effective method for leveling and increase in power density. At I²CNER, we are developing innovative materials and processes such as solar cells that efficiently convert solar energy to electricity, and steam electrolysis that can convert to hydrogen as an energy carrier. Considering CO_2 as a carbon resource and also a hydrogen carrier, the efficient conversion process of CO_2 to useful compounds are also developing. In particular, we are working on the development of materials that can separate CO_2 which is diluted, such as in the atmosphere.

On the other hand, we are also investigating the development of new interdisciplinary science for innovative photocatalysts such as dye modification and enzyme, which can directly convert solar energy into hydrogen. Finally, underground storage of CO_2 will also be necessary for net decrease of CO_2 emission, and therefore, storage technology and the stability of stored CO_2 underground are further studied. We will contribute to a carbon-neutral society in a holistic approach, by creation of innovative science and engineering with interdisciplinary sciences at different time and distance scales.

In the last 13 years, I²CNER has been focused on the creation of high efficiency in conversion technology for realization of carbon-neutral energy society. As a next step, we newly added rapid conversion as a keyword and also focus on the energy that is not being used effectively, cultivating a new academic field by integrating disciplines. We aim to contribute to realizing a carbon-neutral energy society by novel concepts including a scenario and design for renewable society.

Professor Tatsumi Ishihara
Director, International Institute for Carbon-Neutral Energy Research (I²CNER)

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 a recent inductee 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. I²CNER is furthering this analysis across the spectrum of available technologies, with a focus on the technologies being developed within I²CNER. 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 I²CNER's international identity. The members of this platform, who are world experts with a solid record of international research experiences, collaborate with I²CNER'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 I²CNER scientific advances

to applicable technology transfer through a large and growing network of I²CNER 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, I²CNER 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)<launched in Apr. 2016>

NEXT-RP is an international research center that develops and evaluates next-generation refrigerants to solve global environmental issues and future energy crises. Our essential duty is to find the following next generation refrigerants: (i) Lower ODP (Ozone Depletion Potential), (ii) Lower GWP (Global Warming Potential), (iii) Non-flammable or Mildly flammable, (iv) No toxicity or Lower toxicity.

Mitsui Chemicals, Inc.-Carbon Neutral Research Center (MCI-CNRC)<launched in Nov. 2021>

MCI-CNRC, in collaboration with Mitsui Chemicals Inc., will develop and acquire cutting-edge environmental infrastructure technologies that will contribute to carbon neutrality, as well as pursue the practical use and commercialization of these technologies. By carrying out focused and efficient research into the elemental technologies needed to achieve carbon neutrality, the center will speed up the process of getting these technologies adopted in society.

Center for Energy Systems Design (CESD) <launched in Nov. 2022>

CESD hopes to promote research on carbon-neutral technologies required for social implementation by collaborating with six research organizations (Hokkaido University, Tohoku University, Tokyo Institute of Technology, Kumamoto University, RIKEN, and National Institute for Materials Science). This center consists of six research teams. The teams of "Light Energy Conversion", "Electric Energy Conversion", "Material Conversion", and "Materials, Storage and Transport" conduct research to enable "high-speed conversion". The "Energy Analysis" research team is responsible for the design of energy research by back-casting. The "Data Science" research team supports each research team by promoting data science, leading to discontinuous innovation. Not only achieving innovative outcomes, but the center also aims to foster the scientists of the future by making the center a field where young researchers can actively participate.

CENTERS FOR COMMON EDUCATION AND RESEARCH

Research Center for Negative Emissions Technologies (K-NETs)<launched in Apr. 2021>

This center aims to develop negative emissions technologies of greenhouse gases, i.e., developing technologies for CO_2 capture directly from the atmosphere, conversion and storage of the captured CO_2, and utilization of renewable energy. CO_2 can be captured anywhere since air exists ubiquitously on the earth. This nature of ubiquitous existence will enable the construction of an energy-robust society through local production for local consumption of carbon resources and contribute to the control of global warming by underground storage of excess emissions. This research project is supported by the Moonshot Research and Development Program launched by the Cabinet Office of Japan.

I²CNER Carbon Neutral Vision

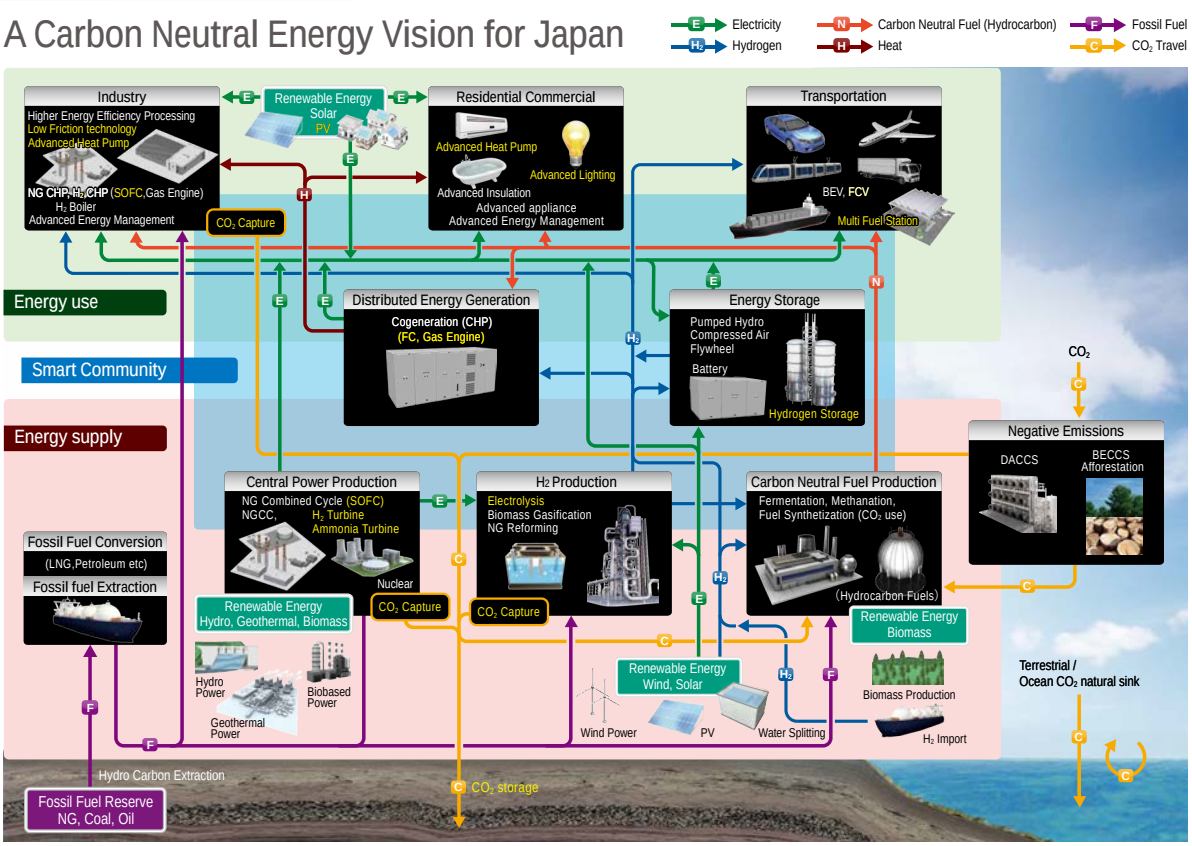


Figure 4.1. Parameter Space of Technology Options.

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), converting captured CO_2 to useful C-Fuels, 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 will 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 emissions since a large unused capacity although somewhat accelerated, 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

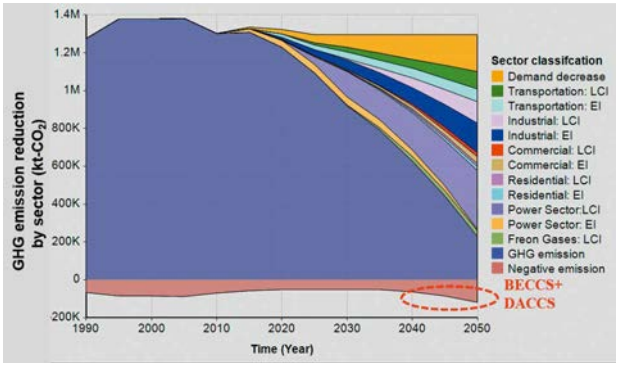


Figure 4.2. CO_2 reduction relative to 2010 by sector in Scenario A.

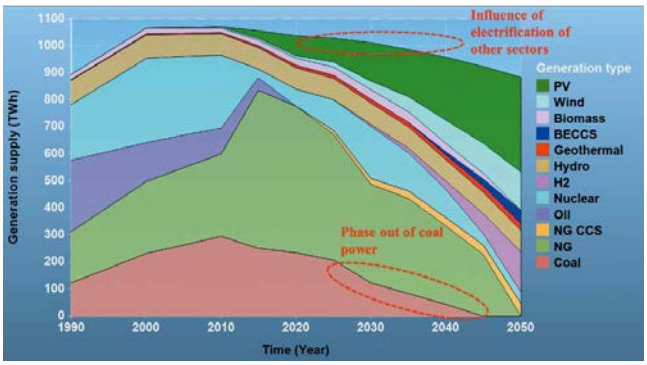


Figure 4.3. Electricity mix by generation type in Scenario A.

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

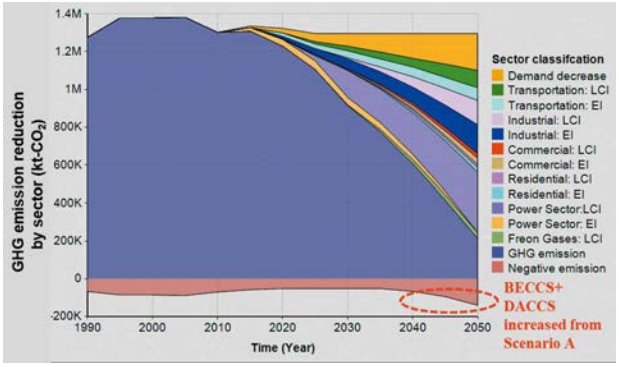


Figure 4.4. CO_2 reduction relative to 2010 by sector in Scenario B.

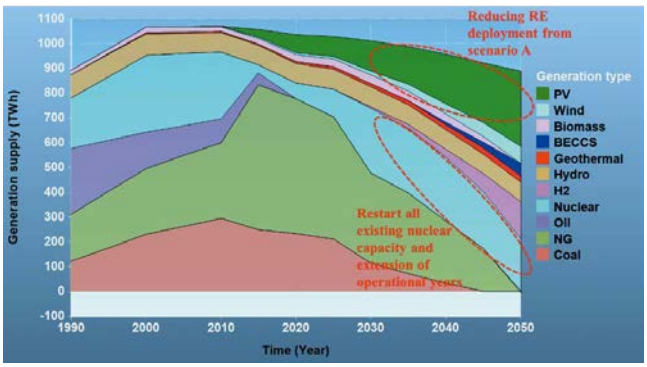


Figure 4.5. Electricity mix by generation type in Scenario B.

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.

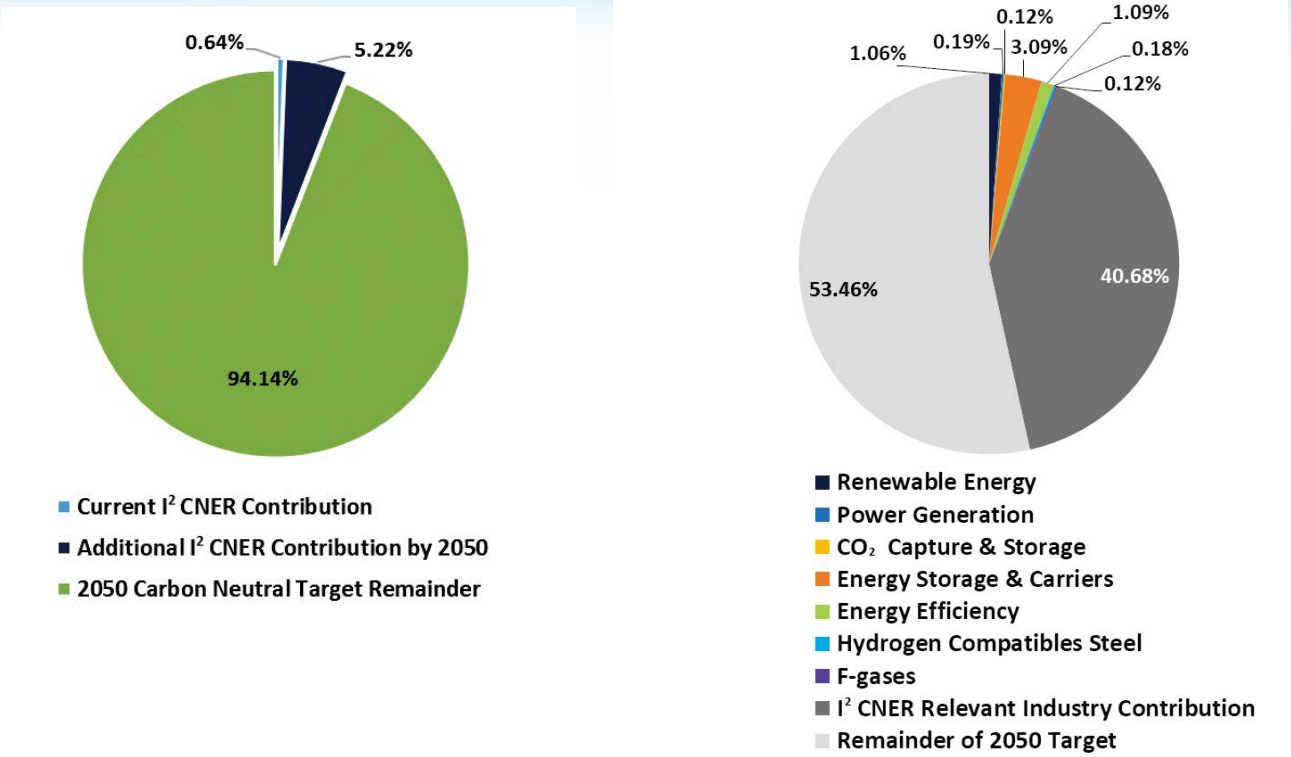
I²CNER's Contribution to the 2050 CO_2 Reduction Target

Based on our analysis of current and future achievements, approximately 0.64% 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 40.7% 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 5.68% reported in the 2021 Annual Report to 5.86%) is that 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, and due to the progress of I²CNER research roadmaps. This implies the research direction of I²CNER is suitable for an energy transition to a carbon-neutral energy society.

As shown in Fig. 5b, 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 2021 Annual Report are primarily due to scenario and incremental research achievement influences, shown as follows. The contribution of energy storage and carriers increases (from 3.0% to 3.09%) due to the necessity of a larger introduction of low carbon hydrogen. The contribution of CO_2 capture and storage did not change, as issues such as long lead times for implementation and limited availability of storage sites persist. The contribution of energy efficiency (1.09%) has increased moderately, while the contribution of renewable energy increases (from 1.03% to 1.06%) due to a slightly larger anticipated introduction of PV. The contribution of hydrogen compatibles steel increases marginally (from 0.17% to 0.18%) again due to a larger introduction of low carbon hydrogen. The contribution of power generation (0.19%) is similar because the decrease in natural gas power generation (SOFC) and the increase in hydrogen power generation (hydrogen turbine) cancel each other out. The contribution of F-gases (0.12%), which includes the development of new refrigerants for heat pumps with lower GWP, is unchanged from 2021. Finally, the contribution to the overall relevant industry efforts increases (to 40.7%) due to complementary industry efforts toward decarbonization. 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.



(a) Current and Future Contributions

(b) Overall Contributions to 2050 CO_2 Reduction Target

Figure 5. I²CNER's current and future contributions to CO_2 reduction in Japan.

Advanced Energy Materials

1. Tailoring composition and deformation modes at the microstructural level for next generation low-cost high-strength austenitic stainless steels (PI Sofronis, PI Somerday, PI Stubbins, Prof. Tsuchiyama, PI Kubota, Prof. Aravas)

In this collaborative effort we are exploring the concept that the hydrogen-induced degradation of austenitic steels is advanced by hydrogen enhanced localized plasticity (HELP) and it is the intrinsic and concerted action of chemical composition with HELP that seems to govern the mechanical phenomena such as the onset of fracture. It is exactly this intrinsic character of the embrittlement that this initiative aims to elucidate in an austenitic steel and accordingly assess the correlation and importance of classic metrics such as thermodynamic stability, stacking fault energy (SFE), and martensite formation with embrittlement. More specifically we are working to establish detailed relationships specific to the effects of alloy composition, short-range ordering (SRO), and microsegregation in the presence of hydrogen on the transition between homogeneous deformation and localized plasticity in shear bands. We have developed a suite of four model alloys, all of which satisfy the aforementioned classic metrics of hydrogen resilience. Comparing the tensile properties of these alloys in both annealed and hydrogen charged conditions (Fig. 6.1), reveal a range of responses, which we are beginning to understand in the context of nanoscale chemical heterogeneities that have been characterized by an emerging scanning transmission electron microscopy technique. Ultimately, through our collaboration we are deliberately developing cost-effective, hydrogen resistant alloys capable of meeting the goal of an economical outgrowth of hydrogen applications and delivery systems.

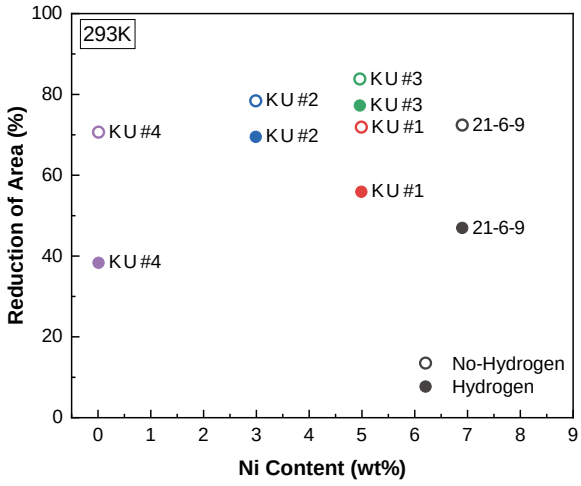


Fig. 6.1. Performance of the four model alloys designed for this study, many of which show surprising resilience to hydrogen embrittlement (little change in reduction of area once charged with hydrogen, filled data points) despite exceptionally low nickel concentrations making them more economically viable while also providing a platform to understand the impact of localize chemical heterogeneity on the deformation mechanisms.

To understand the effect of the presence of the SRO domains on the macroscopic flow localization in the austenitic steels under consideration, we investigated the interaction of the local dislocation structure evolution with SRO in the presence of hydrogen. This interaction derives from the local SRO stress fields arising from the associated misfit strains and the difference of the SRO's elastic moduli from those of the surrounding matrix. The magnitude of these local strains and moduli, which depends on the SRO composition and its interaction with hydrogen, is calculated by atomistic calculations and experimental measurements. We study how the hydrogen-enhanced dislocation generation rate and potentially the hydrogen-weakened SRO misfit strains reduce the critical applied stress required for a dislocation pileup to break through the repulsive stress field of an SRO domain. The potential reduction of this critical applied stress has strong implications for changing the macroscopic deformation mode from homogenous to localized into bands of intense shear. By quantifying the micromechanics of the dislocation/hydrogen/SRO interactions, we find that the presence of the SRO domains can induce shear localization. Moreover, the presence of hydrogen reduces the macroscopic strain for the onset of localization (Fig. 6.2).

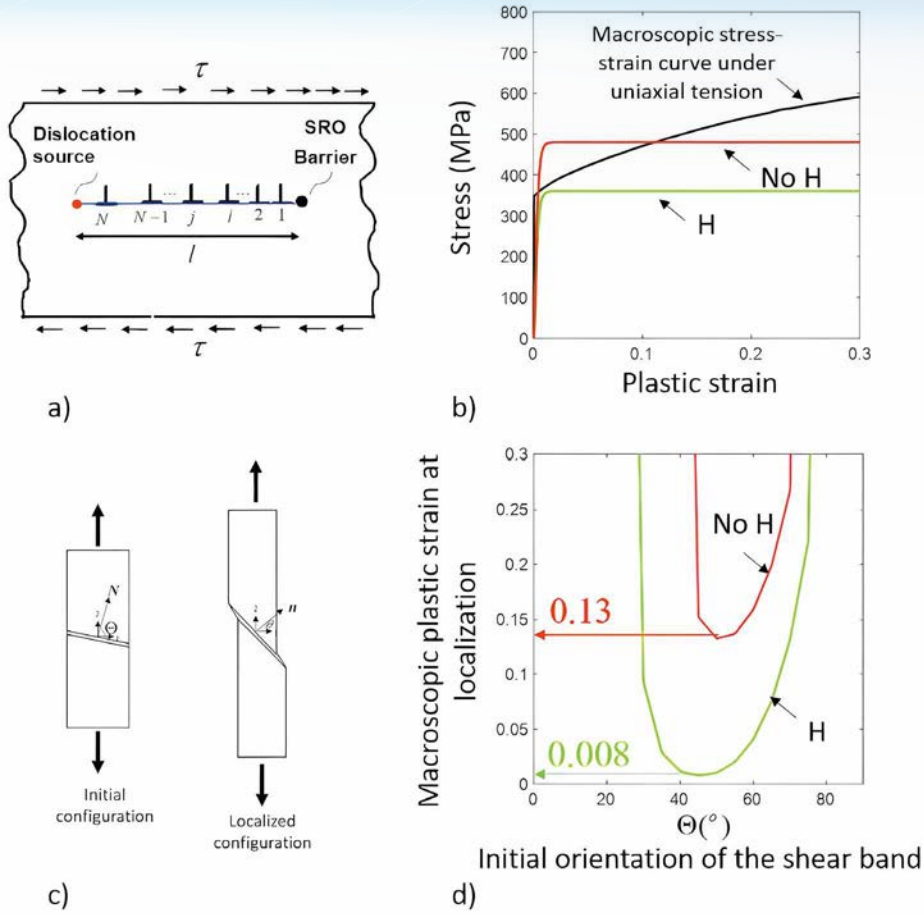


Fig. 6.2. Study of the onset of shear localization in uniaxial macroscopic tension: (a) interaction of a dislocation pileup with an SRO domain in which hydrogen leads to easier emission of dislocations and causes weakening of the SRO stress field. The ensuing stress-strain curve at the microscale is shown in (b), where the effect of hydrogen is to lower the critical stress required to overcome the SRO stress field. The micromechanical model in (b) is used to study whether macroscopic homogeneous deformation in uniaxial tension is compatible with a band of localized shear as shown in (c). The effect of hydrogen on the critical strain for the onset of localization for different band orientations.

2. Safe, One-Pot, Homogeneous Direct Synthesis of H_2O_2 (PI Ogo)

Hydrogen peroxide is an environmentally friendly oxidizing agent but current synthetic methods are wasteful. This is a result of the high flammability of H_2/O_2 mixtures and/or the requirement for cocatalysts. In this paper, we report the synthesis of H_2O_2 by means of a homogeneous catalyst, which allows a safe, one-pot synthesis in water, using only H_2 and O_2. This catalyst is capable of removing electrons from H_2, storing them for the reduction of O_2, and then permitting the protonation of the reduced oxygen to H_2O_2. The turnover number (TON) is 910 under an H_2/O_2 (95/5) atmosphere (1.9 MPa) for 12 h at 23 °C, which is the highest of any homogeneous catalyst. Furthermore, we propose a reaction mechanism based on two crystal structures.

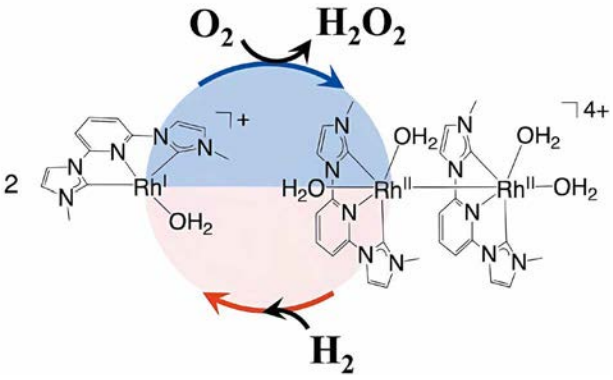


Fig. 6.3. Proposed catalytic reaction mechanism of a synthesis of H_2O_2 from H_2 and O_2 in water. Acetate ions could replace with aqua ligands, but this has no apparent effect on the catalytic mechanism.

