

Energy Outlook

International Institute for Carbon-Neutral Energy Research

March
2020

I²CNER 10th Anniversary Issue

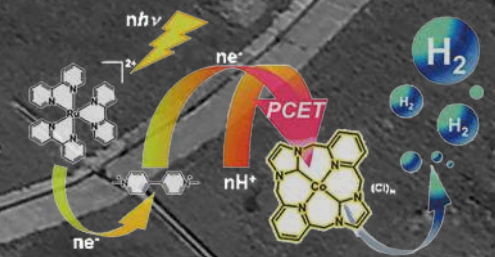
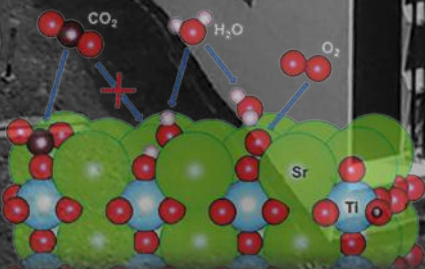