These results meet the short- and a mid-term milestone for molecular modification of biological and synthetic H_2 and CO_2 catalysts in Project 1 of the Advanced Energy Materials Thrust's roadmap.

The importance of this study is that a new homogeneous catalyst enables the safe and direct synthesis of hydrogen peroxide.

Disciplines: Inorganic Biochemistry, Coordination chemistry, material synthesis

3. Understanding the roles of hydroxide in CO_2 electroreduction on Cu electrode for achieving variable selectivity (PI Yamauchi and PI Staykov)

Hydroxide-derived copper (OH/Cu) electrodes exhibit excellent performance for electrocatalytic CO_2 reduction reaction (CO_2RR). However, the role of hydroxide (OH) in CO_2RR remains controversial and therefore the origin for the selectivity enhancement emerging on OH/Cu has not been fully understood. In the present work, we quantitatively evaluated surface OH by electroadsorption and established a direct correlation between the OH amount and selectivity for the production of CH_4 and C_{2+} on OH/Cu with the help of computational investigations concerning work functions of the surface. Based on these findings, we demonstrated variable selectivity using OH/Cu electrodes having a controlled OH amount; three OH/Cu electrodes realized their distinct selectivity such as Faradaic efficiency (FE) for the production of CH_4 (CH_4 FE) of 78%, C_{2+} FE of 71%, and the ratio of C_{2+}-to-CH_4 >355. The proposed simple strategy for the selectivity control would contribute to further quantity synthesis of value added chemicals using CO_2RR.

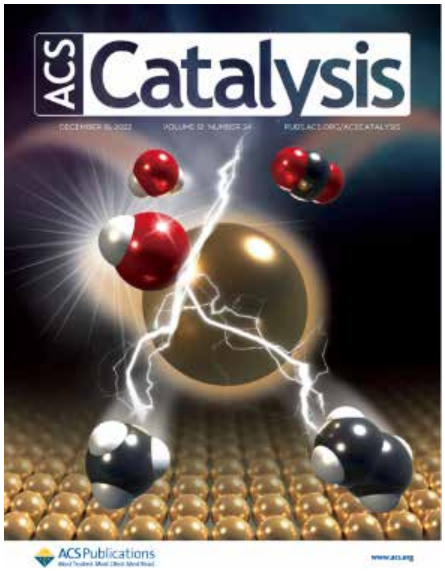


Fig. 6.4. Hydroxide exerts a significant influence on the performance of the electrochemical reduction of CO_2, but its specific role is unclear. Here, Mingxu Sun, Aleksandar Staykov and Miho Yamauchi present how hydroxide on Cu electrodes works in CO_2 electroreduction to achieve selectivity control of the products.

4. Development of hydrogen-compatible SUS304 (Prof. Macadre, Prof. Tsuchiyama, Prof. Masumura)

This research was supported by Kakenhi JP20K04178.

Combining relatively simple processes (high temperature nitrogen addition and cold-rolling), a low-nickel austenitic stainless steel, SUS304, was processed to become hydrogen compatible. Several nitrogen contents were investigated (0.25 mass%, 0.36mass%, and 0.44mass%). The grain size decreased slightly with increasing nitrogen content. The 0.36mass% nitrogen material displayed the smallest decrease of elongation by hydrogen, so it was chosen for grain refinement (Fig. 6.5 Left). The grain size without annealing twins was 120μm and 50~70μm when counting annealing twins. After cold-rolling and recrystallization, the grain size was 11μm. Fig. 6.5 Right shows the hydrogen compatibility evaluated by the chemical composition (nickel equivalent) and the reduction of ductility by hydrogen (reduced reduction of area, RRA). Increasing the nitrogen content improved the hydrogen compatibility, but above 0.25~0.30mass% nitrogen, the hydrogen compatibility decreased. This was cancelled by significant grain refinement.

This research has shown several important points for the development of hydrogen-compatible alloys:

- There is an upper limit to the amount of nitrogen added for hydrogen compatibility, at 0.30mass%.
- This upper limit can be extended with grain refinement, and the resulting alloy combines good yield stress (~490MPa), no decrease of elongation, and no embrittlement in hydrogen.
- The nickel equivalent is useful for a first evaluation, but tensile measurements are necessary for final judgement of hydrogen compatibility.

This achievement is toward the short-term milestone of Project 4 (alloy design of low-Ni high-SFE austenitic stainless steels).

This research received an "Excellent Poster Presentation Award" at the 6th International Conference on Materials and Reliability (ICMR2022).

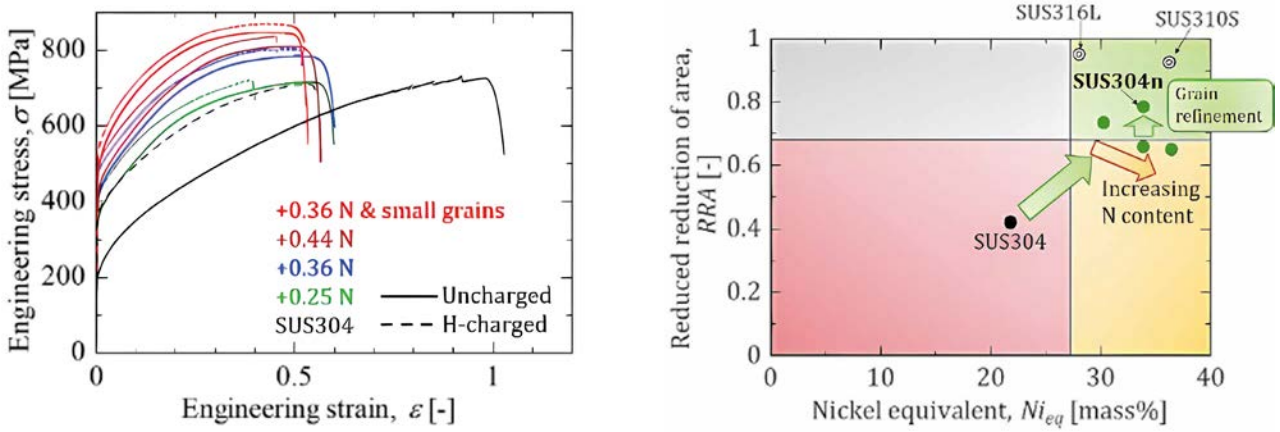


Fig. 6.5. Left: Effect of solute nitrogen content and grain size on the tensile properties of SUS304 with and without hydrogen (indicated nitrogen contents in mass%); Right: Evaluation of the hydrogen compatibility with both chemical composition criterion (Nickel equivalent) and ductility criterion (Reduced reduction of area) (Increasing the nitrogen content decreases the hydrogen compatibility, but this is cancelled by reduced grain size) (Only the green zone is hydrogen compatible).

5. Development of a Novel Photoenergy Conversion System by Plasmon-Induced Charge Separation Using Sunlight as an Energy Source (Prof. Takahashi)

This works aims to develop photoenergy conversion devices with high efficiencies. Although the total amount of sunlight is large, the energy density per unit area is small and the supply is unstable. Therefore, it is important in practical use to devise some means to store and increase the energy density. The localized surface plasmon resonance (LSPR) of metal nanoparticles increases the density of solar energy, and the phenomenon of plasmon-induced charge separation (PICS), which occurs when metal nanoparticles are combined with semiconductors, can be used to convert light energy into electrochemical energy.[3] We previously reported that conventional PICS was applicable to site-selective nanoscale-polymerization (Fig. 6.6a).[4,5] However, conventional PICS has some problems due to the use of n-type semiconductors. One is the low stability of metal nanoparticles. Since oxidation reactions occur on the metal nanoparticles, it may cause the metal nanoparticles themselves to dissolve, even silver nanoparticles, which are known to be relatively stable. Second is the low efficiency of the charge separation. The photoelectric conversion efficiency (η) of the conventional PICS was approximately 1%.[3] In titanium dioxide photocatalysts, metal nanoparticles supported on the photocatalyst function as an electron pool that suppresses recombination of excited electrons and holes, as evidenced by their use as reduction sites.[6] Therefore, electrons transferred to the semiconductor after charge separation by conventional PICS are likely to undergo reverse electron transfer to the metal nanoparticles (recombination in the broad sense). We therefore propose that the above problem can be solved by using a p-type semiconductor, which reverses the charge transfer, because the reduction reaction can proceed on the metal nanoparticles used in PICS (Fig. 6.6b)[7,8]. These results meet the short-term milestone "Establish novel photoenergy conversion system based on charge separation at the nanointerface" in Project 2 of the Thrust's roadmap.

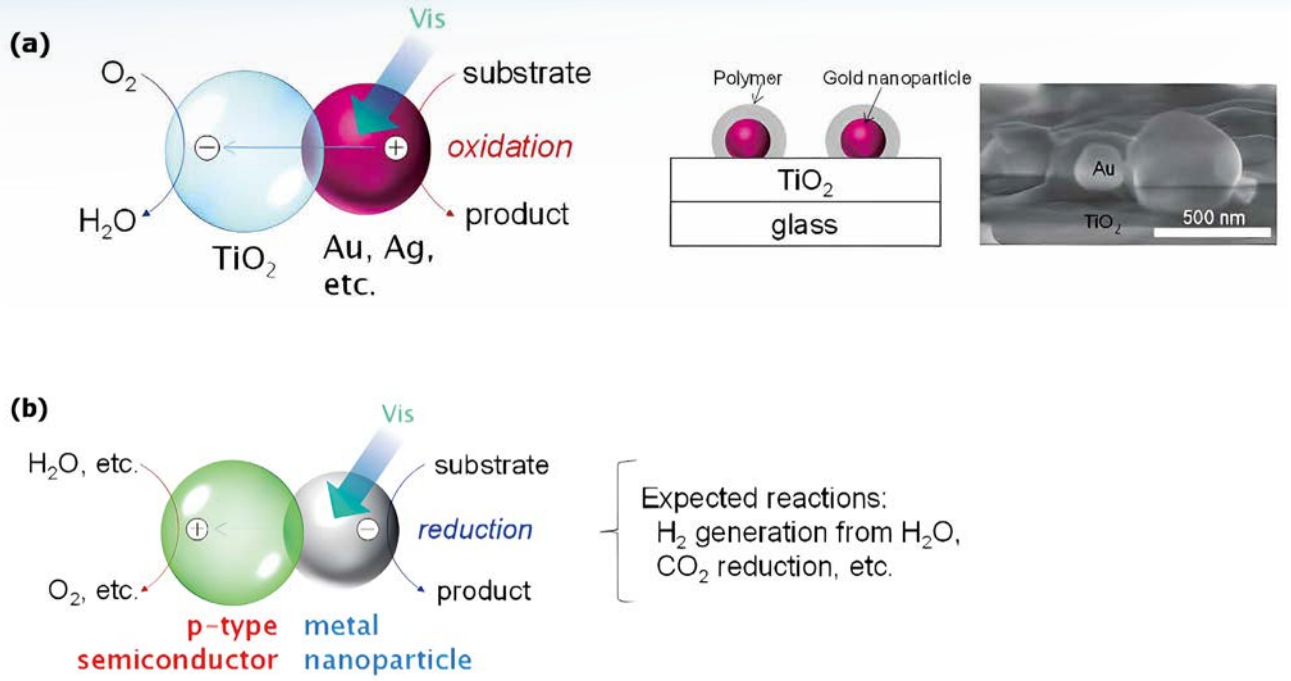


Fig. 6.6. Schematic illustration of (a) conventional PICS with an n-type semiconductor and (b) novel PICS with a p-type semiconductor.

6. Catalyst activation for CO decomposition under chemomechanical effects of fretting and improvement of fretting fatigue strength (PI Kubota and Prof. Komoda)

This study reports the first experimental result showing that the addition of carbon monoxide (CO) to hydrogen gas (H_2) significantly improves fretting fatigue strength (Fig. 6.7). Specifically, the fretting fatigue limit in the CO mixed H_2 was 240 MPa, whereas it was 205 MPa in the H_2. Initially, we anticipated that the hydrogen effect during fretting fatigue test would be mitigated based on our previous accomplishments, which demonstrated that gas molecules with higher affinity for the iron surface preferentially adsorb onto it, resulting in a reduction of hydrogen uptake in the material. Consequently, hydrogen embrittlement was alleviated. However, in this fretting fatigue test, a completely different mechanism was at play. The improvement in fretting fatigue strength was achieved by a reduction in the friction force between the contacting surfaces, brought about by the accumulation of amorphous carbon particles between them. The plausible mechanism for the production of carbon particles involved the decomposition of CO on the iron surface, where the catalytic action was activated by fretting. The accumulation of carbon was not observed in the crack growth test and fracture toughness test conducted in the CO mixed H_2 gas. Therefore, fretting induced a unique chemomechanical effect that activated the catalytic action of the iron for CO decomposition. Initially, the iron surface was deactivated by natural oxide layer covering it, which fretting removes. Additionally, fretting continuously refreshes the catalytic surface by removing reaction products through fretting wear. This study opens up new possibilities in science and engineering by demonstrating that the catalytic actions of metal surfaces can be activated by tribological effects.

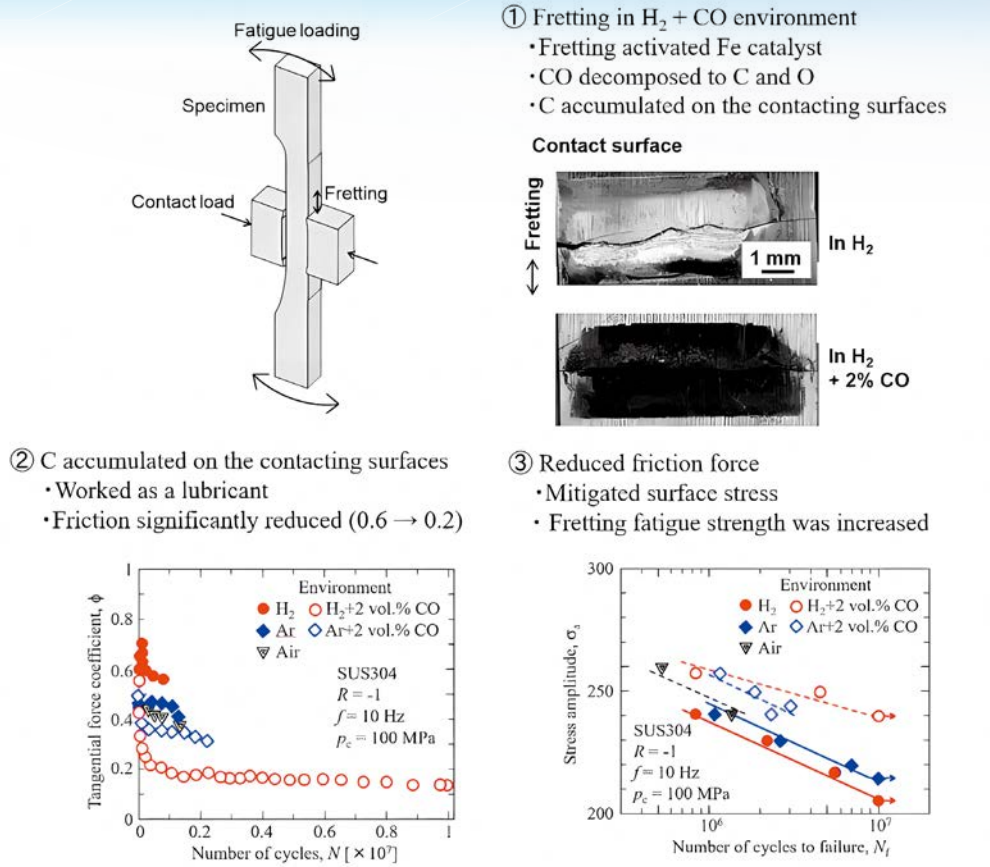


Fig. 6.7. Improvement of fretting fatigue strength in CO-mixed H_2 gas. Fe catalyst for CO decomposition activated through chemomechanical effect of fretting. Production of amorphous carbon on the contacting surfaces reduced the surface stress through the reduction in friction force, resulting in the significant increase of fretting fatigue strength.

References

[1] Ogo S., Yatabe T., Tome T., Takenaka R., Shiota Y, Kato K. (2023), Safe, One-Pot, Homogeneous Direct Synthesis of H_2O_2, Journal of the American Chemical Society, 145(8), 4384-4388. DOI: 10.1021/jacs.2c13149.

[2] Sun M., Staykov A., Yamauchi M. (2022), Understanding the Roles of Hydroxide in CO_2 Electroreduction on a Cu Electrode for Achieving Variable Selectivity, ACS Catalysis, 12(24), 14856-14863. DOI: 10.1021/acscatal.2c03650.

[3] Tian Y., Tatsuma T. (2005), Mechanisms and Applications of Plasmon-Induced Charge Separation at TiO2 Films Loaded with Gold Nanoparticles, Journal of the American Chemical Society, 127(20), 7632-7637. DOI: 10.1021/ja042192u.

[4] Takahashi Y., Furukawa Y., Ishida T., Yamada S. (2016), Site-selective nanoscale-polymerization of pyrrole on gold nanoparticles via plasmon induced charge separation, Nanoscale, 8(16), 8520-8524. DOI: 10.1039/c6nr01531j.

[5] Takahashi Y., Sota Y., Ishida T., Furukawa Y., Yamada S. (2020), Oxidative Reaction Energy in Photopolymerization Inspired by Plasmon-Induced Charge Separation, Journal of Physical Chemistry C, 124(7), 4202-4205. DOI: 10.1021/acs.jpcc.9b09738.

[6] Kubo W., Tatsuma T. (2005), Photocatalytic remote oxidation with various photocatalysts and enhancement of its activity, Journal of Materials Chemistry, 15(30), 3104-3108. DOI: 10.1039/b504752h.

[7] Takahashi Y. (2023), Development of a Highly Efficient Hydrogen Generation System by Plasmon-Induced Charge Separation Using Sunlight as an Energy Source, Readout: Horiba technical reports, 57, 29-32.

[8] Takahashi Y., Yamadori Y., Murayama T., Shingo S., Yamada S., Article in Press.

[9] Kubota M., Komoda R., Nakamura Y. (2022), Improvement of Fretting Fatigue Strength by Carbon Monoxide and Catalyst Activation under Chemomechanical Effects of Fretting, Theoretical and Applied Fracture Mechanics, 121, 103460. DOI: 10.1016/j.tafmec.2022.103460.

Advanced Energy Conversion Systems

1. Defect passivation greatly increases efficiency and long-term stability of perovskite solar cells (PI Adachi and Prof. Matsushima)

The defects in the light-harvesting perovskite absorber layer play a key role in limiting power conversion efficiencies and long-term stability of lead halide perovskite solar cells. Although organic ammonium halides have been widely used for defect passivation in high-performance perovskite solar cells, the stability issue is still a challenge. Herein, we develop a novel material of pyridine-carbazole to passivate defects *via* coordination bonding [1]. With this passivation, the photoluminescence intensity of perovskite films was increased. In addition, the formation of under-coordinated Pb^{2+} defects in perovskite films was reduced significantly, enabling high-performance and long-term stable perovskite solar cells. Three different sets of perovskite solar cells were constructed, namely, without passivation, with phenethylammonium iodide (commonly used for passivation), and with pyridine-carbazole passivation. Remarkably, the perovskite solar cells fabricated using the pyridine-carbazole passivation not only achieved power conversion efficiencies of over 20% but also retained 85% of their initial performances over more than 5000 h (Fig. 6.8). In contrast, the perovskite solar cells without or with phenethylammonium iodide passivation degraded quickly during the long-term operational stability test under light illumination.

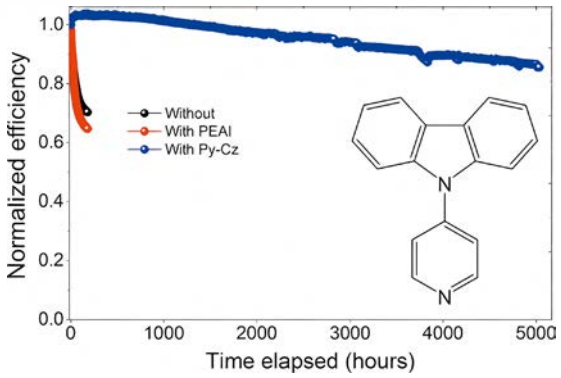


Fig. 6.8. Operational stability of perovskite solar cells under illumination. Pyridine-carbazole (Py-Cz) or phenethylammonium iodide (PEAI) passivation was used.

This method opens up a new opportunity to develop highly efficient and operationally stable perovskite solar cells and is directed to the short-term milestone of Project 5 "Solar energy harvesting for eco-friendly power generation"

2. Mechanism of homogeneous ionomer distribute in the catalyst layer in polymer electrolyte membrane fuel cell (PI Fujigaya)

Catalyst layers (CL) composed of catalyst composites and an ionomer are key components in polymer electrolyte membrane fuel cells (PEMFCs). In particular, the preparation conditions of the CL, starting from the dispersion of the catalyst composite with an ionomer, largely affect the PEMFC performance. In this research, the effects of alcohol content in the dispersion solvent using two binary mixtures composed of water and ethanol were studied. Additionally, Pt-loaded carbon black (CB) and Pt-loaded polymer-wrapped CB were used as the catalyst composites to study the effects of alcohol content on the interaction between the ionomer and the surface of the carbon supports. The CL prepared using the water-rich (80 wt.% water) solvent achieved higher PEMFC performance compared to that prepared using the alcohol-rich (13 wt.% water) solvent. We found that this difference is ascribed to the stronger interaction between the ionomer and CB surface under water-rich conditions. Of interest, when using the polymer-wrapped CB, the difference in PEMFC performance between the CLs from the water-rich and alcohol-rich dispersions was minimal because of the comparable interaction between the ionomer and wrapping polymer surface

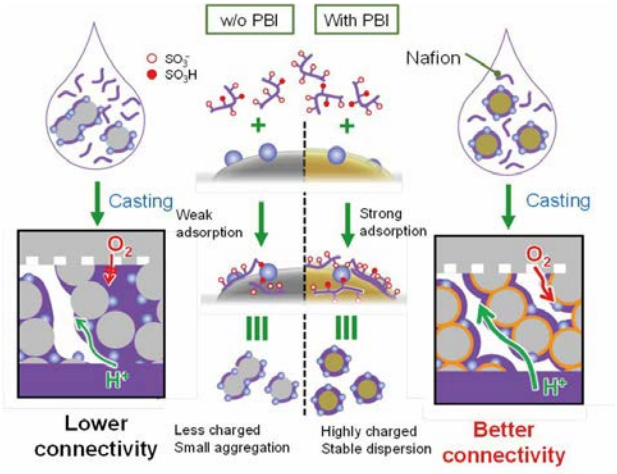


Fig. 6.9. Schematic illustration of a steam electrolysis cell with a proton conductor and a flat 50 × 50 mm^2 electrolyte cell

in both solvents. Therefore, we concluded that controlling the interaction between the ionomer and catalyst composites is crucial for lowering the cost of PEMFC.

These results pave the way for low-cost fabrication of polymer electrolyte membrane fuel cells and are directed to the midterm milestone of Project 2 "Lowering catalyst loading and new design of catalyst layer"

3. CO_2 photoreduction on a high-entropy oxynitride (Prof. Edalati and PI Ishihara)

CO_2 photoreduction on photocatalysts is a nature-friendly solution to decrease the CO_2 amount, however the method still has low efficiency because of difficult separation and easy recombination of charge carriers in available catalysts. In this study, a high-entropy oxynitride was introduced as an active photocatalyst for photoreduction. The material had a chemical composition of $TiZrNbHfTaO_6N_3$ and was produced by a high-pressure torsion method followed by oxidation and nitriding. It showed higher photocatalytic CO_2 to CO conversion compared to corresponding high-entropy oxide, benchmark photocatalyst P25 TiO_2, and almost all catalysts introduced in the literature. The high activity of this oxynitride, which also showed good chemical stability, was attributed to the large absorbance of light and easy separation of electrons and holes, the low recombination of charge carriers, and the high CO_2 adsorption on the surface. These findings introduce high-entropy oxynitrides as promising photocatalysts for CO_2 photoreduction.

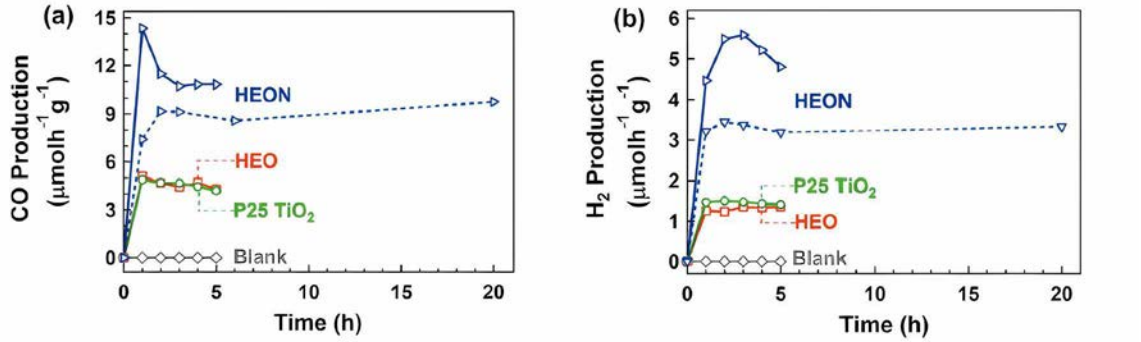


Fig. 6.10. Photocatalytic CO_2 reduction on TiO_2, high entropy oxide(HEO), and high entropy oxynitride (HEON)

4. Solvated Structure of Hybrid Tetraglyme-Aqueous Electrolyte Dissolving High-Concentration LiTFSI-LiFSI for Dual-Ion Battery (PI Ishihara)

The solvated structure of a highly concentrated hybrid tetraglyme (G4)-water electrolyte was studied for an increasing cycle stability and performance of a KS6 used dual-ion battery. Hybrid solvent of G4 and water with a weight ratio of 2 to 8 was able to dissolve 9LiFSI-1LiTFSI supporting salts up to 37 mol kg^{-1} (37 mol kg^{-1} G2W8). In spite of such high concentration of supporting salts, reasonable charge and discharge performance of dual-ion battery (discharge capacity of ≈40 mAh g^{-1} and coulombic efficiency of 90%) were exhibited over 300 cycles. This was attributed to the decreased hydrogen evolution reaction (HER) potential to –1.05 V vs. Ag/AgCl by addition of G4. From Fourier-transform infrared, nuclear magnetic resonance, and Raman spectroscopies, G4 molecules were more strongly coordinated to Li^+ to form ion pairs of $[Li(G4)x(H_2O)y]+$ complex in hybrid G4-water electrolyte. Co-intercalation of bis(trifluoromethanesulfonyl)I mide ($TFSI^-$) and bis(fluorosulfonyl)imide (FSI^-) into graphitic carbon KS6 cathode was confirmed in hybrid aqueous electrolyte.

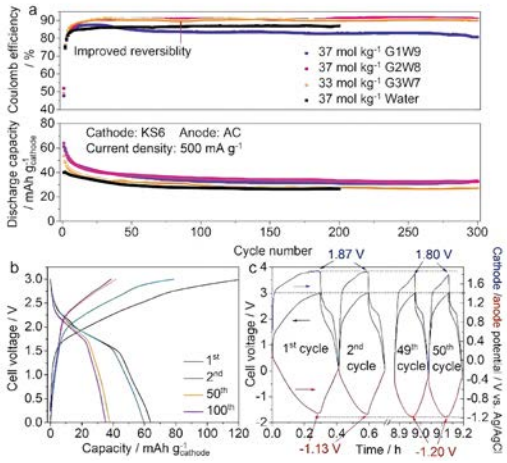


Fig. 6.11. (a) Effect of water/G4 ratio on discharge capacity and coulombic efficiency as a function of cycle number. (b) Charge–discharge profiles of the KS6/AC full cell with 37 mol kg^{-1} G2W8 electrolyt. (c) Potential of cathode, anode, and full cell at different cycle number.

5. Photo-enhanced ionic conductivity (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. Specifically, we demonstrate the increase of the grain boundary conductance of a 3 mol% Gd-doped ceria thin film by a factor of approximately 3.5 at 250 °C and the reduction of its activation energy from 1.12 to 0.68 eV under illumination, while light-induced heating and electronic conductivity could be excluded as potential sources for the observed opto-ionic effect. 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.

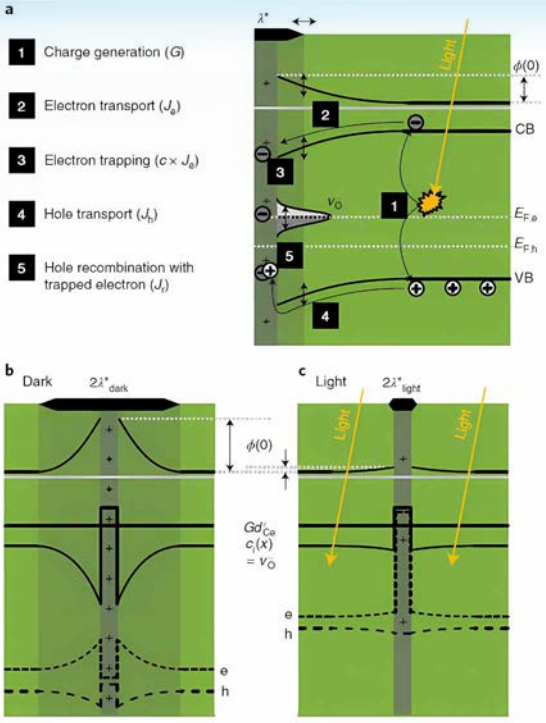


Fig. 6.12. Suggested mechanism of the opto-ionic effect and the consequences for potential distribution and charge carrier concentrations. a, Individual steps responsible for the reversible decrease in the grain boundary potential barrier shown in combined schematics of potential (above the grey line) and charge carrier concentrations (below the grey line). The thin double arrows indicate the opposing consequences due to steps 3 (trapping of electrons) and 5 (recombination), respectively, for potential distribution, density of states (oxygen vacancies) in the grain boundary core and band bending. b,c, Grain boundary potential ϕ and the space charge width, as well as concentrations of Gd dopants on Ce sites (Gd'Ce), doubly positively charged oxygen vacancies (ci(x) = VO..), holes (h) and electrons (e) in the dark (b) and under illumination (c). Panel c shows an extreme case of a nearly fully collapsed grain boundary potential barrier, for which the concentration of accumulated electrons in the grain boundary core nearly matches the concentration of oxygen vacancies under equilibrium (dark). Quasi-Fermi energies for electrons and holes (EF,e, EF,h), depletion width in the dark (λ*dark) and under light (λ* light).

6. Oxygen Reduction Reaction and Electronic Properties of LnO-Terminated Surfaces of Pr_2NiO_4 and La_2NiO_4 (PI Staykov)

Density functional theory calculations were performed to elucidate the origin of catalytic activity of the pristine LnO-terminated surfaces of two Ruddlesden–Popper phase oxides of industrial interest. The direct comparison of molecular oxygen interaction with La_2NiO_4 and Pr_2NiO_4 allowed us to evaluate the electronic effect on the oxygen reduction reaction energetics. We have further addressed the surface catalytic activity as a function of interstitial oxygen occupancy in the rock salt layer and provided a possible explanation for the limits of the interstitial oxygen concentration. The oxide ion transport in the rock salt layer was compared for $La_2NiO_{4.125}$ and $Pr_2NiO_{4.125}$. The diffusion difference was attributed to the electronic structure of the valence shells of Pr and La. The different polarizability of those elements would lead to the opposite effect on the transition state stability. In-depth understanding of the La_2NiO_4 and Pr_2NiO_4 (including $La_2NiO_{4.125}$ and $Pr_2NiO_{4.125}$) electronic properties allowed us to refer electronic and hole conductivities to the computed band gaps and the electronic structure of the valence bands. Our study shows that while La_2NiO_4 and Pr_2NiO_4 share a similar crystallographic structure, the most important properties, such as surface catalytic activity, ionic diffusivity, and electron transport, are a direct consequence of the valence shell structure of the Ln cations: La and Pr (J. Phys. Chem. C 2022, 126, 7390).

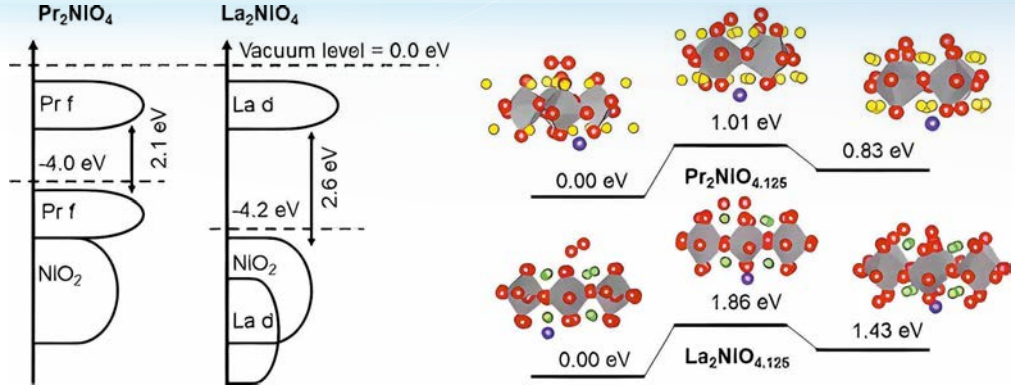


Fig. 6.13. Relative alignment of bands in La_2NiO_4 and Pr_2NiO_4 and their effect on the surface catalytic activity.

These results provide crucial understanding for surface catalysis and and elemental composition in SOFC electrodes.

7. Advanced Processing of Proton Conducting Electrochemical Devices with Optimized Electrode/Electrolyte Interfaces (PI Matsumoto and Prof. Kwati)

Ceramic proton-conducting oxides are a highly promising class of materials with great potential for a wide range of intermediate-temperature electrochemical applications, including producing large-scale clean hydrogen by steam electrolysis. Interest in this material class stems from its low activation energy for proton transport, which enables high proton conductivity between 300-600°C. Operating within this optimal temperature range offers numerous advantages, including promoting facile chemical kinetics and thermal integration with high-value waste-heat sources. Additionally, this range provides significantly higher thermodynamic efficiency than low-temperature electrolysis technologies. Despite these advantages, processing and scaling up such electrolytes for industrial purposes poses several challenges. We demonstrate an effective tape-casting route that produces flat, planar protonic electrolysis half-cells with impressive dimensions of up to 100 mm x 100 mm x 0.5 mm. Thanks to our successful international collaboration with IEK-1 Forschungszentrum Jülich. Generally, half-cell flatness is critical to cell performance. Our processed cells, with a final size of 50 × 50 mm^2, showed a total flatness of around 0.2 mm, as shown in Fig. 7(a). Leak rate testing of the half-cells with helium showed very good gas tightness of the sintered electrolyte layer, well within the threshold necessary for cell operation (~5 × 10^{-5} hPa dm^3 (s cm^2)$^{-1}$). Using $Ba_{0.5}La_{0.5}CoO_{3-\delta}$ as the air electrode demonstrates remarkable capabilities and endurance within the 450-550°C temperature range, as indicated by its current-voltage characteristics and hydrogen evolution rates.

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 operating at 500°C by applying mixed-conducting protonic electrode."

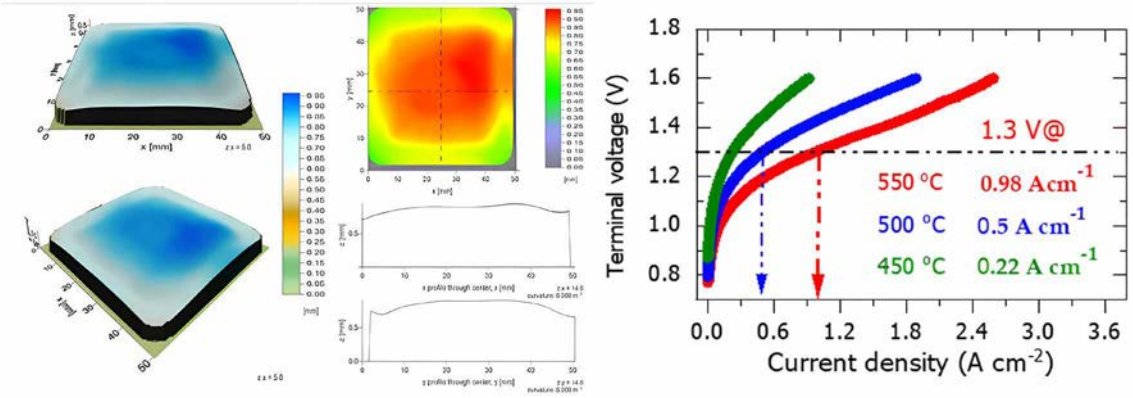


Fig. 6.14. (a) 50 × 50 mm^2 half-cell flatness evaluated after co-sintering at 1300 °C/5h (b) steam electrolysis current-voltage characteristics measured from 450-550°C.

References

[1] Tumen-Ulziia G., Auffray M., Klotz D., Harrington G.F., Chen X., Balijapalli U., Vediyappan V., Nakamura N., Feng Z., Takekuma K., Fujita Y., Wang P., Yamada S., Tamada K., Batmunkh M., Zhong Y., Mathevet F., Matsushima T., Adachi C. (2022), Defect passivation by pyridine-carbazole molecules for efficient and stable perovskite solar cells, ACS Applied Energy Materials, 5(12), 15819-15827. DOI: 10.1021/acsaem.2c03364.

[2] Wu D., Kayo N., Jayawickrama S.M., Phua Y.K., Tanaka N., Fujigaya T. (2022), Effect of Alcohol Content on the Ionomer Adsorption of Polymer Electrolyte Membrane Fuel Cell Catalysts, International Journal of Hydrogen Energy, 48(15), 5915-5928. DOI: 10.1016/j.ijhydene.2022.11.116.

[3] Akrami S., Edalati P., Shundo Y., Watanabe M., Ishihara T., Fuji M., Edalati K. (2022), Significant CO_2 photoreduction on a high-entropy oxynitride, Chemical Engineering Journal, 449, 137800. DOI: 10.1016/j.cej.2022.137800.

[4] Yang D., Li H., Shen X., Watanabe M., Ishihara T. (2023), Solvated Structure of Hybrid Tetraglyme-Aqueous Electrolyte Dissolving High-Concentration LiTFSI-LiFSI for Dual-Ion Battery, ChemSusChem, 16(4), e202201805. DOI: 10.1002/cssc.202201805.

[5] Defferriere T., Klotz D., Gonzalez-Rosillo J.C., Rupp J.L.M., Tuller H.L. (2022), Photo-enhanced ionic conductivity across grain boundaries in polycrystalline ceramics, Nature Materials, 21(4), 438 -444. DOI: 10.1038/s41563-021-01181-2.

[6] Leonard K., Okuyama Y., Ivanova M.E., Meulengberg W.A., Matsumoto H. (2022), Anode Supported Planar 5 × 5 cm^2 $SrZr_{0.5}Ce_{0.4}Y_{0.1}O_{2.95}$ Based Solid Oxide Protonic Fuel Cells via Sequential Tape-Casting, Solid State Ionics, 379, 115918. DOI: 10.1016/j.ssi.2022.115918.

[7] Leonard K., Okuyama Y., Ivanova M.E., Meulengberg W.A., Matsumoto H. (2022), Tailored and improved protonic conductivity through $Ba(Z_xCe_{10-x})_{0.08}Y_{0.2}O_{3-\delta}$ ceramics perovskites type oxides for electrochemical devices, ChemElectroChem, 9(4), e202101663. DOI: 10.1002/celc.202101663.

Multiscale Science and Engineering for Energy and the Environment

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

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) . Although conventional DAC technologies are mainly based on sorbent-based systems, we have first proposed membrane-based DAC (m-DAC) process in last year. In this year, we have investigated the detail condition of m-DAC process and revealed the key factors of this process.[1] The analysis showed that application of a multi-stage separation process can enable the preconcentration of atmospheric CO_2 (0.04%) to more than 40%. This possibility and combination of the membranes with advanced CO_2 conversion may lead to realistic means for opening a circular CO_2 economy.

In order to realized m-DAC process, highly-permeable nanomembranes of poly(dimethylsiloxane) (PDMS) with sufficient mechanical durability are necessary for practical use. We have developed mechanically reinforced PDMS nanomembranes by thin layers of carbon nanotube (CNT), giving CO_2 permeability and gas selectivity of 42,500 GPU and 10 (CO_2/N_2), respectively in the case of the 27-nm-thick, composite membrane.[2]

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.

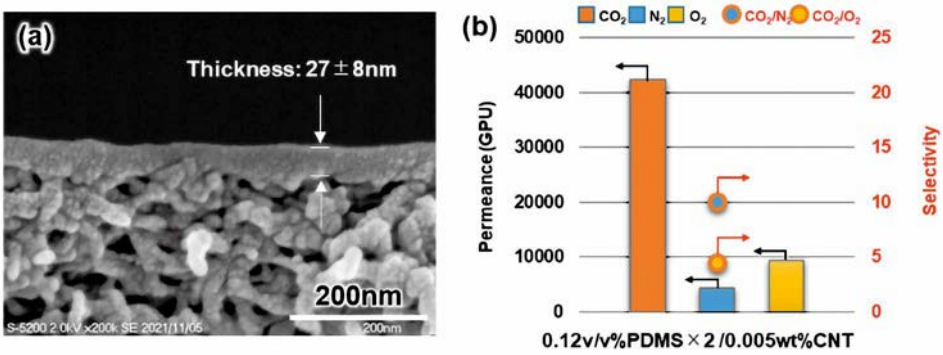


Fig. 6.15. A cross section of PDMS/CNT membrane on a porous support (a) and its gas permeance properties (b).

2. Minimal seismic source for continuous injected CO_2 monitoring (PI Tsuji and Prof. Ikeda)

The monitoring of stored CO_2 is crucial for predicting CO_2 leakage, preventing CO_2 injection-induced earthquakes, and ensuring effective CO_2 storage, such as the selection of CO_2 injection wells. To continuously monitor the injected CO_2 with low cost, we have developed a Portable Active Seismic Source (PASS) specifically designed for monitoring CO_2 storage reservoirs at a depth of approximately 1 km. By stacking the signals generated by the PASS, we have significantly improved the signal-to-noise ratio of the seismometer data, even at far distances from the source. In a previous study [3], we confirmed that signals propagated up to ~80 km when using a seismic source of 8000N at 20 Hz, after stacking four months of data. However, since the CO_2 storage reservoirs are much smaller in size compared to the signal propagation range, we downsized the seismic source and developed a centimeter-scale PASS. Utilizing the minimal PASS with 19N at 50 Hz, we observed signal propagation of approximately 1 km for horizontal distances [4]. The reduced size and lower cost of the PASS make it feasible for permanent deployment at multiple locations to ensure continuous monitoring of CO_2 storage reservoirs.

This achievement directly addresses the short-term milestone "Develop effective monitoring system using continuous source system and fiber optic cable," in the Project "Monitoring of CO_2 saturation and pore pressure" of the Thrust's roadmap.

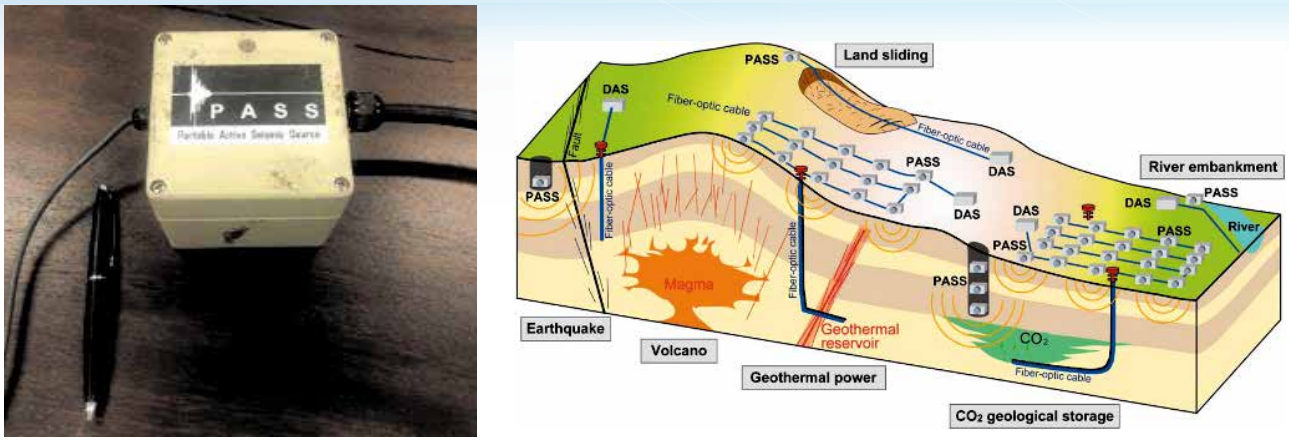


Fig. 6.16. (Left) Picture of PASS. (Right) Conceptual image of the continuous monitoring based on PASS.

3. Materials Performance Evolution to Support the Energy Transition (PI Stubbins)

To develop the necessary technologies to address climate change, there is a growing need for materials and components that operate in high temperature adverse atmospheres for efficient energy conversion and associated processing applications. These materials applications include enhanced efficiency, high temperature heat exchange and advanced energy production with high operating temperatures. For many crucial industrial activities, process heat is critical to efficient product generation and often reliant on high temperature heat sources which are not available from most renewable resources such as wind, solar, geothermal and hydro.

To meet this challenge, much of our research during this past year has been directed at analyzing and developing materials and components for elevated temperature applications. This included the development of processing for the fabrication of compact heat exchangers with materials that are capable of operating at temperatures above 700°C in extreme atmospheres including corrosion, mechanical loading and irradiation. A significant achievement in the past year is to develop 3D imaging of advanced energy materials to understand mechanical deformation processes. An example is shown of a Fe-9Cr steel that has been irradiated to 0.1 displacements per atom (dpa) at 450°C and deformed while being imaged in both near-field and far-field synchrotron beams. Using these techniques, we can develop a full 3D, grain-by-grain deformation map of the alloy's deformation response. This technique is a key, new process for understanding advanced energy materials' performance. It has been applied to several systems including high temperature, irradiation and hydrogen exposure.

This achievement directly addresses the mid-term milestone "Modeling of emerging and disruptive technologies," in the Project "Energy Transitions" of the Thrust's roadmap.

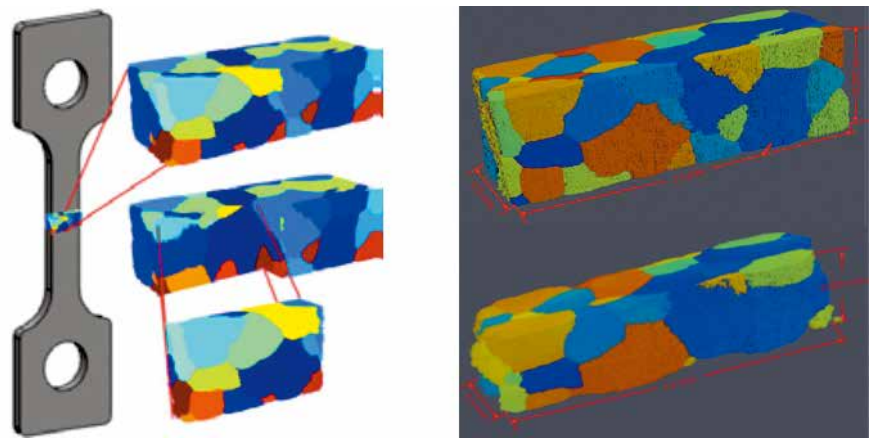


Fig. 6.17. the orientation of slices of a Fe-9Cr steel irradiated to 0.1 dpa at 450°C and the grain modification before (above) and after (below) 4% tensile deformation.

4. Adsorption of Volatile Organic Compounds onto Biomass-Derived Activated Carbons (PI Saha)

Volatile organic compounds (VOCs) are a class of hazardous gaseous materials emitted from certain solids or liquids. They are thought to possess serious short- or long-term adverse effects on human health. Two biomass-derived activated carbons synthesized from mangrove wood and waste palm trunk precursors are chosen, and four types of VOCs (ethanol, dichloromethane, acetone, and ethyl acetate) adsorption to them are measured experimentally using the inverse gas chromatography technique. The zero uptake adsorption enthalpy and specific entropy of the adsorption are theoretically computed for all the samples. After that, these data are compared with the obtained data for Maxsorb III, which is the best commercially available activated carbon with a high price, to assess the performance of the biomass-derived activated carbons. Results show that, for all the VOCs, the cost-effective mangrove-based activated carbon can be an excellent alternative to the high-priced Maxsorb III when employed as an adsorbent material for VOC removal. The results have been disseminated in ASME Open Journal of Engineering, Vol. 1, 011032-1-7, 2022.

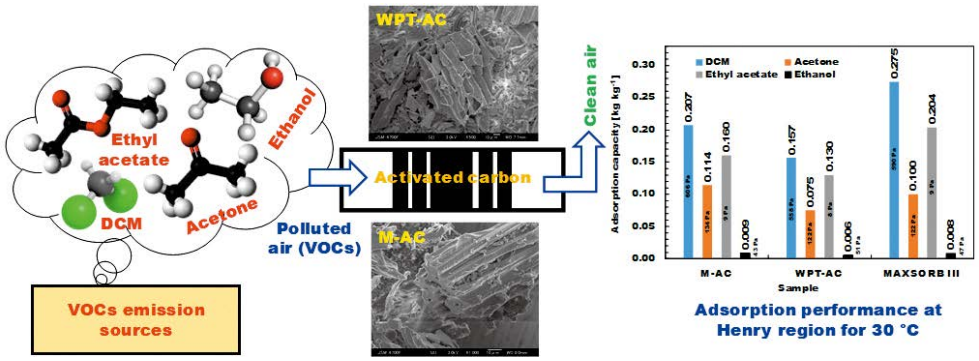


Fig. 6.18. Schematic illustration of VOC adsorption on biomass-derived activated carbons and their sorption behavior.

This achievement directly addresses the short-term milestone "Clear understanding of adsorption/desorption process of functional adsorbents," in the Project "Heat Mass Transfer: Adsorption" of Thrust's roadmap.

References

[1] Fujikawa S., Selyanchyn R. (2022), Direct Air Capture by Membranes, MRS Bulletin, 47(4), 416-423. DOI: 10.1557/s43577-022-00313-6.

[2] Ariyoshi M., Fujikawa S., Kunitake T. (2022), Nanomembranes of poly(dimethysiloxane) reinforced with carbon nanotubes and their potential for CO_2 capture, Chemistry Letters, 51(9), 962–965. DOI: 10.1246/cl.220296.

[3] Tsuji T., Ikeda T., Matsuura R., Mukumoto K., Lawrens H. F., Kimura T., Yamaoka K., Shinohara M. (2022), Continuous monitoring system for safe managements of CO_2 storage and geothermal reservoirs, Scientific Reports, 11(1), 19120. DOI: 10.1038/s41598-021-97881-5.

[4] Tsuji T., Tsuji S., Kinoshita J., Ikeda T., Ahmad A. B. (2023), 4 cm Portable Active Seismic Source (PASS) for Meter- to Kilometer-Scale Imaging and Monitoring of Subsurface Structures, Seismological Research Letters, 94(1), 149-158. DOI: 10.1785/0220220049.

[5] Lan K. C., Chuang C. P., Tung H. M., Mo K., Miao Y., Liu X., Lee H., Park J. S., Almer J., Stubbins J. F. (2022), A study on texture stability and the biaxial creep behavior of as-hydrided CWSR Zircaloy-4 cladding at the effective stresses from 55 MPa to 65 MPa and temperatures from 300°C to 400°C, Journal of Nuclear Materials, 564, 153688. DOI: 10.1016/j.jnucmat.2022.153688.

[6] Romnes C. J., Stubbins J. F., Mireles O. R. (2022), Tuning the Properties of Additively Manufactured Tungsten Ultra-fine Lattices by Adjusting Laser Energy Density and Lattice Geometry, Journal of Materials Engineering and Performance, 31(8), 6256-6269. DOI: 10.1007/s11665-022-07126-3.

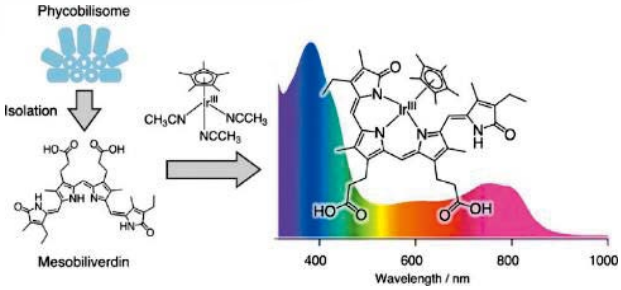
[7] Feng L., Xu Y., Qiu J., Liu X., Wen C., Qian Z., Liu W., Yan W., Li Y., Wang Z., Zheng S., Guo S., Shi T., Lu C., Gou J., Li L., Shan J., Stubbins J. F., Gu L., Yun D. (2022), A novel approach on designing ultrahigh burnup metallic TWR fuels: Upsetting the current technological limits, MRS bulletin, 47(11), 1092-1102. DOI: 10.1557/s43577-022-00420-4.

[8] Rupam T. H., Saha B. B., Palash M. L., Pal A. (2022), Adsorption of Volatile Organic Compounds Onto Biomass-Derived Activated Carbons: Experimental Measurement and Comparison, ASME Open Journal of Engineering, 1, 011032. DOI: 10.1115/1.4055182.

Advanced Energy Materials

Cp*Ir Complex with Mesobiliverdin Ligand Isolated from Thermoleptolyngbya sp. O-77 (PI Ogo and Prof. Yoon)

We developed a new method to isolate a natural pigment of mesobiliverdin IXα (MBV) directly from phycocyanin of Thermoleptolyngbya sp. O-77 and synthesized a water-soluble Cp*Ir complex with the isolated MBV ligand. To obtain a high yield of MBV, we modified the conventional method by adding additional two steps: the protease digestion of phycocyanin by trypsin and the isolation of MBV by hydrophobic and silica gel column chromatographies. The Cp*Ir complex with MBV ligand was characterized by electrospray ionization-mass spectrometry, ultraviolet-visible-near-infrared absorption spectroscopy, X-ray photoelectron spectroscopy, 1H NMR spectroscopy, and H-H correlation spectroscopy. This is the first example of a platinum-group metal complex with MBV as a ligand.[1]



Disciplines: Biology, biochemistry, structural biology

Fig. 7.1. Chemically derived MBV from PCB extracted from purified phycocyanin of Thermoleptolyngbya sp. O-77 and synthesized a water-soluble Cp*Ir complex using the isolated MBV as a natural pigment ligand. The synthesized Cp*Ir complex with MBV is water-soluble and exhibits a wide range of absorption from 300 to 900 nm.

Heterointerface created on Au cluster-loaded unilamellar hydroxide electrocatalysts as a highly active site for the oxygen evolution reaction (PI Yamauchi, PI Staykov)

The oxygen evolution reaction (OER) is a critical element for all sorts of reactions that use water as a hydrogen source, such as hydrogen evolution and electrochemical CO_2 reduction, and novel design principles that provide highly active sites on OER electrocatalysts will push the limits of their practical applications. Herein, we demonstrate Au-cluster loading on unilamellar exfolied layered double hydroxide (ULDH) electrocatalysts for the OER to fabricate a heterointerface between Au clusters and ULDHs as an active site, which is accompanied by the oxidation state modulation of the active site and interfacial direct O-O coupling (interfacial DOOC). The Au cluster-loaded ULDHs exhibits excellent activity for the OER with an overpotential of 189 mV at a current density of 10 mA cm^{-2} and a durability of 12 h. X-ray absorption fine structure measurements reveal that charge transfer from the Au clusters to ULDHs modifies the oxidation states of trivalent metal ions, which can be an active site on the ULDHs. The present study supported by density functional theory calculations indicates that active sites at the interface between the Au clusters and ULDHs promote a novel OER mechanism through interfacial DOOC, thereby achieving outstanding catalytic performance.

Disciplines: Catalysis, Electrochemistry, Quantum chemistry

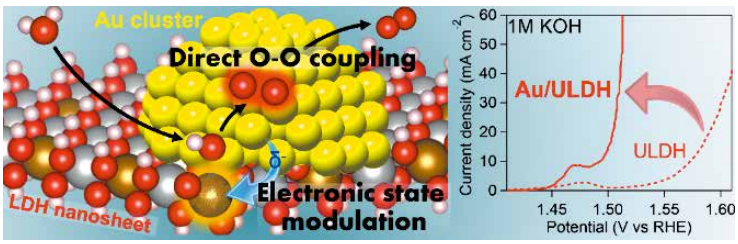


Fig. 7.2. The material design for interface active sites to allow a novel oxygen evolution reaction (OER) mechanism is proposed. The Au cluster-loaded unilamellar layered double hydroxide (LDH) nanosheet electrocatalysts create interfacial active sites which exhibit interfacial direct O-O coupling and excellent OER performance.

References

[1] Yamada K., Yatabe T., Yoon K., Ogo S. (2022), Cp*Ir complex with mesobiliverdin ligand isolated from Thermoleptolyngbya sp. O-77, Journal of Organometallic Chemistry, 964, 122302. DOI: 10.1016/j.jorganchem.2022.122302.

[2] Kitano S., Noguchi T., Nishihara M., Kamitani K., Sugiyama T., Yoshioka S., Miwa T., Yoshizawa K., Staykov A., Yamauchi M. (2022), Heterointerface Created on Au-Cluster-Loaded Unilamellar Hydroxide Electrocatalysts as a Highly Active Site for the Oxygen Evolution Reaction, Advanced Materials, 34(16), 2110552. DOI: 10.1002/adma.202110552.

Advanced Energy Conversion Systems

1. Ideal cell concept for high performance solid oxide cell (PI Matsumoto, PI Ishihara, Prof. Kwati)

Converting renewable energy to hydrogen is strongly required for net zero society, intermediate temperature solid oxide cell which is reversible operation of fuel cell is expecting to be applied because of high efficiency and stability. Oxide ion conductor, in particular, Y_2O_3 stabilized ZrO_2 has been widely used for electrolyte [1], however, large degradation ratio is the current most significant issues which is assigned to the sintering of Ni in fuel electrode. Recently, oxide proton conductor is also studied from high efficiency at low temperature. However, because of partial hole conduction, deviation of H_2 formation amount from Faraday's law is serious issues for the electrolyzer using oxide proton conducting electrolyte [2]. In this study, combination of oxide ion conductor and proton conductor film is studied for solving the issues of both type electrolyzer. For fabrication of the double electrolyte cell so-called "Ideal cell", $BaZr(Ce, Y, Yb)O_3$ film prepared in Forschungszentrum Jülich GmbH under collaboration of Dr. Leonard and Dr. Meulenberg is used and $LaGaO_3$ thin film was deposited by pulsed laser deposition (PLD) method. If this approach will be going successfully, increase in open circuit potential and also electrochemical performance such as efficiency is expected and open new concept of solid oxide cell.

2. HPT for advanced photocatalysts for CO_2 conversion and water splitting (Prof. Edalati, PI Ishihara, Prof. Watanabe)

The effect of HPT in synthesizing new materials, introduction of defects and stabilization of high-pressure phases was used to develop new photocatalysts. This study combined materials science with chemistry.

3. Automatized Optimization of Ring-Opening Reactions in Lactone Derivatives (PI Staykov) in collaboration with IMI

Cyclization and cycloreversion of organic compounds are fundamental kinetic processes in the design of functional molecules, molecular machines, nanoscale sensors and switches in the field of molecular and nano electronics. We present a fully automatic computational platform for the design of a class of 5- and 6-membered ring lactones by optimizing the ring-opening reaction rate. Starting from a minimal initial parent set, our algorithm generates iteratively cascades of pools of candidate lactone derivatives where optimization and down-selection are performed without human supervision. We employ density functional theory combined with transition state theory to elucidate the exact mechanism leading to the lactone ring opening reaction. Based on the analysis of the reaction pathway and the frontier molecular orbitals, we identify a simple descriptor which can easily correlate with the reaction rate. Consequently, we can omit computationally expensive transition state calculations and deduce the reaction rate from simple ground state and ionic calculations. To accelerate the platform, we use a dataset of the order of 800 molecules to train machine learning models for the prediction of targeted chemical properties reducing the computational time by a 90% factor. We developed an evolutionary algorithm capable of generating datasets three orders of magnitude larger than the initial parent set. Thus, we can explore a large domain of the chemical space using minimal computational effort. Our entire platform is modular and our current implementation for lactone can be further generalized to more complex systems via substitution of the quantum chemical and fingerprinting modules.

Disciplines: chemistry, quantum mechanics, applied mathematics, machine learning

4.Understanding the Roles of Hydroxide in CO_2 Electroreduction on a Cu Electrode for Achieving Variable Selectivity (PI Staykov and PI Yamauchi)

Hydroxide-derived copper (OH/Cu) electrodes exhibit excellent performance for the electrocatalytic CO_2 reduction reaction (CO_2RR). However, the role of hydroxide (OH) in CO_2RR remains controversial; therefore, the origin of the selectivity enhancement emerging on OH/Cu has not been fully understood. In

the present work, we quantitatively evaluated surface OH by electroadsorption and established a direct correlation between the OH amount and selectivity for the production of CH_4 and C_{2+} on OH/Cu with the help of computational investigations concerning work functions of the surface. Based on these findings, we demonstrated variable selectivity using OH/Cu electrodes having a controlled OH amount; three OH/Cu electrodes realized their distinct selectivity such as Faradic efficiency (FE) for the production of CH_4 (CH_4 FE) of 78%, C_{2+} FE of 71%, and the ratio of C_{2+}-to-CH_4 >355. The proposed simple strategy for selectivity control would contribute to further quantity synthesis of value-added chemicals using CO_2RR.

Disciplines: theoretical chemistry, electrodynamics, synthesis, characterization

References

[1] Ishihara T., Tan Z., Song J.T., Takagaki A. (2022), Sequential-infiltration of Ce and Ni in NiO-YSZ fuel electrode for tubular type solid oxide reversible cells (SORC) using $LaGaO_3$ electrolyte film, Solid State Ionics, 379, 115914. DOI: 10.1016/j.ssi.2022.115914.

[2] Leonard K., Ivanova M.E., Weber A., Deibert W., Meulenberg W.A., Ishihara T., Matsumoto H. (2022), Anode supported planar 5 × 5 cm^2 $SrZr_{0.5}Ce_{0.4}Y_{0.1}O_{2.95}$ based solid oxide protonic fuel cells via sequential tape-casting, Solid State Ionics, 379, 115918. DOI: 10.1016/j.ssi.2022.115918.

[3] Edalati P., Itagoe Y., Ishihara H., Ishihara T., Emami H., Arita M., Fuji M., Edalati K. (2022), Visible-light photocatalytic oxygen production on a high-entropy oxide with multiple-heterojunction introduction, Journal of Photochemistry and Photobiology A: Chemistry, 433, 114167. DOI: 10.1016/j.jphotochem.2022.114167.

[4] Akrami S., Edalati P., Shundo Y., Watanabe M., Ishihara T., Fuji M., Edalati K. (2022), Significant CO_2 photoreduction on a high-entropy oxynitride, Chemical Engineering Journal, 449, 137800. DOI: 10.1016/j.cej.2022.137800.

[5] Akrami S., Murakami Y., Watanabe M., Ishihara T., Arita M., Guo Q., Fuji M., Edalati K. (2022), Enhanced CO_2 conversion on highly-strained and oxygen-deficient $BiVO_4$ photocatalyst, Chemical Engineering Journal, 442, 136209. DOI: 10.1016/j.cej.2022.136209.

[6] Akrami S., Murakami Y., Watanabe M., Ishihara T., Arita M., Fuji M., Edalati K. (2022), Defective high-entropy oxide photocatalyst with high activity for CO_2 conversion, Applied Catalysis B: Environmental, 303, 120896. DOI: 10.1016/j.apcatb.2021.120896.

Multiscale Science and Engineering for Energy and the Environment

1. Theoretical molecular design of polydimethylsiloxane structures toward preferential CO_2 permeation. (PI Fujikawa, Prof. Staykov)

Enhancement of CO_2 selectivity over other gas species on PDMS nanomembranes is a next step to develop membrane-based direct air capture system. Especially, gas-polymer matrix of membranes plays an important role on gas selectivity. In this study we employ density functional theory to investigate the binding interaction between polydimethylsiloxane and CO_2 for application in gas separation membranes. The binding strength has been studied systematically as a function of the monomer conformational rotations in the polymer chain. Our work identified major differences between the CO_2 interaction with the helical conformation and the linear conformation of polydimethylsiloxane polymer chains. We have further estimated dependence between the CO_2 binding strength and the polydimethylsiloxane polymer chain curvature by systematically evaluating the CO_2 binding to cyclic polydimethylsiloxane oligomers. The enhanced CO_2 interaction with helical chains and cyclic oligomers was attributed to cooperative, confinement effects, and local electron density distribution at the Si–O–Si fragments. The binding modes were identified using vibration frequency analysis.

Disciplines: Polymer chemistry, surface science, nanomaterial chemistry, theoretical chemistry

2. Cultural and Demographically Aware Energy System Design (PI Chapman)

Future energy system design is an imperfect science, with many considerations required for an energy system that will meet environmental targets, while also achieving national level economic and social goals. This research, conducted in collaboration with UIUC partners from Dr Caleb Brooks Lab, seeks to address this issue.

The research combines a national survey of the united states, seeking to understand people's preferences toward energy technologies which can meet carbon neutrality targets and ideals in regard to economic and social outcomes. This research is unique in that it considers culture and demographics, i.e., respondent's race, location, income, education background and etc. to develop a model to design the ideal future energy system. Outcomes define an energy system which can be considered fair by all stakeholders, and one which engenders a larger amount of renewables than the current US plan, while retaining sufficient baseload power generation sources to ensure a resilient and stable energy system.

Disciplines: Energy Economics, Energy Modelling, Statistical Analysis

3. Materials Performance Evolution to Support the Energy Transition (PI Stubbins)

For a major energy transition, the use of elevated temperature materials and systems for industrial applications is of critical importance. Most high temperature processes are combustion-type processes which require fossil fuels or possibly hydrogen as a by-product to a separate reforming process (which might also generate emissions). The energy transition in this sector, compared to transportation, domestic and commercial energy uses, is difficult to address with typical large-scale renewable sources. Most renewables are capable of producing electricity, but not high process temperatures required for many industrial applications.

The University of Illinois are developing a micro-nuclear-reactor program which will eventually construct a small, 10MW gas-cooled nuclear reactor system. The gas-cooling allows for high temperature operation and the generation of high temperature working fluid in a He to molten salt heat exchanger. This project will provide a high temperature heat source that will be able to drive a number of high temperature processes including hydrogen production, steam production, and process heat for biomaterials processing, all without GHG release. This will be a first of a kind (FOAK) nuclear system and is a large collaborative project with several industrial partners

and led by Prof. Brooks with a large group of faculty support.

One important aspect of this and similar projects is the development of compact heat exchangers (CHX) for very efficient high temperature heat transfer. We are the University of Illinois lead on a $3M-3yr US DOE project to develop bonding processes to withstand temperatures above 750°C for 20 or more year component lives. This work would revolutionize high temperature heat transfer between a variety of working fluids and gases. This work is complementary to the major I^{2}CNER effort for low temperature heat exchange. It involves a large working group in the US across several major universities and national laboratories.

Disciplines: Energy Efficiency Technologies, Energy Transition for GHG Reduction, Materials Science, High Efficiency Power Generation Systems.

4. Synthesis of green transition metal doped MIL-100(Fe) (PI Saha)

Metal-organic framework (MOF)-water working pairs have been envisaged to provide the next revolutionary advancement in the existing sorption-based thermal energy storage and conversion systems. Herein, a promising MOF for high water sorption, MIL–100(Fe), and its transition metal-doped (Ni^{2+} and Co^{2+}) derivatives are produced following a green synthesis procedure. The synthesized materials were tested in water sorption measurements using a thermogravimetric technique. The experimentally obtained adsorption data were correlated with the Sun-Chakraborty adsorption isotherm model. As an example of thermal energy conversion, an adsorption chiller is considered, and hence cooling cycles were drawn using the sorption data. The cooling cycles revealed that the nickel-doped MIL–100(Fe) demonstrates the highest value of the specific cooling effect (450.79 kJ kg^{-1}) among the studied MOFs. An inverse gas chromatography technique was employed to investigate the surface free energy of the parent and doped MIL–100(Fe) MOFs. It was found that nickel-doped MIL–100(Fe) had the highest total surface free energy of 105.41 mJ m^{-2}. Surfaces' Lewis acid-base activities and the work of cohesion and adhesion (towards water molecules) were investigated. The surfaces' properties were correlated with the water adsorption isotherms, which can provide crucial information for developing optimal adsorbents targeting water as the adsorbate for efficient and effective thermal energy storage and conversion systems.

Disciplines: Material science, thermal engineering, physical chemistry

References

[1] Vaishnav A., Fujikawa S., Staykov A. (2023), Curvature Effect in Polydimethylsiloxane Interaction with CO_2. Insights from Theory, Journal of Physical Chemistry A, 127(4), 876-885. DOI: 10.1021/acs.jpca.2c07001.

[2] Chapman A., Shigetomi Y., Karmaker S.C., Saha B.B., Brooks C. (2023), Cultural and demographic energy system awareness and preference: Implications for future energy system design in the United States, Energy Economics, 112, 106141. DOI: 10.1016/j.eneco.2022.106141.

[3] Elbakhshwan M., Desorcy L., Jentz I., Anderson M., Gao F., Allen T., Messner et B., Keating B., McKillup S. (2023), Advancing diffusion bonded compact heat exchangers for high temperature applications, Advanced Materials and Processes, 181(4), 14-18. DOI: 10.31399/asm.amp.2023-04.p014.

[4] Rupam T. H., Steenhaut T., Palash M. L., Filinchuk Y., Hermans S., Saha B. B. (2022), Thermochemical energy applications of green transition metal doped MIL -100(Fe), Chemical Engineering Journal, 448, 137590. DOI: 10.1016/ j.cej.2022.137590.

Advanced Energy Materials

1. Developments of Nanostructured Materials for Energy Storage/Catalysis Applications (Prof. Kobayashi)

For energy storage and catalysis applications, we have designed and created innovative solid-solution alloy nanoparticles (NPs) in which the constituent elements do not mix in the bulk state. The novel alloy NPs were synthesized using our original non-equilibrium synthesis techniques or through hydrogen absorption/desorption processes [1-5]. Notably, our studies have contributed to remarkable advancements in various catalytic reactions (Fig. 8.1(a)). For example, PtW solid-solution alloy NPs have demonstrated excellent performance in the hydrogen evolution reaction, attributed to the presence of negatively charged Pt active sites induced by W doping [1]. Additionally, CuRu solid-solution alloy NPs have exhibited higher CO oxidation activity compared to Ru NPs, which are known as one of the best monometallic CO oxidation catalysts [2,3].

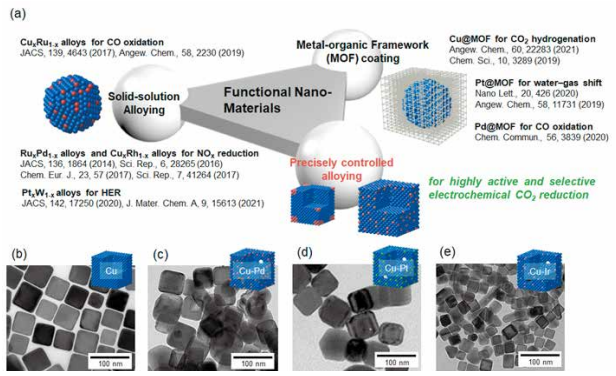


Fig. 8.1. (a) Developments of nanostructured materials for catalysis applications and TEM images of shape-controlled nanocrystals for electrochemical CO_2 reduction catalysts, (b) Cu cubes, (c) Cu-Pd, (d) Cu-Pt and (e) Cu-Ir NCs.

In addition to alloy nanoparticles, we have explored multifunctional composite nanomaterials incorporating metal-organic frameworks (MOFs) [6-9]. One notable example is Pd@copper(II) 1,3,5-benzenetricarboxylate (HKUST-1), a novel hydrogen storage material. By coating Pd nanocrystals with HKUST-1, we have significantly enhanced the hydrogen-storage capacity and speed through a charge transfer process between the Pd nanocrystals and HKUST-1 [6]. Another material of interest is Cu/ZnO@$[Zr_6O_4(OH)_4(BDC)_6]$ (BDC = benzenedicarboxylate) (UiO-66), which has demonstrated higher activity in methanol synthesis from CO_2 and H_2 compared to benchmark catalysts such as Cu/ZnO/γ-Al_2O_3 [7,8]. This finding shows promise for utilizing CO_2 in the production of valuable chemicals, contributing to a more sustainable and environmentally friendly approach.

For further development of advanced materials and the realization of a carbon resource-recycling society, our focus lies in creating highly active and selective electrochemical catalysts for converting CO_2 into useful chemical feedstocks under mild conditions. We aim to achieve this by precisely controlling the reaction field, facets and active sites of the catalyst at the atomic level (Fig. 8.1(b)-(e)).

References

[1] Kobayashi D., Kobayashi H., Wu D., Okazoe S., Kusada K., Yamamoto T., Toriyama T., Matsumura S., Kawaguchi S., Kubota Y., Aspera S., Nakanishi H., Arai S., Kitagawa H. (2020), Significant Enhancement of Hydrogen Evolution Reaction Activity by Negatively Charged Pt through Light Doping of W, Journal of the American Chemical Society, 142(41), 17250-17254. DOI: 10.1021/jacs.0c07143.

[2] Huang B., Kobayashi H., Yamamoto T., Toriyama T., Matsumura S., Nishida Y., Sato K., Nagaoka K., Haneda M., Xie W., Nanba Y., Koyama M., Wang F., Kawaguchi S., Kubota Y., Kitagawa H. (2019), Copper Substitution Induced CO Adsorption Site Change of a Ruthenium Catalyst for Highly Enhanced CO Oxidation Activity, Angewandte Chemie - International Edition, 58(8), 2230 -2235. DOI: 10.1002/anie.201812325.

[3] Huang B., Kobayashi H., Yamamoto T., Matsumura S., Nishida Y., Sato K., Nagaoka K., Kawaguchi S., Kubota Y., Kitagawa H. (2017), Solid-Solution Alloying of Immiscible Ru and Cu with Enhanced CO Oxidation Activity, Journal of the American Chemical Society, 139(13), 4643-4646. DOI: 10.1021/jacs.7b01186.

[4] Kobayashi H., Yamauchi M., Ikeda R., Yamamoto T., Matsumura S., Kitagawa H. (2018), Double Enhancement of Hydrogen Storage Capacity of Pd Nanoparticles by 20 at% Replacement with Ir; Systematic Control of Hydrogen Storage in Pd -M Nanoparticles (M = Ir, Pt, Au), Chemical Science, 9(25), 5536-5540. DOI: 10.1039/c8sc01460d.

[5] Kobayashi H., Kusada K., Kitagawa H. (2015), Creation of Novel Solidsolution Alloy Nanoparticles on the Basis of Density-of-states Engineering by Interelement Fusion, Accounts of Chemical Research, 48(6), 1551–1559. DOI: 10.1021/ar500413e.

[6] Li G., Kobayashi H., Taylor J. M., Ikeda R., Kubota Y., Kato K., Takata M., Yamamoto T., Toh S., Matsumura S., Kitagawa H. (2014), Hydrogen Storage in Pd Nanocrystals Covered with a Metal -organic Framework, Nature Materials, 13(8), 802–806. DOI: 10.1038/nmat4030.

[7] Mitsuka Y., Ogiwara N., Mukoyoshi M., Kitagawa H., Yamamoto T., Toriyama T., Matsumura S., Haneda M., Kawaguchi S., Kubota Y., Kobayashi H. (2021), Fabrication of Integrated Copper-Based Nanoparticles/Amorphous Metal -Organic Framework by a Facile Spray-Drying Method: Highly Enhanced CO_2 Hydrogenation Activity for Methanol Synthesis, Angewandte Chemie - International Edition, 60(41), 22283-22288. DOI: 10.1002/anie.202110585.

[8] Kobayashi H., Taylor J. M., Mitsuka Y., Ogiwara N., Yamamoto T., Toriyama T., Matsumura S., Kitagawa H. (2019), Charge Transfer Dependence on CO_2 Hydrogenation Activity into Methanol in Cu Nanoparticles Covered with Metal-Organic Framework Systems, Chemical Science, 10(11), 3289-3294. DOI: 10.1039/c8sc05441j.

[9] Ogiwara N., Kobayashi H., Concepcion P., Rey F., Kitagawa H. (2019), The First Study on the Reactivity of Water Vapor in a Metal -Organic Framework with Platinum Nanocrystals, Angewandte Chemie - International Edition, 58(34), 11731–11736. DOI: 10.1002/anie.201905667.

2. Direct Synthesis of Hydrogen Peroxide by Means of a Rhodium Homogeneous Catalyst (Prof. Yatabe)

This work reports the first example of a safe, one-pot synthesis of H_2O_2 in water, using only H_2 and O_2. This H_2O_2 synthesis catalyzed by a Rh homogeneous catalyst. The Rh catalyst extracts electrons of H_2, uses them for the reduction of O_2, and acquires protons from water to release H_2O_2. The catalytic reaction depends on the pressure of H_2/O_2 mixture, and the maximum turnover number (TON) is 910 under an H_2/O_2 (95/5) atmosphere (1.9 MPa) for 12 h at 23 °C in water. The TON is the highest of any homogeneous catalyst for H_2O_2 synthesis. The reaction mechanism has been proposed based on the structure of intermediates as well as spectroscopic data. The Rh catalyst stores the electrons of H_2 as mononuclear form, RhI species, and the mononuclear form returns the starting dinuclear form, RhII species, concomitant with the reduction of O_2 to H_2O_2. This reaction system gives us the chance to use H_2O_2 for bench-top oxidation reactions of organic materials under safe conditions from only H_2 and O_2 without using complicated equipment. This result also serves the basis for new synthetic methodology using H_2 as an electron source.

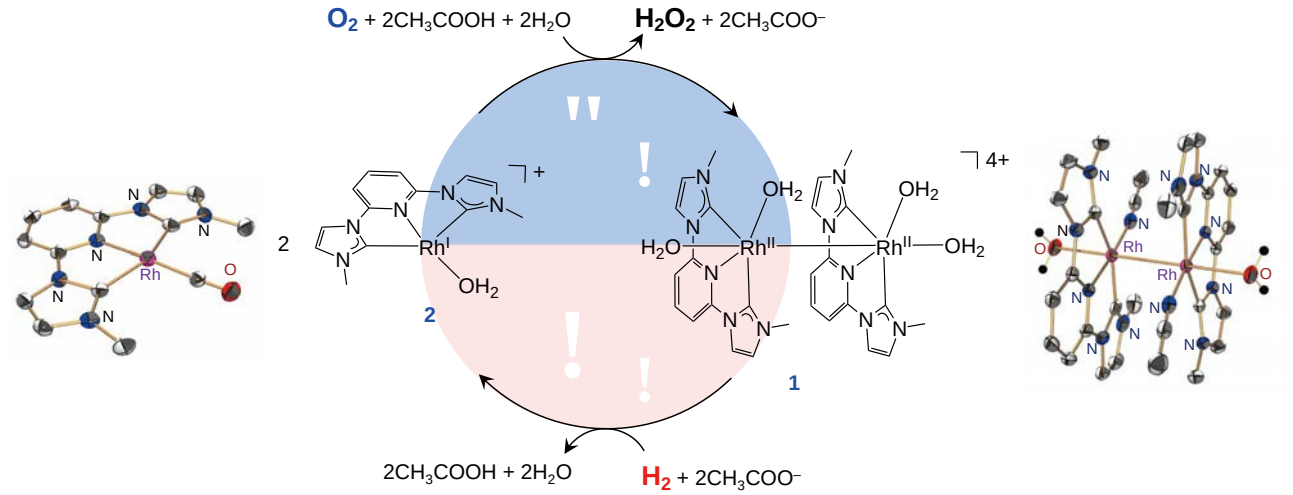


Fig. 8.2. A proposed catalytic reaction mechanism of a synthesis of H_2O_2 from H_2 and O_2 using Rh homogeneous catalyst in water and crystal structures of Rh complexes.

References

Ogo S., Yatabe T., Tome T., Takenaka R., Shiota Y., Kato K. (2023), Safe, One-Pot, Homogeneous Direct Synthesis of H_2O_2. Journal of the American Chemical Society, 145(8), 4384-4388. DOI: 10.1021/jacs.2c13149.

3. Mechanism-based design against high temperature hydrogen attack (Ph.D. Student, Vijayvargia)

High temperature hydrogen attack (HTHA) is degradation of steels exposed to hydrogen gas at high temperatures and pressures. Hydrogen in steels reacts with carbon from carbides to produce methane gas bubbles typically on grain boundaries which grow and coalesce, leading to loss of strength and fracture toughness (see the microstructural investigation of [1] in Fig. 8.3a through d). Current design practice against HTHA is based on the Nelson curves which define the conditions for safe operation in a temperature/hydrogen-partial-pressure diagram. Nelson curves are empirical in nature and do not account for the underlying failure mechanism(s), material microstructure, carbide stability, applied stresses, time-to-failure etc. To this end, we have developed a void growth model for failure of carbon steels by HTHA [2]. The model is based on growth and coalescence of grain boundary voids under the influence of internal cavity methane gas pressure and applied macroscopic loads. The present model is shown to yield satisfactory agreement with the available experimental data from hydrogen attack of 2¼Cr–1Mo steel (see Fig.8.3e). Also, the model is used to construct Nelson type curves in the temperature/hydrogen-partial-pressure diagram. These curves represent failure times for given applied stresses and triaxiality. Figure 1f shows the Nelson-type curve for stresses and triaxiality in typical pressure vessels used in petrochemical industries. The proposed methodology can be viewed as providing a step toward replacing the current design practice against HTHA while maintaining the simplicity of the original Nelson curve approach which addresses both the short- and long-term milestones of Project 3 (Predictive models of H_2-assisted cracking).

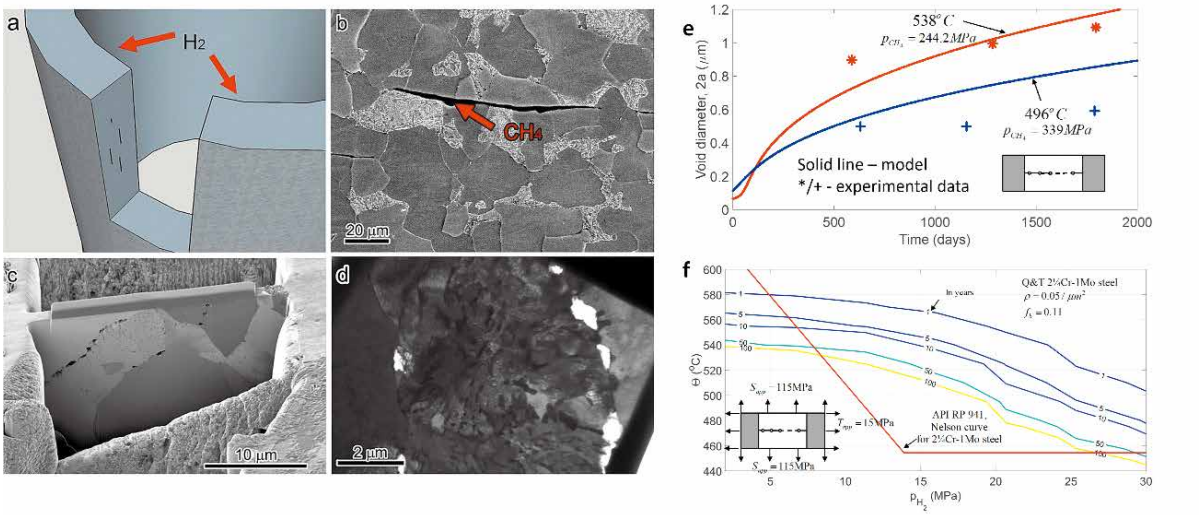


Fig. 8.3. a) Schematic showing orientation of cracks within the wall of the reboiler, b) SEM micrograph showing close-up of intergranular crack, c) FIB image of section showing grain boundary bubbles, d) TEM micrograph showing bubbles surrounding pearlite grain, e) Model predictions for void growth for 2¼Cr-1Mo steel in 20.7MPa hydrogen gas at 496oC and 538oC, f) Contour plots of time to failure in years plotted on a Nelson-type graph for 2¼ Cr-1Mo steel under stresses corresponding to the inner diameter surface of a pressurized cylinder. Contour lines indicate time to failure (1, 5, 10, 50, and 100 years). The Nelson curve from API RP 941 for the 2¼Cr-1Mo steel is also superposed

References

[1] Martin M.L., Dadfarnia M., Orwig S., Moore D., Sofronis P. (2017) A microstructure-based mechanism of cracking in high temperature hydrogen attack, Acta Materialia, 140, 300-304. DOI: 10.1016/j.actamat.2017.08.051.

[2] Vijayvargia K., Dadfarnia M., Sofronis P., Kubota M., Staykov A., Wada K., Pugh J.A., Eason T.J. (2023), Three-dimensional constraint-based void-growth model for high temperature hydrogen attack. International Journal of Fracture, 243(2), 203-228. DOI: 10.1007/s10704-023-00739-2.

Advanced Energy Conversion Systems

1. Visible-light driven photocatalytic water splitting on KTa(Zr)O_3 modified with acene-based organic semiconductors(Prof. Watanabe)

This work provides guidance for the design of photocatalytic water splitting that can efficiently utilize visible light. Inorganic oxide photocatalysts are known to use light to decompose water into hydrogen and oxygen, but most of them use ultraviolet light, and there is a need to develop photocatalysts that can efficiently use visible light. We have previously reported a visible-light-responsive photowater splitting photocatalyst by combining KTa(Zr)O_3, a photocatalyst capable of water splitting, with an organic dye capable of repairing visible light. In this study, we focused on acene organic semiconductors, which are photoconductive materials, with the aim of achieving more efficient charge separation at the dye- KTa(Zr)O_3 interface. The combination of various acenes organic semiconductors with KTa(Zr)O_3 resulted in up to a 14-fold increase in photocatalytic water splitting activity compared to photocatalysts without the addition of dyes. Theoretical calculations suggest that the smaller the reorganization energy between the ground-excited state, the higher the photocatalytic activity shows, indicating that efficient charge transfer is an important factor. The combination of acenic organic semiconductor/ KTa(Zr)O_3 was found to be capable of Z-scheme type photocatalytic water splitting reaction using light up to 720 nm. This result demonstrates that among the sunlight components, acene organic semiconductor/ KTa(Zr)O_3 is a photocatalytic system that can utilize the entire UV-visible light range.

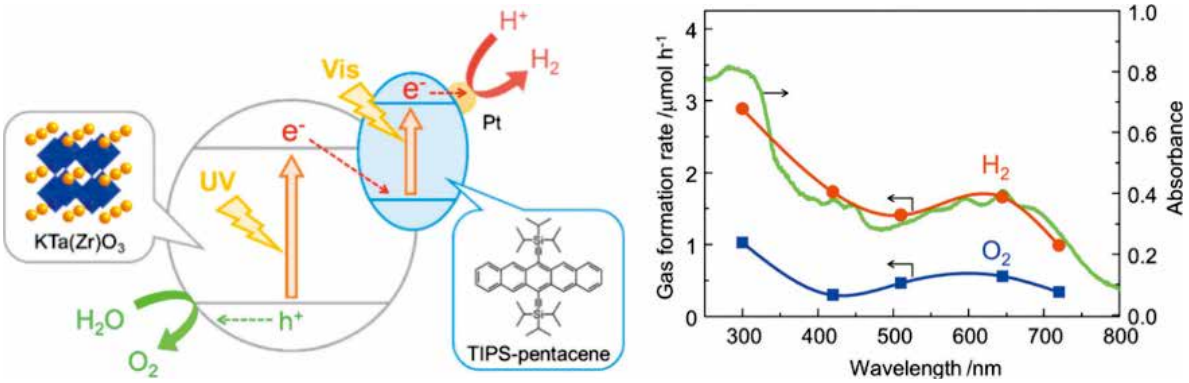


Fig. 8.4. (left) Z-scheme type charge-transfer mechanism in the PtOX/Acene/KTa(Zr)O_3 photocatalyst. (right) H_2 and O_2 formation rates of the water splitting reaction on PtOX /Acene/KTa(Zr)O_3 under double beam excitation conditions with band-pass filter (300 nm + 420, 510, 645, and 720 nm) and the UV–vis diffuse reflectance spectrum of photocatalyst.

Disciplines: Water splitting, Hydrogen, Photocatalyst, Visible light, Z-scheme

References

Hagiwara H., Watanabe M., Kim S., Higashi K., Ishihara T. (2022), Photocatalytic Water Splitting on KTa(Zr)O_3 Modified with Acene-Based Organic Semiconductors, Journal of Physical Chemistry C, 126(23), 9634 -9641. DOI: 10.1021/acs.jpcc.2c02532.

2. Photoreduction of CO_2 on High-Entropy Catalysts (Prof. Edalati)

CO_2 photoreduction on photocatalysts is a clean technology to reduce CO_2 to active gases such as CO or to value-added compounds. However, this technology still has low efficiency for practical applications mainly because of the difficult separation of electrons and holes (i.e. large bandgap) and easy recombination of these charge carriers in existing catalysts. High-entropy photocatalysts were recently introduced in I^{2}CNER as a new family of catalysts with high compositional and electronic structure tunability for different chemical reactions [1-2]. In one of the latest studies in this regard [3], a high-entropy oxynitride was introduced as an active photocatalyst with a low band and high chemical stability for the photoreduction of CO_2. The catalyst had a chemical composition of TiZrNbHfTaO6N3 and was synthesized by a high-pressure torsion method followed by high-temperature oxidation and ammonia-induced nitriding. It showed higher catalytic CO_2 to CO photoreduction compared to corresponding high-entropy oxide, benchmark P25 TiO_2 photocatalyst, and nearly all photocatalysts studied in the literature. The high activity of high-entropy oxynitride photocatalyst, which also exhibited high chemical stability, was attributed to the large light absorbance, easy electron and hole separation, the low recombination rate of electrons and holes, and the high physical and chemical adsorption of CO_2 on the surface. This study introduces high-entropy oxynitrides as a new family of low-bandgap photocatalysts with high activity for CO_2 photoreduction.

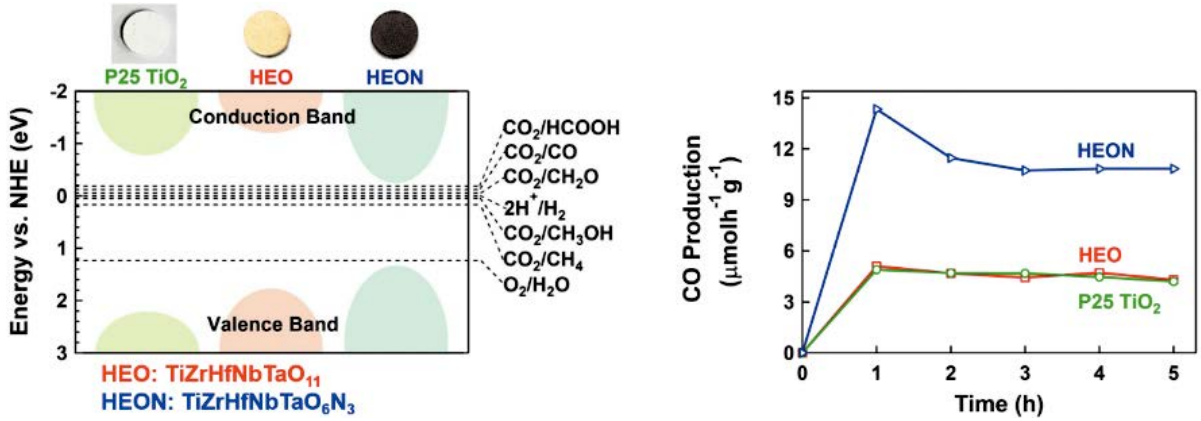


Fig. 8.5. Lower bandgap and higher photocatalytic activity of high-entropy oxynitride compared to high-entropy oxide and benchmark P25 TiO_2 photocatalyst.

References

[1] Edalati P., Shen X.F., Watanabe M., Ishihara T., Arita M., Fuji M., Edalati K. (2021), High-Entropy Oxynitride as Low-Bandgap and Stable Photocatalyst for Hydrogen Production, Journal of Materials Chemistry A, 9(26), 15076-15086. DOI: 10.1039/d1ta03861c.

[2] Edalati P., Itagoe Y., Ishihara H., Ishihara T., Emami H., Arita M., Fuji M., Edalati K. (2022), Visible-Light Photocatalytic Oxygen Production on a High-Entropy Oxide with Multiple-Heterojunction Introduction, Journal of Photochemistry and Photobiology A: Chemistry, 433, 114167. DOI: 10.1016/j.jphotochem.2022.114167.

[3] Akrami S., Edalati P., Shundo Y., Watanabe M., Ishihara T., Fuji M., Edalati K. (2022), Significant CO_2 Photoreduction on a High-Entropy Oxynitride, Chemical Engineering Journal, 449, 137800. DOI: 10.1016/j.cej.2022.137800.

3. Fine bubble technology for electrochemical reactions (Prof. Tomisaki)

Fine bubbles whose diameters are less than 100 μm have specific properties unlike macrobubbles[1]. They have long stagnation in solutions and high internal pressure, and their surface is usually electrochemically charged. For these properties, they were used in many fields, for example, it is used for water treatment and organic synthesis[2]. In electrochemical reactions, there are some problems to be solved from the viewpoint of environmental consideration and reaction efficiency. To promote the specific reactions, complicated catalysts or mediators are used. In the reactions which gaseous species react, low gas solubility can also be an issue. It would be one of the ways to solve these problems by utilizing fine bubbles for electrochemical reactions. In my previous research, electrochemical reduction of carbon dioxide using diamond electrodes were studied. To produce carbon monoxide or formic acid more efficiently, we also used fine bubbles[3]. The overpotential for the reaction was slightly decreased and production of carbon monoxide was promoted. Although the results were not sufficient enough, it opens up possibilities to use fine bubbles in electrochemical reactions. Therefore, I focused on investigating fundamental properties to use fine bubble technology for electrochemical reactions. Fine bubble contained solutions were prepared changing the dissolved gaseous species, flow rate of liquid and gas, or supporting electrolyte by fine bubble generator (Fig. 8.6.). I am collaborating with Professor Mase at Shizuoka University to use fine bubble appropriately for reactions. When fine bubbles were contained in the solutions, the redox reactions were enhanced in some cases. I continue to study the fundamental things, and apply the knowledge to some reactions which gaseous species react and are converted into useful compounds like carbon dioxide.

In addition, collaborative works with Professor Einaga at Keio University and Dr. Jiwanti at Airlangga University were conducted. With Professor Einaga, electrochemical carbon dioxide reduction using diamond electrodes modified with organic compound was studied[4]. With Dr. Jiwanti, carbon-based electrodes which can be used for electrochemical sensing of medicines or electrolytic synthesis of useful compounds were investigated.

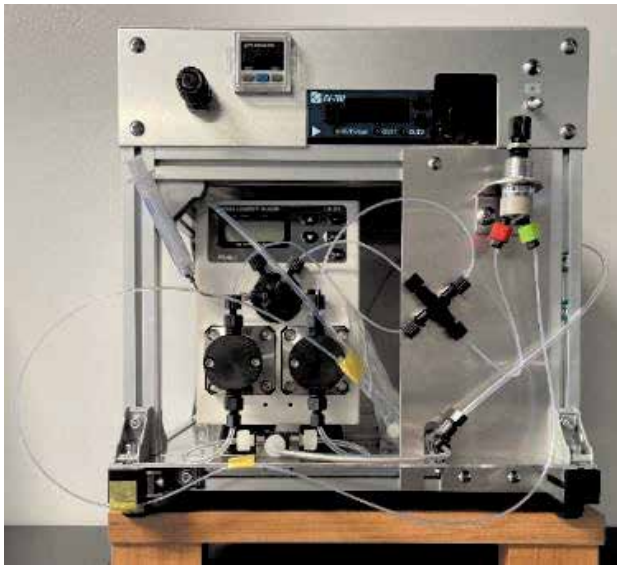


Fig. 8.6. Fine bubble generator (PMT Co., Ltd.)

References

[1] Takahashi M. (2005), ζ Potential of Microbubbles in Aqueous Solutions: Electrical Properties of the Gas-Water Interface, Journal of Physical Chemistry B, 109(46), 21858-21864. DOI: 10.1021/jp0445270.

[2] Mase N., Mizumori T., Tatemoto Y. (2011), Aerobic copper/TEMPO-catalyzed oxidation of primary alcohols to aldehydes using a microbubble strategy to increase gas concentration in liquid phase reactions, Chemical Communications, 47(7), 2086-2088. DOI: 10.1039/c0cc04377j.

[3] Tomisaki M., Natsui K., Fujioka S., Terasaka K., Einaga Y. (2021), Unique properties of fine bubbles in the electrochemical reduction of carbon dioxide using boron-doped diamond electrodes, Electrochimica Acta, 389, 138769. DOI: 10.1016/j.electacta.2021.138769.

[4] Mikami T., Yamamoto T., Tomisaki M., Einaga Y. (2022), Amine-Functionalized Diamond Electrode for Boosting CO_2 Reduction to CO, ACS Sustainable Chemistry and Engineering, 10(45), 14685-14692. DOI: 10.1021/acssuschemeng.2c02532.

Multiscale Science and Engineering for Energy and the Environment

1. Dynamic Optical Wireless Power Transfer for Transportation Electrification (Prof. Nguyen Dinh Hoa)

The study in [1] is the first to propose a dynamic optical wireless power transfer (OWPT) system to simultaneously and wirelessly charge both ground and aerial electric vehicles (EVs), as illustrated in Fig. 8.7. This dynamic OWPT system includes an overhead facility to locate laser transmitters, renewable energy resources and energy storage devices. As such, clean energy is used for EV charging. A number of laser transmitters are on the roof of the facility, which point upward to wirelessly charge aerial EVs, while the other laser transmitters are mounted on the facility's ceiling and point downward to wirelessly charge ground EVs. All laser transmitters are able to rotate around the normal direction to track and continuously charge aerial and ground EVs while they are moving, owing to the attached tracking cameras. Analytical mathematical formulas are then derived for the wirelessly transmitted power and energy, based on which the unique existence of maximum power and energy points are proved. Moreover, those maximum points are shown to be inversely linearly dependent on the environment attenuation coefficient, i.e. on weather conditions. Such maximum points can be numerically found utilizing bisection methods.

The proposed dynamic OWPT system can be used to assist the cooperation of aerial and ground EVs [2] and can be further enhanced by employing the concept of bidirectional OWPT [3]. In addition, the proposed system is part of a larger infrastructure [4] to contribute for the anywhere, anytime availability of energy so that the comfort of EV users is increased while the range anxiety is significantly reduced.

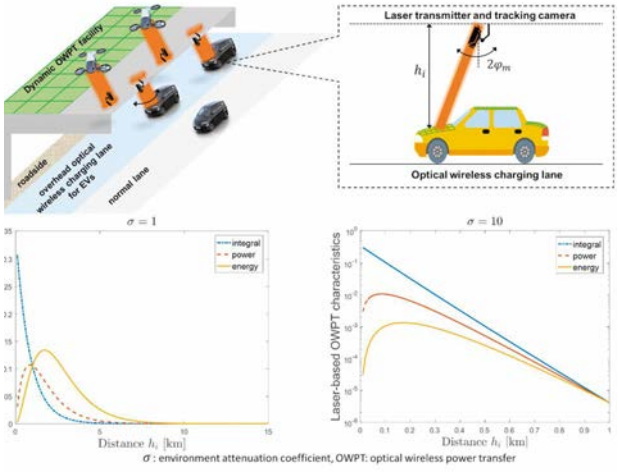


Fig. 8.7. Proposed dynamic optical wireless charging system for ground and aerial electric vehicles, with simulation results showing the dependence of received power and energy on the environment condition and transmitting distance.

References

[1] Nguyen D.H. (2023), Dynamic Optical Wireless Power Transfer for Electric Vehicles, IEEE Access, 11, 2787-2795. DOI: 10.1109/ACCESS.2023.3234577.

[2] Nguyen D.H. (2023), A Nature-Inspired Distributed Robust Control Design for Ground-Aerial Vehicle Cooperation, IEEE Transactions on Intelligent Transportation Systems, 24(4), 4454-4463. DOI: 10.1109/TITS.2022.3229336.

[3] Nguyen D.H. (2022), Bidirectional Optical Wireless Power Transfer via Optical Transceiver, The Proceedings of the 4th Optical Wireless and Fiber Power Transmission Conference (OWPT2022), part of the Optics and Photonics International Congress 2022 (OPIC2022), Yokohama, Japan, April 18-21.

[4] Nguyen D.H. (2022), Wireless power transfer and renewables for energy mobility, flexibility, and sustainability, 2022 I²CNER-IMI Joint International Workshop, Fukuoka, Japan, January 26.

2. A comprehensive description of flame morphology in a gravitational field for efficient, stable and safe combustion process (Prof. Matsue)

Combustion is one of the most important technologies for efficient, stable and safe energy generations. Recently, application of CO_2-free fuels such as hydrogen, ammonia and blended mixtures including these gases are ones of the central issues in combustion research towards the reduction of global warming gases. On the other hand, flame morphology, the essence to control combustion process, involves plenty of physicochemical factors including mixture properties, and understanding of its global picture is limited and challenging due to difficulties of experiments and of flame descriptions in mathematical/numerical studies.

The work [1] by Matsue and Matalon firstly achieves a comprehensive description of flame propagations in a gravitational field. In [1], the flame morphology depending on combustible mixtures and their diffusion properties, as well as the gravitational parameter representing the ratio of buoyancy to inertial forces is considered under the assumption of small thermal expansion. In this setting, the bifurcation theory in advanced applied mathematics can be applied, and relevant (steady and oscillatory) flame morphology is described for all parameter values in typical ranges including their persistence and structural change, under the change of the above parameters.

The present research provides an expectation of flame morphology for a broad class of mixtures including prospective gas mixtures, and an approach to study flame morphology with interactions between flames and other physicochemical factors, such as sound, towards the development of sustainable combustion technologies in industry.

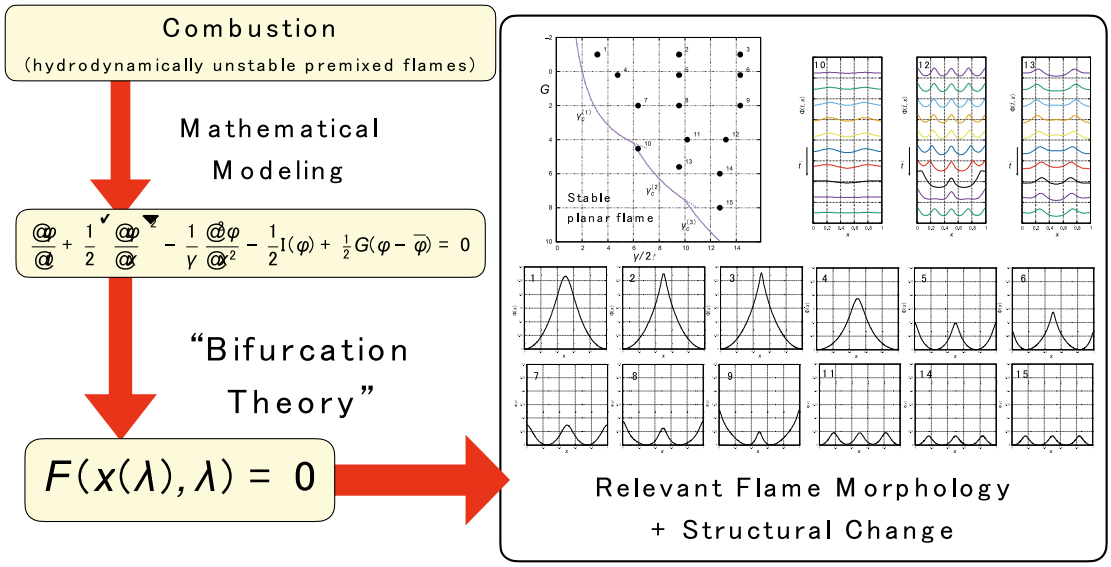


Fig. 8.8. Complex combustion process is reduced to a differential equation describing the displacement of planar flame fronts. Bifurcation theory then systematically and comprehensively unravels the flame morphology for various parameters.

References

[1] Matsue K., Matalon M. (2023), Dynamics of hydrodynamically unstable premixed flames in a gravitational field - Local and global bifurcation structures, Combustion Theory and Modelling, 27(3), 346-374. DOI: 10.1080/13647830.2023.2165968.

3. Thermodynamic properties of a new low-GWP refrigerant, HFO1132(E) (Prof. Sakoda)

Hydrofluorocabons (HFCs) are widely used as working fluids for refrigerators, air-conditioners, and heat-pump systems. However, there is a need to reduce their use due to their large global warming potentials (GWPs) according to the Paris Agreement and Kigali Amendment. Hydrofluoroolefins (HFOs) with a carbon-carbon double bond have low-GWPs, and they are expected to be promising HFC alternatives. HFO1132(E) (C2H2F2, trans-1,2-difluoroethene) has a relatively low normal boiling temperature, 220 K and is expected for low-temperature applications. There is no accurate equation of state (EOS) for HFO1132(E) at present, and reliable experimental data of the thermodynamic properties are essential for the formulation of the EOS. In this study, PvT properties in both of the vapor and liquid phases, saturated densities, and critical parameters of HFO1132(E) were measured [1, 2]. The PvT properties (relation of pressure-specific volume-temperature) were measured along eight isochores between 65 and 832 kg m-3 in the temperature range from 310 to 400 K and at pressures up to 6.5 MPa by the isochoric method. Fig. 8.9 shows the obtained PvT property data on the temperature-pressure diagram. The uncertainties in the temperature and pressure measurements are 5 mK and 1 kPa, respectively. The uncertainty in the density measurement is within 0.15 %. The saturated densities were determined by the visual observation of meniscus disappearance and also by the intersection of the saturation-pressure curve and the isochores of the PvT properties. Finally, the critical parameters were determined in consideration of the meniscus disappearing level as well as the intensity of critical opalescence. These data are useful for the formulation of an accurate multi-parameters EOS. These results were accomplished by Research Center for Next Generation Refrigerant Properties (NEXT-RP), and contribute to the short-term milestone "Accumulation of thermodynamic and transport properties of new refrigerants, and development of their accurate EOS" in Project 7 " Thermophysical properties of new working fluids" of the Thrust's roadmap.

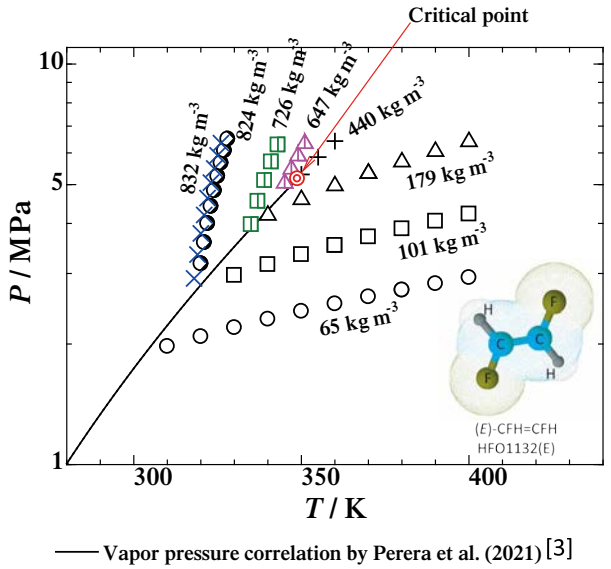


Fig. 8.9. Experimental results for the PvT properties along eight isochores from 65 to 832 kg m^{-3} and the critical point of R1132(E) [1, 2] on the temperature-pressure diagram.

References

[1] Sakoda N., Perera U.A., Thu K., Higashi Y. (2022), Measurements of PvT properties, saturated densities, and critical parameters of R1132(E), International Journal of Refrigeration, 140, 166-171. DOI: 10.1016/j.ijrefrig.2022.05.012.

[2] Sakoda N., Higashi Y. (2021), Thermodynamic Properties Measurement of HFO1132(E), Proceedings of the 2nd IIR Conference on HFOs and Low GWP Blends, 1024. DOI: 10.18462/iir.HFO.2021.1024.

[3] Perera U.A., Sakoda N., Miyazaki T., Thu K., Higashi Y. (2022), Measurements of Saturation Pressures for the Novel Refrigerant R1132(E), International Journal of Refrigeration, 135, 148-153. DOI: 10.1016/j.ijrefrig.2021.12.014.

Returning Results to Society

The relevance of I²CNER's research efforts and objectives in FY2022 toward enabling the green innovation initiative of the government of Japan is evidenced through 4 new collaborative projects with industry as well as some 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 2022, I²CNER filed for 12 patents, and was granted 20, bringing the total number of patent applications since inception to 367 and patents awarded to 138.

1. Development of high-performance adsorption systems (PI Saha)

PI Saha continued his industrial collaboration with Bry Air Asia on the development of high-performance adsorption systems. Adsorption-based systems are useful in environments where adsorbate is required to be temporarily or periodically stored and released. The collaborative project relates to adsorbent-based heat exchanger systems for adsorption cooling and heat pump applications and it contributes significantly to the performance enhancement of the systems. We developed hybrid adsorber heat exchanging device in which the coating steps were completed first, the coating on the metallic portions was dried, and the interstitial spaces were filled in with conventional granular adsorbent materials (shown in Fig. 9.1.).

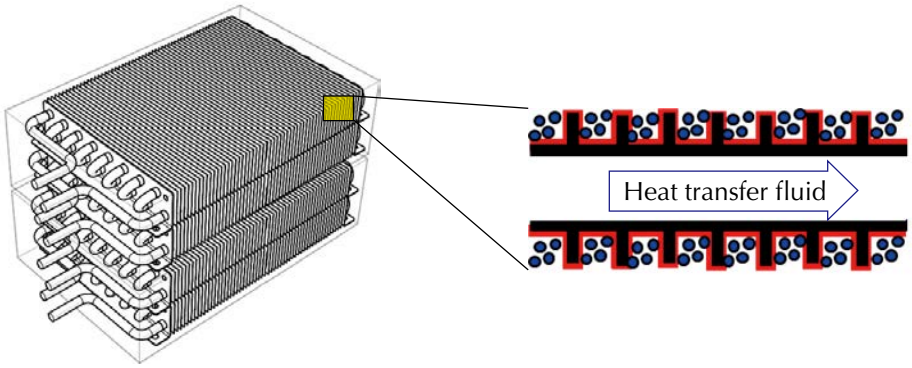


Fig. 9.1. Block diagram of hybrid adsorber heat exchanger.

2. Development of high-efficiency refrigeration and air-conditioning technology for practical use of next-generation low-GWP refrigerants(Prof. Higashi)

NEXT-RP, which was established in 2016 as a research center affiliated with I²CNER, is the only public research institute for the evaluation of refrigerant thermophysical properties in the world. NEXT-RP collaborates with domestic and international thermophysical property research institutes to evaluate new next-generation refrigerants with low GWP (Global Warming Potential) without depleting the ozone layer. Currently, NEXT-RP is participating in the New Refrigerants Research Project, a national project of the Ministry of Economy, Trade and Industry (METI), and is implementing the project of "Development of high-efficiency refrigeration and air-conditioning technology for practical use of next-generation low-GWP refrigerants" from 2023 to 2027.

For the joint research with the refrigerant manufacturers and the air-conditioning manufacturers, several projects are currently in progress. For example, in the joint research with Daikin Industries, Osaka, Japan, NEXT-RP has been involved in the evaluation of thermophysical properties of new refrigerant R1132(E) and new refrigerant blends, R474A, R474B, and R479A, in the development stage. The results have been presented at international conferences and published in international journals. In 2022, JARef Vol. 5, a data book on thermophysical properties of HFO and HCFO refrigerants, was published by the Japan Society of Refrigerating and Air Conditioning Engineers (JSRAE). In addition, NEXT-RP played an essential role in the certification process of ISO 17584, revised in August 2022, and has contributed globally to the intellectual infrastructure project of low-GWP refrigerants.

Fig. 9.2. New refrigerant sample of R1132(E).

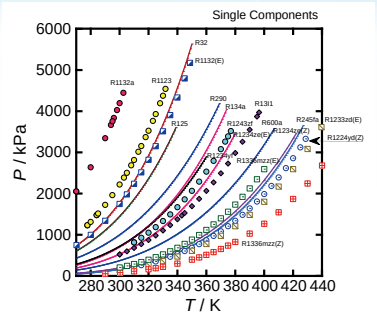


Fig. 9.3. Vapor pressure curves measured in NEXT-RP.

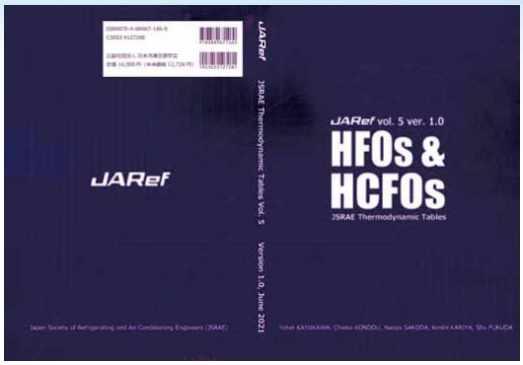


Fig. 9.4. HFO and HCFO data book edited by NEXT-RP.

3. Quantitative characterization of oxygen effect within fatigue crack growth in hydrogen-blended natural gas (PI Kubota and Prof. Komoda with JFE Steel Corporation)

Prof. Kubota (I^2CNER) and Komoda (I^2CNER and Kyushu Institute of Technology) continued their industrial collaboration with JFE Steel Corporation on the characterization of fatigue crack growth in hydrogen-blended natural gas. In 2013, Profs. Somerday, Sofronis and Kirchheim (PIs of I^2CNER) along with their colleagues invented an analytical formula that quantitatively describes the amount of oxygen needed to mitigate the hydrogen effect on fatigue crack growth, considering specific hydrogen pressure, frequency and magnitude of loading, and material strength (Acta Materiallia 2013). In this collaboration, the pivotal outcome from I^2CNER's research was applied to studying the crack growth in hydrogen-blended natural gas, which led to successful determination of the oxygen contents governing hydrogen-assisted fatigue crack growth.

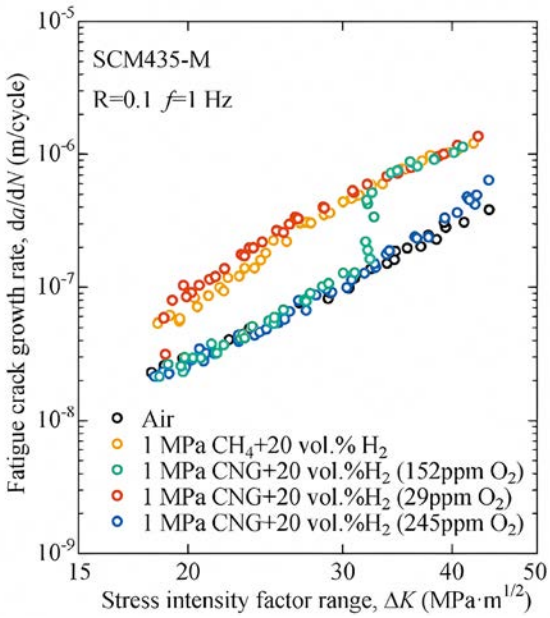


Fig. 9.5. Fatigue crack growth rate (da/dN) versus stress intensity factor range (ΔK) for SCM435 in 20 vol.% H_2 contained natural gases with different O_2 concentrations

Network of International Collaborations

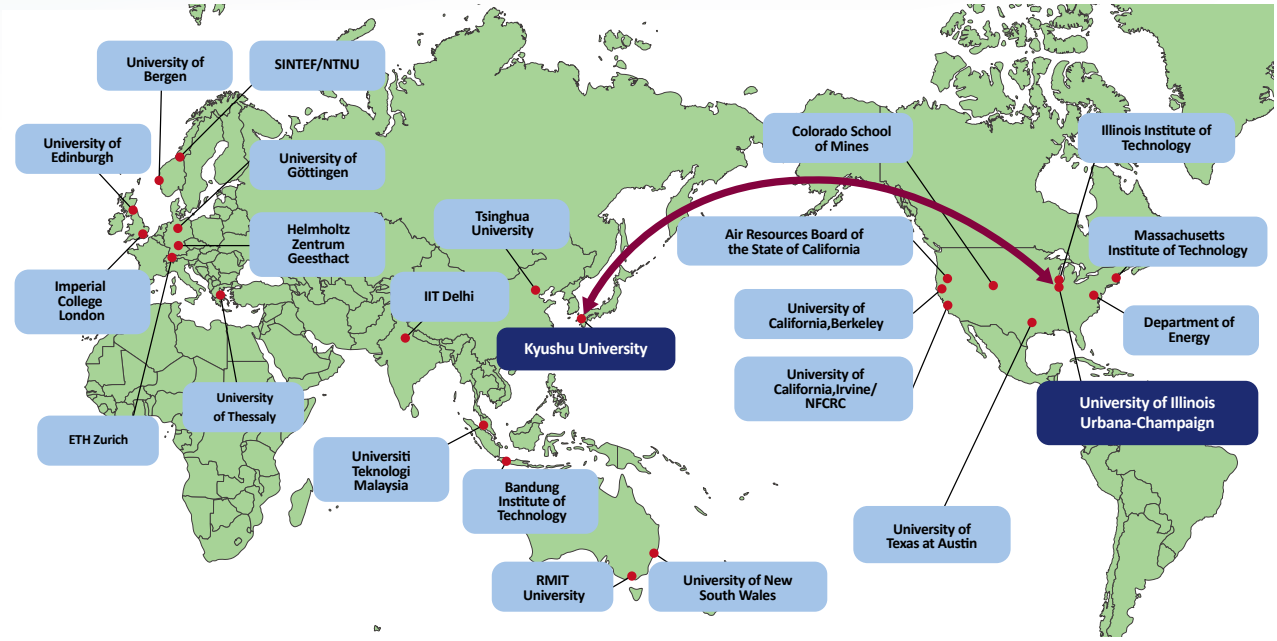


Fig. 10.1. This map includes the home institutions of I²CNER's foreign WPI faculty as well as those institutions with which I²CNER has academic agreements.

Globalization by the Numbers

In FY2022, 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 8 international conferences (240 in total since inception); 8 international conference sessions/symposia or workshops (349 since inception); and 6 I²CNER international workshops (92 since inception).
- Our researchers have given 42 keynote, plenary, and invited presentations in international conferences and fora (843 since inception).
- Our researchers have joint publications with researchers from 168 institutions (1127 in total since inception).
- Between its inception and March 31, 2023, the Institute has hosted a total of 99 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), 17 (FY2019) and 10 (FY2022). Of these, 71 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.*

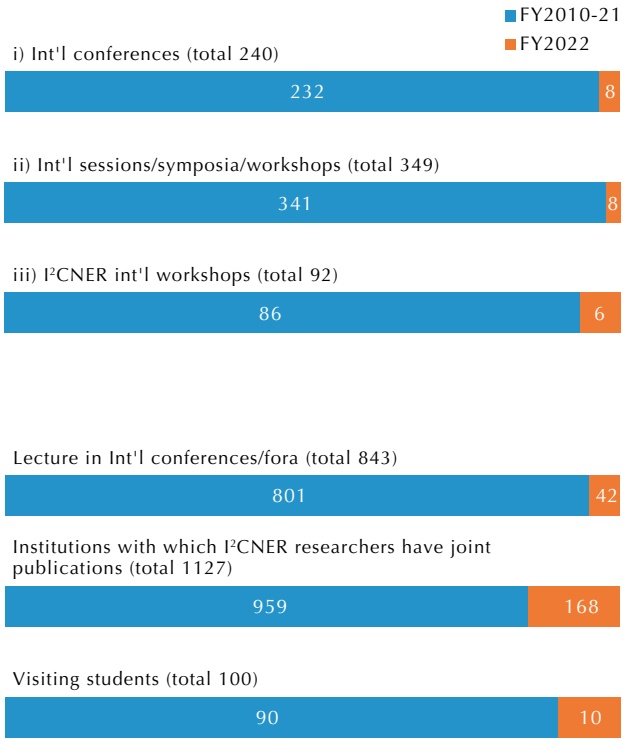
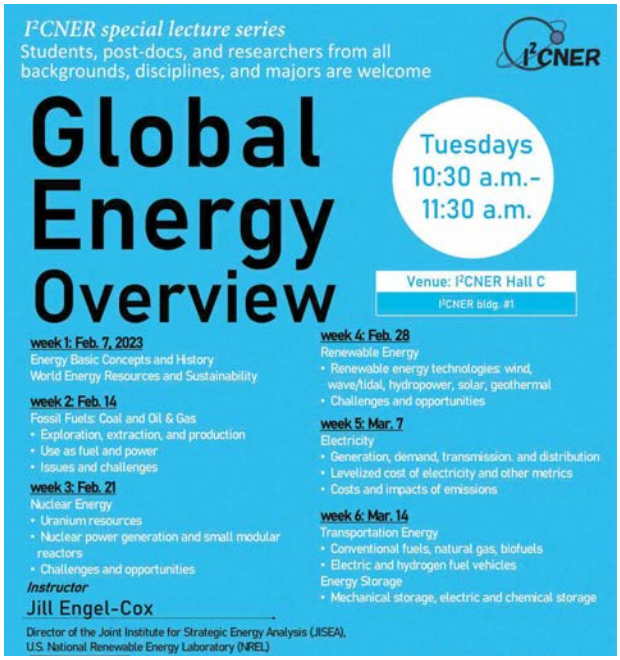


Fig. 10.2. Details of international activities

I²CNER special lecture series "Global Energy Overview" from Visiting Professor, Dr. Jill Engel-Cox

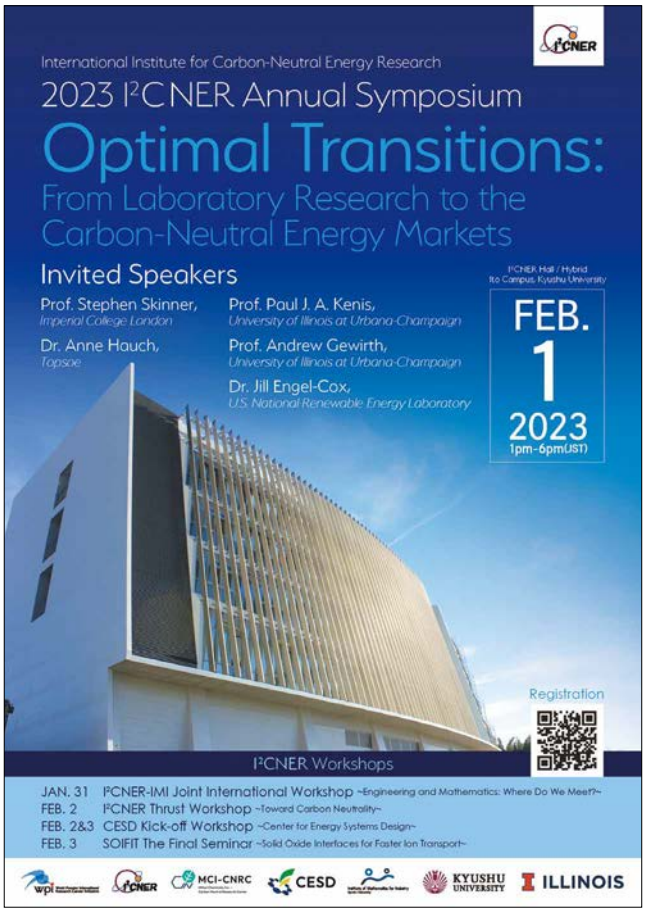
From January through March 2023, I²CNER hosted a Visiting Professor, Dr. Jill Engel-Cox from the National Renewable Energy Laboratory, Golden, Colorado, USA. The 10 week extended residency enabled in-depth discussions with faculty, mentoring of students, seminars to share knowledge, and collaboration on research. During her stay, Dr. Engel-Cox conducted a 6-week lecture series on global energy to approximately 40 students from across Kyushu University, covering energy history, policy, and technologies. The seminar series provided the students with a broad overview of the energy sector and opportunity for discussion about issues and trends in global energy development. In addition to the seminar series, Dr. Engel-Cox presented on energy technology innovation at I²CNER's annual symposium and participated in a workshop on energy economics with Kyushu University and Kyoto University on energy and social issues.

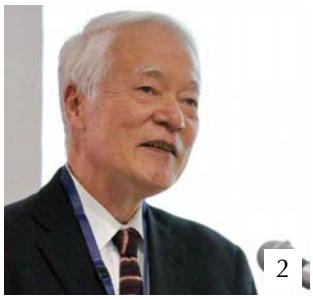


In addition to the seminar series, she collaborated with Dr. Andrew Chapman on writing a thought paper on energy, population, and economics, comparing the differences and similarities of development between three countries – Japan, the United States, and Bangladesh. The paper is expected to be published in a journal in 2023. Dr. Engel-Cox, Dr. Chapman, and several I²CNER students also started collaborations on analysis of decisionmaking on sustainable energy and planned meetings in Colorado later in 2023. Multiple mentoring meetings were held with I²CNER students on their research and careers.

While in Kyushu, Dr. Engel-Cox gave a joint talk with Dr. Akari Hayashi at an event in March on the topic of women in science, technology, engineering, and math (STEM), sponsored by the U.S. Consulate and held at the American Center in Fukuoka. Representatives from three universities, including Kyushu University, also spoke about their STEM programs. In addition, Dr. Engel-Cox conducted a webinar on careers in science and engineering on International Women's Day for the American Consulate in Okinawa.

Optimal Transitions: From Laboratory Research to the Carbon-Neutral Energy Markets
(2023 I²CNER Annual Symposium)





(photos, from the upper left to the lower right)
1. Dr. Tatsuro Ishibashi, President, Kyushu University
2. Dr. Akira Ukawa, WPI Program Director
3. Mr. Chuka Asike, Principal Officer to the U.S. Consulate Fukuoka
4. Mr. Shingo Shibata, Managing Executive Officer, Center Executive, R&D Center, Mitsui Chemicals, Inc.
5. Prof. Andrew Gewirth, Department of Chemistry, University of Illinois Urbana - Champaign (UIUC)
6. Dr. Anne Hauch, Senior Group Manager, SOEC Cell Performance Group - Power-to-X Topsoe

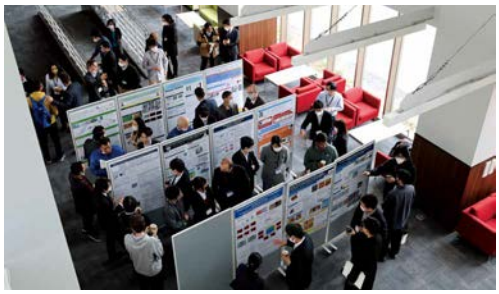
Since its inception, I²CNER has held an annual symposium, which has evolved over time from an event that celebrates the current research achievements of its thematic research areas (three thrusts) to an exploratory forum that focuses on a single research topic that is highly relevant to I²CNER's research 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, "Optimal Transitions: From Laboratory Research to the Carbon-Neutral Energy Markets" held on February 1, 2023. In this symposium, the latest research results were presented in the four research areas of the Mitsui Chemicals, Inc. – Carbon Neutral Research Center (MCI-CNRC), which was established within I²CNER to accelerate the implementation of carbon neutral technologies in society. World-class researchers from research institutions in the U.S., Europe, and Asia were invited to the conference, where they engaged in lively discussions from their respective standpoints.

Program *February 1, 2023*

MC: PI Tatsumi Ishihara, I²CNER

Opening Remarks	**Dr. Tatsuro Ishibashi,** *President, Kyushu University* **Dr. Akira Ukawa,** *WPI Program Director* **Mr. Chuka Asike,** *Principal Officer to the U.S. Consulate Fukuoka* **Mr. Shingo Shibata,** *Managing Executive Officer, Center Executive, R&D Center, Mitsui Chemicals, Inc.* **PI Petros Sofronis,** *Director, I²CNER, Kyushu University*
Introduction	**Prof. Toshihiro Takai,** *Director, MCI-CNRC, I²CNER, Kyushu University* *"Establishment of Mitsui Chemicals, Inc.–Carbon Neutral Research Center (MCI-CNRC)"*
Session I: Green Hydrogen Production and Utilization	**Prof. Stephen Skinner,** *Imperial College London* *"Investigating surface and interface properties and their impact on solid oxide cell electrodes"* **Dr. Anne Hauch,** *Senior Group Manager, SOEC Cell Performance Group - Power-to-X Topsoe* *"Current Status of SOEC Development in Denmark; from research at DTU to up-scaling and commercialization at Topsoe"* **Prof. Kaveh Edalati,** *I²CNER, Kyushu University* *"Active photocatalysts by high-pressure torsion"*
Session II: CO_2 Separation and Capture	**Prof. Paul Kenis,** *Elio Eliakim Tarika Endowed Chair and Department Head in Chemical and Biomolecular Engineering, University of Illinois Urbana-Champaign (UIUC)* *"Towards Integration of CO_2 capture and conversion technology"* **PI Bidyut Baran Saha,** *I²CNER, Kyushu University* *"Prospect of functional adsorbents in attaining environmental sustainability"*
Session III: CO_2 Conversion and Fixation	**PI Andrew Gewirth,** *Department of Chemistry, UIUC* *"Electrodeposited Composite Catalysts for CO_2 and methanol electrolyzers"* **Prof. Junji Nakamura,** *MCI-CNRC, I²CNER, Kyushu University* *"Conversion of carbon dioxide to methanol using Cu/ZnO catalysts"*
Session IV: Advanced Analysis and Evaluation	**Dr. Jill Engel-Cox,** *Director of the Joint Institute for Strategic Energy Analysis, U.S. National Renewable Energy Laboratory* *"From Research to Markets: Case studies of Clean Energy Technologies"* **PI Andrew Chapman,** *I²CNER, Kyushu University* *"Achieving a Sustainable Transition: Energy System Design, Behavior and Innovation"*
Closing Remarks	**PI Tatsumi Ishihara,** *I²CNER, Kyushu University*



Poster session

Scene during a coffee break

Group photo

Distinguished Visitors

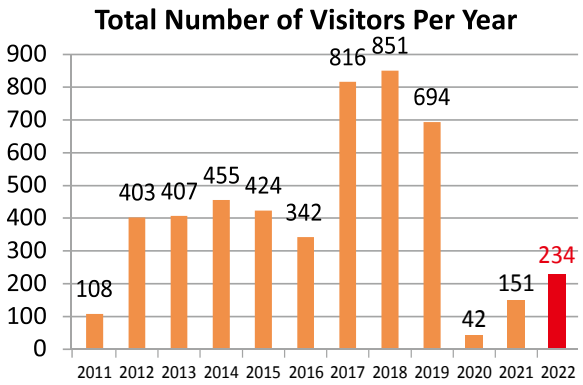
May 18, 2022 Dr. Michael Jacob (second from left), Innovation and Science Counsellor at the Embassy of Sweden in Tokyo.

June 6, 2022 Dr. Gediminas Ramanauskas (center), First Counsellor of the Delegation of the European Union to Japan.

June 30, 2022, Mr. Takashi Nishiyama (second from right), Director of Basic and Generic Research Division, Research Promotion Bureau of Research Promotion Bureau of Minister of Education, Culture, Sports, and Technology in Japan

September 22, 2022, Dr. Se Jung Oh (second from left), President, Seoul National University.

November 8, 2022, Mr. Nobuhiro Ishikawa, (center), Vice President, Toagosei co., ltd.



Although COVID-19 pandemic still persisted, the number of visitors increased in 2022 compared to the previous year.

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 FY2022, the Institute hosted 11 speakers (11 non-Japanese) for I²CNER Seminars. Cumulatively, 190 speakers have presented at 187 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

April 6, 2022

Prof. John A. Kilner
Senior Research Investigator, Imperial College London, UK
Title: Optimising Ion Transport in Ceramics for Energy Conversion and Storage Applications

June 1, 2022

Prof. Robert O. Ritchie
Professor, University of California / Lawrence Berkeley National Laboratory, USA
Title: Mechanisms of Fracture and Damage-Tolerance in New Metallic Alloys

October 12, 2022

Prof. Daniel Orejon
Associate Professor, University of Edinburgh, UK
Title: Droplets on Micro-decorated Surfaces: Wetting and Phase-Change

November 16, 2022

Prof. Erwin Reisner
Professor, University of Cambridge, UK
Title: Solar Panels for Light-to-Chemical Conversion

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, 368 speakers have presented at 232 seminars. In FY2022, 17 speakers presented at 17 Institute Interest Seminars. Even during the pandemic, Zoom seminars effectively reached 303 attendees.

Selected IISS speakers

May 17, 2022

Dr. Shamal Chandra Karmaker
Multiscale Science and Engineering for Energy and the Environment
Title: Energy poverty and cultural impact on the energy system

June 8, 2022

Prof. Junji Nakamura
Mitsui Chemicals, Inc.- Carbon Neutral Research Center
Title: Bridge Between Catalytic Chemistry and Surface Science

July 6, 2022

Asst. Prof. Mai Tomisaki
Advanced Energy Conversion Systems
Title: Electrochemical Conversion of Carbon Dioxide Using Diamond Electrodes

November 2, 2022

Asst. Prof. Zhenying Wang
Multiscale Science and Engineering for Energy and the Environment
Title: Wetting Dynamics of Droplets with Interfacial Phase Change: Fundamentals and Implications for Industrial Application

November 30, 2022

Dr. Nan Zhang
Advanced Energy Materials
Title: Ammonia effect on hydrogen embrittlement mitigation and induction

March 29, 2023

Assoc. Prof. Hirokazu Kobayashi
Advanced Energy Materials
Title: Developments of Novel Metal Nanostructured Materials for Energy/Catalysis Applications

Conferences and Symposia

The 13th Asian Thermophysical Properties Conference (ATPC2022)

September 26-30, 2022
Hybrid meeting (onsite and online), organized by Prof. Takahashi. K.
https://www.atpc2022.org/index.html

SNU – Kyushu Joint Symposium

September 23, 2022 in Fukuoka, Japan
Satellite session organizing by PI Fujikawa.

HYDROGENIUS, I²CNER, HYDROMATE, and SINTEF Joint Research Symposium 2023 on Hydrogen-Materials Interactions

February 2-3, 2023, Online
Chaired by PI Somerday and Prof. Matsunaga,
This symposium series has garnered significant attention from the stakeholders within academia, industry and government who are advocating for the utilization of hydrogen.

10th International Symposium on Fretting Fatigue (ISFF-10)

September 19-21, 2022 in Leuven, Belgium
PI Kubota, International Science Committee,
The ISFF is a renowned conference series dedicated to the study on fretting fatigue, and it has been held since 1993. This conference is highly regarded as a gathering of distinguished researchers in the field of fretting fatigue from around the world.

47th International Conference and Expo on Advanced Ceramics and Composites (ICACC2023), S3: 20TH INTERNATIONAL SYMPOSIUM ON SOLID OXIDE CELLS (SOC): MATERIALS, SCIENCE AND TECHNOLOGY

January 22-27, 2023 in Daytona, U.S.A.
Session organized by PI Ishihara

Solid Oxide Interfaces for Faster Ion Transport (SOIFIT) with the 6rd edition of the "Power of Interfaces" workshop

October 6-7, 2022 in Mallorca, Spain
PI Matsumoto

The final seminar of Core-to-Core program SOIFT

February 3, 2023
PI Matsumoto

Plenary and Keynote Presentations

PI Kubota, "Creep in High-Temperature Hydrogen" The 6th International Conference on Materials and Reliability (ICMR2022), Yamaguchi, Japan, December 7-9, 2022

PI Stubbins, "Advances in the Understanding of Mechanical Behavior of Materials for Advanced Energy Systems"(Plenary), International Association of Advanced Materials, 2022 Baltic Conference Series, Stockholm Sweden, August 28-31, 2022.

PI Takahashi, K. "Nanomaterials for phase change heat transfer" (Keynote), 13th Asian Thermophysical Properties Conference (ATPC2022) (Online), September 26, 2022

Prof. Takata "Enhancement of Boiling Heat Transfer by Surface Wettability Control" (Plenary), Energy Technologies Symposium 2022, Tokyo, December 12, 2022

PI Fujikawa, "Membrane-based Direct Air Capture -Possibilities and Prospect-" (Plenary), RadTech Asia 2022, Tsukuba, Japan, August 25, 2022

PI Saha, Adsorption technology toward achieving carbon-neutral energy society, BCSIR Congress 2022, Theme: Integrated Approach for Adapting 4IR, Keynote Lecture, KN-D2, Dhaka, 1-3 December 2022.

PI Ishihara, Photobiocatalyst for water splitting to green hydrogen with high efficiency, 2022 International Symposium on Carbon-neutral Energy Virtual Symposium, Online, June, 2022

PI Ishihara, Strain Effects on Surface Activity and Oxide Ion Conductivity, 23rd International Conference on Solid State Ionics (SSI-23), Bonston, USA, July, 2022(Plenary)

PI Kilner, "Grain Boundaries in MIECs; A Help or a Hindrance?", SSI-23 23rd International Conference on Solid State Ionics, Boston USA, 17-22nd July 2022

Prof. Skinner, Impact of operating environment on key electrochemical processes in solid oxide cells, Solid State Ionics, Boston, USA, 2022

Selected Awards

Date	Recipient's name	Name of award
March 8, 2023	Toshihiro Tsuchiyama	**Distinguished Article Award, ISIJ, The Iron and Steel Institute of Japan**
February 14, 2023	Hideaki Teshima	**JSME Young Engineers Award, Japan Society of Mechanical Engineers**
February 8, 2023	Chihaya Adachi	**Kenjiro Sakurai Memorial Award**
November 15, 2022	Chihaya Adachi	**Highly Cited Researchers 2022, Clarivate**
October 18, 2022	Yukina Takahashi	**Masao Horiba Award**
October 11, 2022	Chihaya Adachi	**2022 (92nd) Hattori Hokokai "Hoko Award"**
May 23, 2022	Yasuyuki Takata	**Honorary Member, Japan Society of Mechanical Engineers (JSME)**
May 23, 2022	Yasuyuki Takata	**Honorary Member, Heat Transfer Society of Japan (HTSJ)**
May 19, 2022	Yasuyuki Takata, Biao Shen	**Scientific Contribution Award, Heat Transfer Society of Japan**
April 30, 2022	Akio Miyara	**JSME Contribution Award, Japan Society of Mechanical Engineers**

Prof. Adachi receiving Kenjiro Sakurai Memorial Award

Prof. Takahashi receiving Masao Horiba Award

Outreach Activities

Outreach Events

Students from Oita Prefecture visited I²CNER (August 17, 2022)

A total of 22 students from O-Labo in Oita Prefecture visited I²CNER and other facilities at Kyushu University's Ito Campus on August 17, 2022 as part of a local government-run active learning program for children in the area. In a bid to make the students familiar with the importance of realizing a carbon-neutral society, I²CNER introduced its research efforts and activities through a variety of programs, including a mini lecture, a hands-on experiment, I²CNER lab tours and a roundtable talk. The students seem to have learned about the research activities at I²CNER and have taken their first steps to thinking about societal issues and their future.

WPI Symposium for High School Students (November 23, 2022)

A hybrid symposium "Science Opens Up Infinite Possibilities" was held on November 23, 2022 hosted by the International Research Center for Neurointelligence (WPI-IRCN), the University of Tokyo. The symposium was mainly targeted at high school students and teachers. Prof. Chapman from I²CNER gave a keynote lecture, titled "Energy transition toward carbon neutrality" along with two other speakers representing institutions of WPI. At the end of the symposium, the students and researchers engaged in a lively question and answer session.

Energy Week 2023 (January 30 - February 3, 2023)

Kyushu University Energy Week 2023 was held January 30 to February 3, 2023, featuring symposia concerning energy on the theme of "Energy Intelligence beyond Borders: Opening the Path to Future Energy and Energy Security with Integrative Knowledge." At this symposium, energy-related organizations inside and outside the university collaborated to hold international workshops, industry-academia-government collaboration workshops, etc., and played a role as a place for interaction that functions as an international hub for energy researchers. The I²CNER Annual Symposium, I²CNER Thrust Workshop, I²CNER-HYDROGENIUS Joint Research Symposium and I²CNER-IMI Joint International Workshop, were all held during Energy Week. This time, the 7th time, it was mostly held in a hybrid format including researchers who are active in Japan and overseas, as well as researchers, students, industry, and others who are engaged in a wide range of energy-related research. A total of approximately 2,000 people attended the event.

Students from Oita Prefecture Visiting I²CNER

WPI Symposium for High School Students

I²CNER Thrust Workshop during Energy Week 2023

Press Releases and Media Coverage

Press Releases in FY2022

DATE	DESCRIPTION
May. 16, 2022	**PI Tsuyohiko Fujigaya** (Advanced Energy Conversion Systems Thrust) Polymer-coated carbon nanotube hybrids with functional peptides for gene delivery into plant mitochondria
Jun. 15, 2022	**PI Andrew Chapman** (Multiscale Science and Engineering for Energy and the Environment Thrust) Shedding Light on the energy-related social equity of nations toward a just transition
Jul. 1, 2022	**Prof. Junji Nakamura** (Mitsui Chemicals, Inc.–Carbon Neutral Research Center) Hydrogenation of Formate Species Using Atomic Hydrogen on a Cu(111) Model Catalyst
Aug. 1, 2022	**PI Andrew Chapman** (Multiscale Science and Engineering for Energy and the Environment Thrust) Listening to the people results in a more sustainable future energy system
Aug. 26, 2022	**PI Chihaya Adachi** (Advanced Energy Conversion Systems Thrust) Small molecules, giant (surface) potential
Sep. 16, 2022	**PI Takeshi Tsuji** (Multiscale Science and Engineering for Energy and the Environment Thrust) Seismic device made for extraterrestrial research can help tackle climate change on earth
Nov. 14, 2022	**Prof. Junji Nakamura** (Mitsui Chemicals, Inc.–Carbon Neutral Research Center) Activating Nitrogen-doped Graphene Oxygen Reduction Electrocatalysts in Acidic Electrolytes using Hydrophobic Cavities and Proton-conductive Particles
Nov. 22, 2022	**PI Tsuyohiko Fujigaya and Prof. Tomohiro Shiraki** (Advanced Energy Conversion Systems Thrust) ortho-Substituted Aryldiazonium Design for the Defect Configuration-Controlled Photoluminescent Functionalization of Chiral Single-Walled Carbon Nanotubes
Feb. 1, 2023	**Dr. Tomoaki Nakaishi** (Mitsui Chemicals, Inc.–Carbon Neutral Research Center) Production efficiency and cost reduction potential of biodiesel fuel plants using waste cooking oil in Japan
Mar. 9, 2023	**PI Seiji Ogo** (Multiscale Science and Engineering for Energy and the Environment Thrust) Safe, One-Pot, Homogeneous Direct Synthesis of H_2O_2
Mar. 22, 2023	**PI Shigenori Fujikawa** (Multiscale Science and Engineering for Energy and the Environment Thrust) Kyushu University, Sojitz, and Kyushu Electric Power Sign MOU for Joint Development and Verification of DAC-U Systems Utilizing Direct Air Capture Technology

Media Coverage in FY2022

DATE	MEDIA OUTLET	DESCRIPTION
May. 19, 2022	Magazine/ Physical science	**Prof. Kwati Leonard** New steam electrolysis devices for efficient hydrogen production
May. 31, 2022	Nihon Keizai Shimbun	**PI Chihaya Adachi and Prof. Tomohiro Shiraki** Kyushu University and Tokyo University of Agriculture and Technology Develop Molecule that Exhibits Giant Positive and Negative Surface Potentials by Simply Depositing a Film
Jun. 21, 2022	NHK-World	**PIs Shigenori Fujikawa and Miho Yamauchi** Science View "A Look at CO_2 Reduction Technology"
Sep. 14, 2022	Nihon Keizai Shimbun	**PI Takeshi Tsuji** University of Tokyo and Kyushu University develop an ultra-compact seismic source device for continuous monitoring of CO_2 geological storage
Dec. 6, 2022	Yahoo! News (my navi news)	**Prof. Tomohiro Shiraki** Future technology using defect chemistry for functionalized carbon nanotubes
Feb. 22, 2023	Nikkan Kogyo Shimbun	**PI Seiji Ogo** A safe synthesis of hydrogen peroxide inspired by nature
Mar. 15, 2023	Magazine/ Junior AERA	**PI Andrew Chapman** Energy transition toward carbon neutrality
Mar. 22, 2023	Nihon Keizai Shimbun	**PI Shigenori Fujikawa** Kyushu University, Sojitz, and Kyushu Electric Power have signed a memorandum


Kyushu University, Sojitz, and Kyushu Electric Power Sign MOU for Joint Development and Verification of DAC-U Systems Utilizing Direct Air Capture Technology

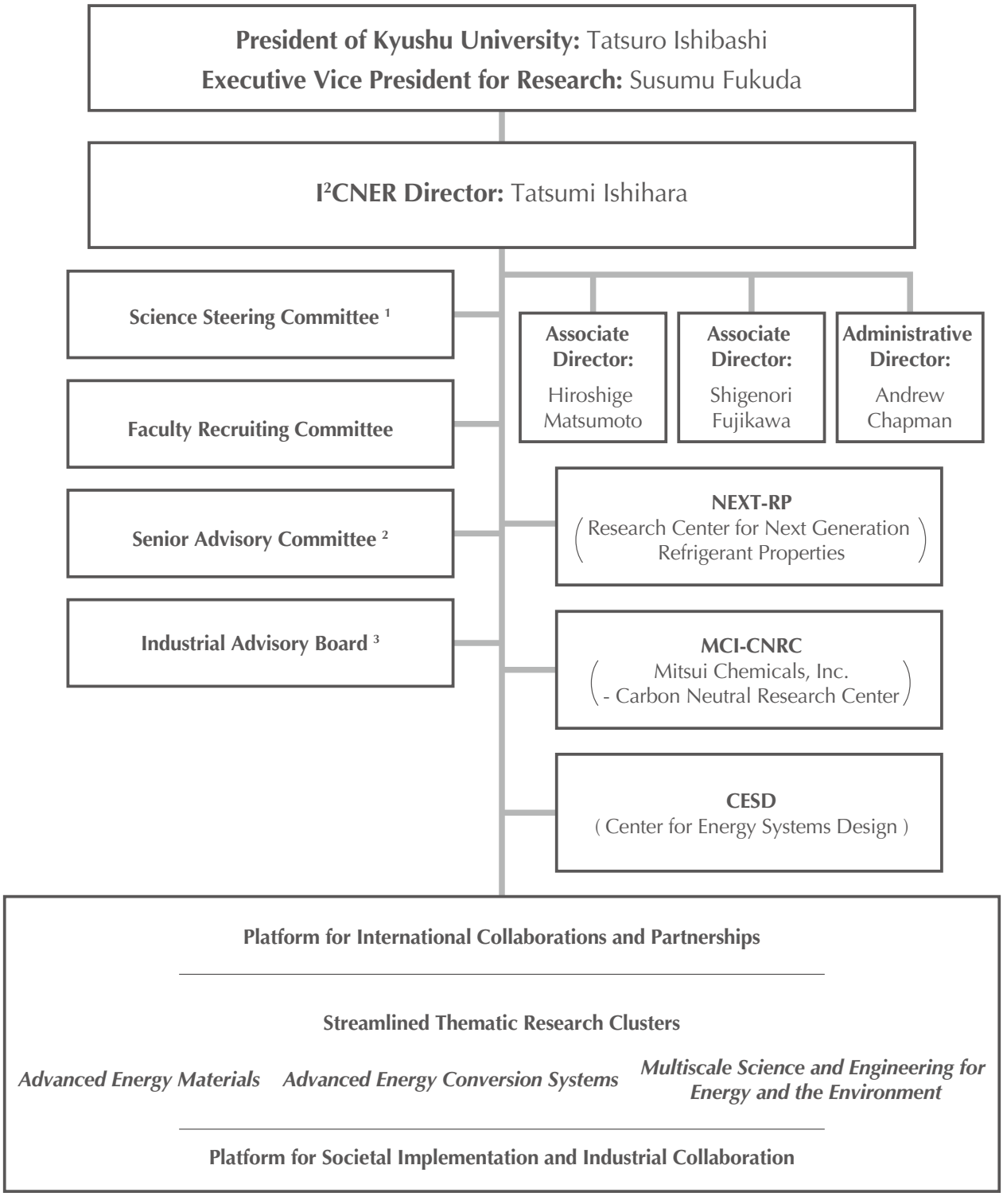
Kyushu University, Sojitz Corporation ("Sojitz"), and Kyushu Electric Power Co., Inc. ("Kyushu Electric Power") have signed a memorandum of understanding for joint development and verification for the application of a Direct Air Capture and Utilization (DAC-U) system. The DAC-U apparatus will combine both: a separation membrane-based direct air capture (m-DACTM) unit currently under development*1 by Kyushu University that allows carbon dioxide to be extracted directly from the atmosphere, with another device that converts the captured carbon dioxide into fuel.

Prof. Shigenori Fujikawa press release (Mar. 22, 2023)

Magazine article covering Prof. Andrew Chapman

I²CNER Structure (as of April 1, 2023)

Organizational Structure



1) The **Science Steering Committee (SSC)** is chaired by the Director, and its members are the two Associate Directors and the 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.

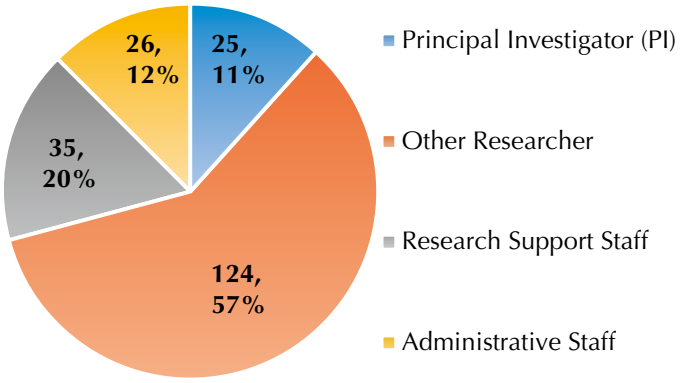
2) The **Senior Advisory Committee (SAC)** makes recommendations on the current status of the Institute and its future directions and provides the Director with a written report detailing their findings and recommendations. The full list of members as of April 1, 2023 is as follows:

- Prof. Petros Sofronis *Chair — University of Illinois at Urbana-Champaign, USA
- Prof. Reiner Kirchheim — University of Göttingen, Germany
- Prof. Robert McMeeking — University of California at Santa Barbara, USA
- Prof. Michael A. Celia — Princeton University, USA
- Prof. Harry Tuller — Massachusetts Institute of Technology, USA
- Prof. John Kilner — Imperial College, London, UK
- Prof. Ian Robertson — University of Wisconsin-Madison, USA
- Prof. Ken Okazaki — Tokyo Institute of Technology, Japan
- Dr. John Kopasz — Argonne National Laboratory, USA

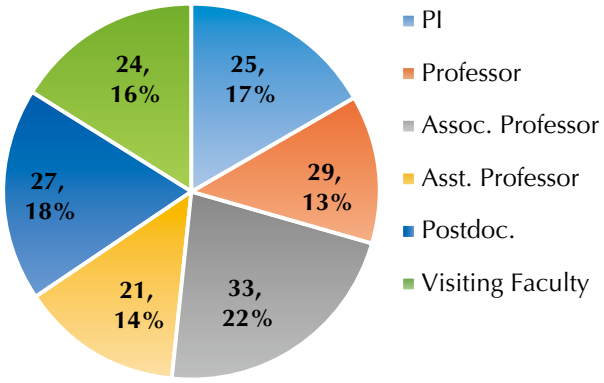
3) In FY2017, I²CNER established **the Industrial Advisory Board (IAB)**, whose members are prominent executives from industry, government agencies, and national laboratories that advise I²CNER on opportunities for interactions with industry and technology transfer. The first IAB meeting was held on February 1, 2018 and was attended by 9 out of 10 IAB members. The meeting provided invaluable inputs to I²CNER researchers on areas that industries would have interest for promoting the development of new technologies.

Personnel (as of April 1, 2023)

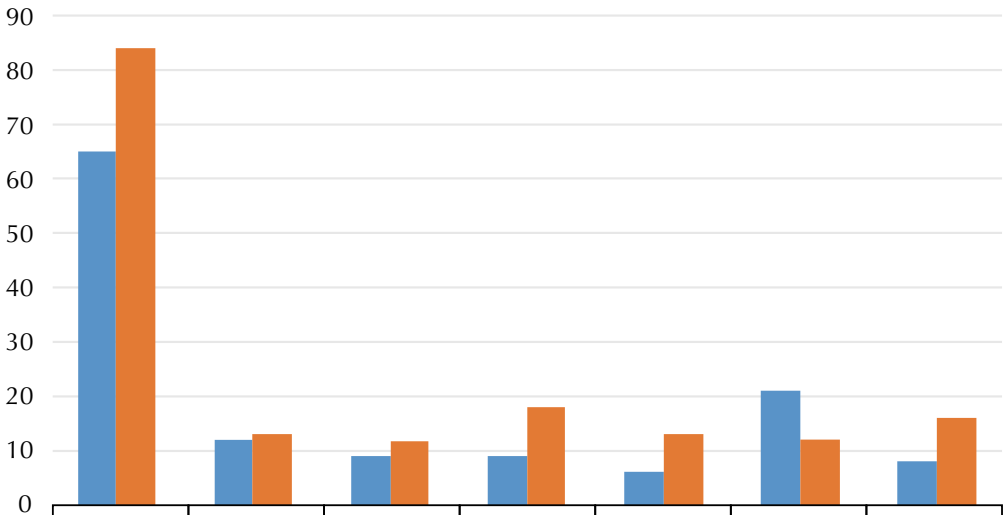
Breakdown of Personnel (Total: 210)



Researchers by Title (Total: 149)



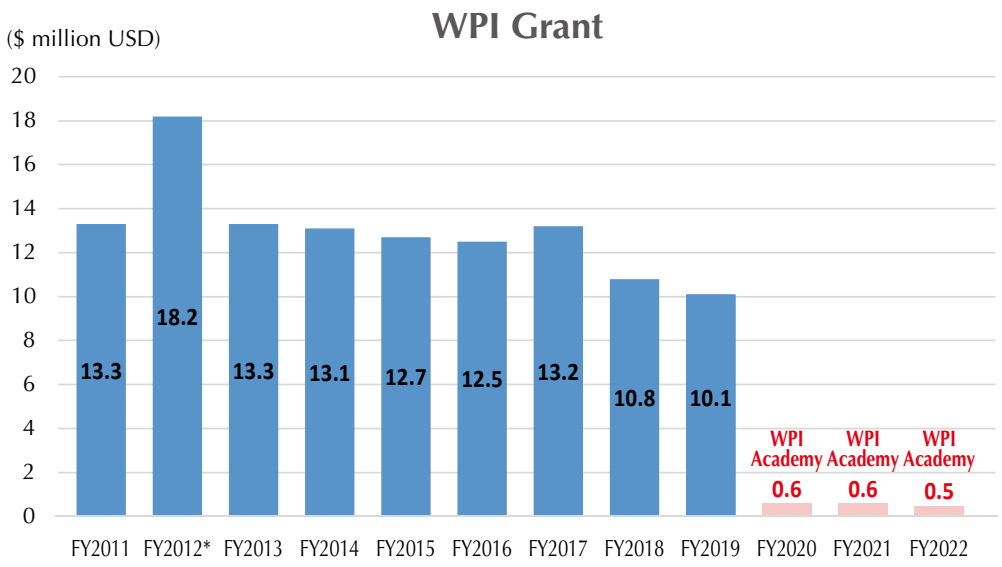
Statistics of Researchers by Title



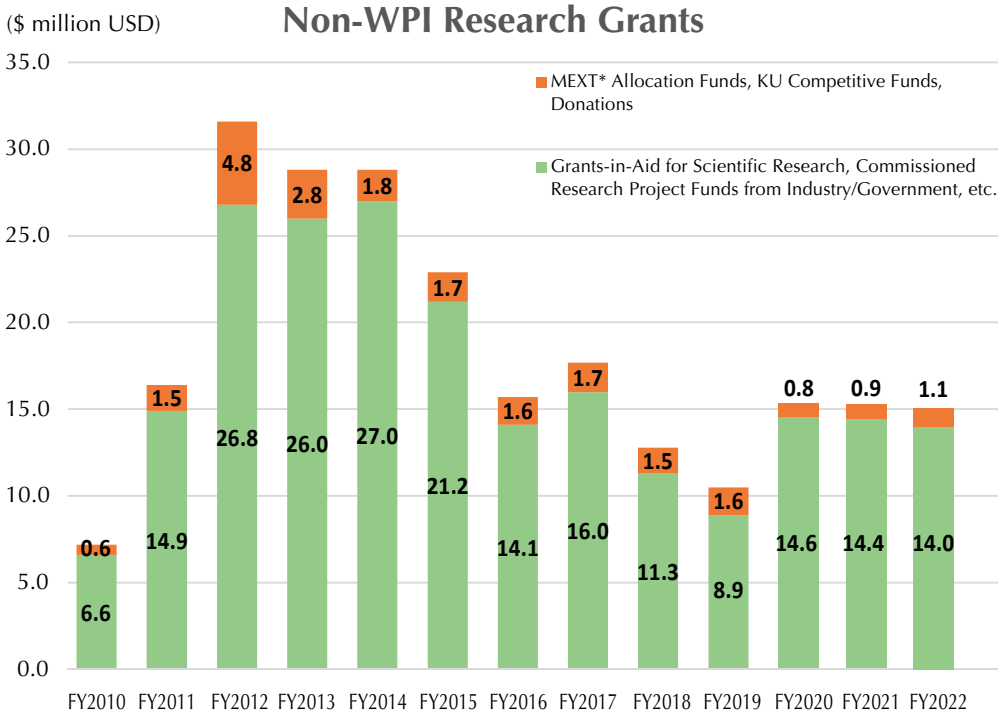
	Total	PI	Prof.	Assoc. Prof.	Asst. Prof.	Postdoc	Visiting Faculty
Overseas	65	12	9	9	6	21	8
Japanese	84	13	12	18	13	12	16
% Overseas	44%	48%	43%	33%	32%	64%	33%
% Female	13%	8%	0%	7%	32%	21%	8%

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, 2023)

Administration

Director
Prof. Tatsumi Ishihara

Associate Directors
Prof. Hiroshige Matsumoto
Prof. Shigenori Fujikawa

Principal Investigators

Advanced Energy Conversion Systems Thrust
Prof. Hiroshige Matsumoto (Thrust Lead PI)
Prof. Tatsumi Ishihara
Prof. Thomas Lippert, *Paul Scherrer Institut, Switzerland*
Assoc. Prof. Aleksandar Tsekov Staykov
Prof. Chihaya Adachi
Prof. Tsuyohiko Fujigaya
Prof. Stephen John Skinner, *Imperial College London, UK*
Prof. Andrew Gewirth, *University of Illinois Urbana-Champain, USA*

Advanced Energy Materials Thrust
Prof. Masanobu Kubota (Thrust Lead PI)
Prof. Toshihiro Tsuchiyama
Prof. Brian P. Somerday, *University of Illinois Urbana-Champain, USA*
Prof. Petros Sofronis, *University of Illinois Urbana-Champain, USA*
Prof. Yoshinori Sawae
Prof. Cynthia A. Volkert, *University of Göttingen, Germany*
Prof. Seiji Ogo
Prof. Miho Yamauchi

Multiscale Science and Engineering for Energy and the Environment Thrust
Prof. Shigenori Fujikawa (Thrust Lead PI)
Prof. Bidyut Baran Saha
Prof. Anutosh Chakraborty, *Nanyang Technological University*
Assoc. Prof. Andrew Chapman
Prof. Koji Takahashi
Prof. Takeshi Tsuji, *University of Tokyo, Japan*
Prof. Yuichi Sugai
Prof. James Stubbins, *University of Illinois Urbana-Champain, USA*
Prof. Paul J. A. Kenis, *University of Illinois Urbana-Champain, USA*

Full-time Faculty & Postdoctoral Associates

Advanced Energy Conversion Systems Thrust
Dr. Adikari Musiyanselage Chathuranganie Senevirathne
Assoc. Prof. Kaveh Edalati
Asst. Prof. Miho Isegawa
Dr. Sovann Khan
Dr. Bhuvaneshwari Manivannan
Assoc. Prof. Toshinori Matsushima
Dr. Yutaka Osaki
Dr. Vediyappan Veeramani
Assoc. Prof. Motonori Watanabe
Dr. Kuan Ting Wu
Dr. Dengyao Yang

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

Multiscale Science and Engineering for Energy and the Environment Thrust
Dr. Jianlei Han
Assoc. Prof. Nguyen Dinh Hoa
Dr. Wing Chung Liu
Dr. Animesh Pal
Prof. Yasuyuki Takata

Platform for International Collaborations and Partnerships
Asst. Prof. Leonard Kwati
Asst. Prof. Mai Tomisaki

Platform for Societal Implementation and Industrial Collaboration
Asst. Prof. Yuto Yamada

Research Center for Next Generation Refrigerant Properties
Prof. Yukihiro Higashi

Mitsui Chemicals, INC. -Carbon Neutral Research Center
Prof. Toshihiro Takai
Dr. Sharif Md Hossain
Dr. Amirul Md.Islam
Dr. Ming-Han Liu
Dr. Mohammad Moniruzzaman
Prof. Junji Nakamura
Dr. Tam Thanh Nguyen
Dr. Thinh Van Nguyen
Dr. Bhim Raju Telugu

Satellite Faculty & Postdoctoral Associates

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

Multiscale Science and Engineering for Energy and the Environment Thrust
Asst. Prof. Kathryn Huff

Part-time Faculty & Postdoctoral Associates

Advanced Energy Conversion Systems Thrust
Asst. Prof. Kenichi Goushi
Prof. Kohei Ito

Prof. Junko Matsuda
Assoc. Prof. Hajime Nakanotani
Prof. Masamichi Nishihara
Prof. Kazunari Sasaki
Assoc. Prof. Tomohiro Shiraki
Asst. Prof. Juntae Song
Asst. Prof. Naoki Tanaka
Prof. Kazunari Yoshizawa

Advanced Energy Materials Thrust
Dr. Akihiko Anzai
Dr. Jiamin Cheng
Asst. Prof. Masaki Donoshita
Dr. Yuu Kajiwara
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
Asst. Prof. Hiroyoshi Tanaka
Assoc. Prof. Tatsuya Uchida
Assoc. Prof. Kazuyuki Yagi
Asst. Prof. Kosei Yamauchi
Assoc. Prof. Seido Yarimitsu
Asst. Prof. Takeshi Yatabe

Multiscale Science and Engineering for Energy and the Environment Thrust
Dr. Yingjun An
Dr. Rasha Afmed Hanafy Bayomi
Assoc. Prof. Tatsunori Ikeda
Dr. Kenshi Itaoka
Prof. Masamichi Kohno
Assoc. Prof. Ken Kojio
Assoc. Prof. Kaname Matsue
Prof. Shoji Mori
Assoc. Prof. Jin Miyawaki
Prof. Takahiko Miyazaki
Assoc. Prof. Qin-Yi Li
Assoc. Prof. Naoya Sakoda
Assoc. Prof. Roman Selyanchyn
Assoc. Prof. Atsuomi Shundo
Dr. Feng Sinan
Prof. Atsushi Takahara
Asst. Prof. Hideaki Teshima
Assoc. Prof. Kyaw Thu
Asst. Prof. Yutaro Umehara
Asst. Prof. Zhenying Wang
Dr. Yucheng Zhang

Mitsui Chemicals, INC. -Carbon Neutral Research Center
Assoc. Prof. Shuntaro Tsubaki

Visiting Professors & Scholars

Advanced Energy Conversion Systems Thrust
Prof. Limin Guo, *Huazhong U. of Science and Technology*
Prof. John A Kilner, *Imperial College London, UK*
Assoc. Prof. Seiichiro Kimura, *Renewable Energy Institute, Japan*
Dr. Kenshi Mitsuishi, *Mitsui Chemicals, Inc., Japan*
Prof. Ken Okazaki, *Tokyo Institute of Technology*
Prof. Harry L. Tuller, *Massachusetts Institute of Technology, USA*
Asst. Prof. Helena Tellez-Lozano

Advanced Energy Materials Thrust
Prof. Nikolaos Aravas, *University of Thessaly, Greece*
Asst. Prof. Mohsen Dadfarnia, *Seattle University, USA*
Prof. Reiner Kirchheim, *University of Göttingen, Germany*
Assoc. Prof. Ryosuke Komoda, *Kyushu Institute of Technology, 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*

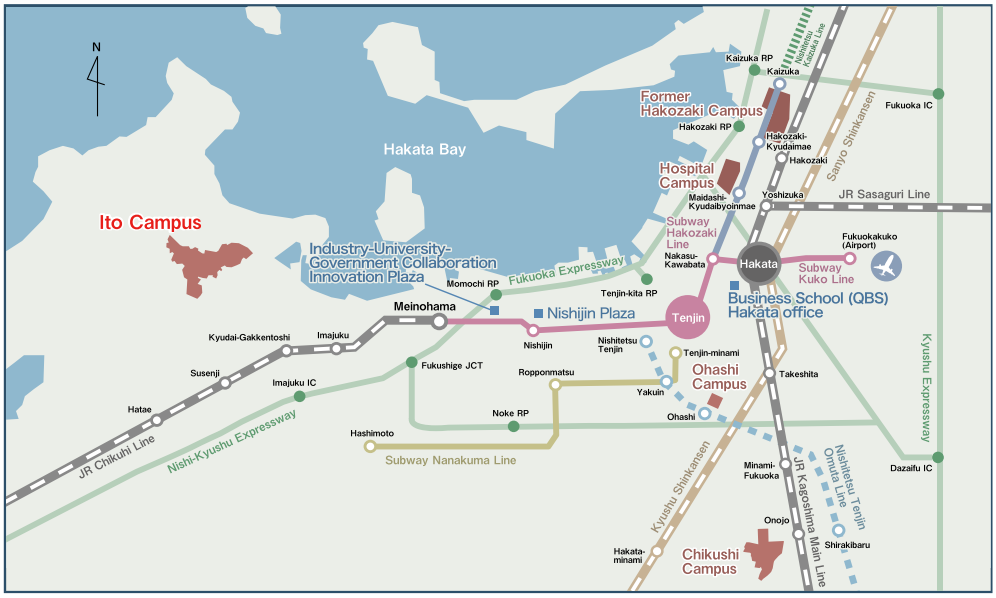
Multiscale Science and Engineering for Energy and the Environment Thrust
Prof. Makoto Akai, *National Institute of Advanced Industrial Science and Technology*
Prof. Jill Engel-Cox, *National Renewable Energy Laboratory, Golden, Colorado, USA*
Assoc. Prof. Jiang Fei, *Yamaguchi University, Japan*
Prof. Benny D. 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*
Asst. Prof. Yutaku Kita, *King's College London, England*
Prof. Toyoki Kunitake, *Kitakyushu Foundation for the Advancement of Industry Science and Technology, Japan*
Prof. Atsushi Kurosawa, *The Institute of Applied Energy, 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*
Dr. Kumi Yoshihara, *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."

34min.

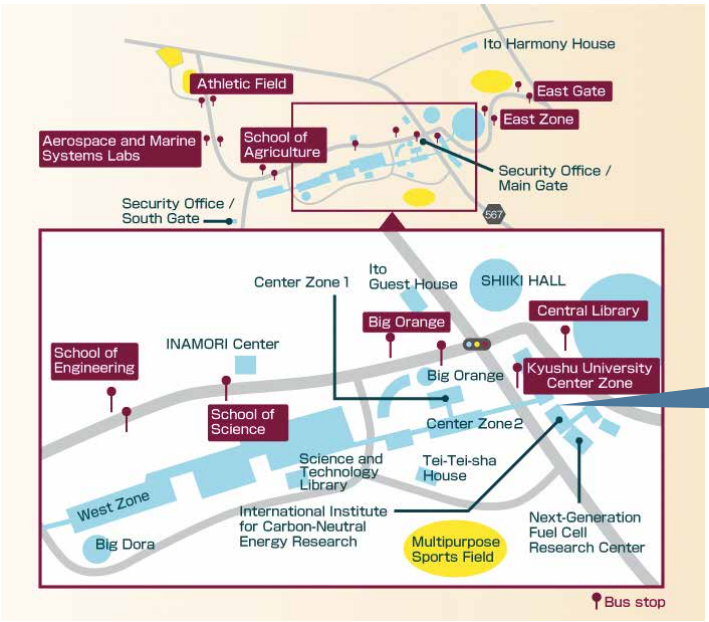
At Meinohama Station:
If your train's destination is "Meinohama," transfer to a JR Kyushu train bound for "Chikuzen-Maebaru/Karatsu/Nishi-Karatsu."

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

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

15min.

Campus Map



International Institute for Carbon-Neutral Energy Research (I²CNER), Kyushu University
Address: 744 Motooka, Nishi-ku, Fukuoka 819-0395, Japan
Phone: +81 (0)92-802-6932 Fax: +81 (0)92-802-6939
Website: i2cner.kyushu-u.ac.jp
Facebook: www.facebook.com/I2CNER.news
Twitter: twitter.com/I2CNER

I²CNER Annual Report 2022

International Institute for Carbon-Neutral Energy Research (I²CNER)
744 Motooka, Nishi-ku, Fukuoka 819-0395 JAPAN
Phone +81 (0)92-802-6932
Fax +81 (0)92-802-6939
Website : i2cner.kyushu-u.ac.jp

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.

International Institute for Carbon-Neutral Energy Research (I²CNER)
744 Motooka, Nishi-ku, Fukuoka 819-0395 JAPAN
Phone +81 (0)92-802-6932
Fax +81 (0)92-802-6939
Website : i2cner.kyushu-u.ac.jp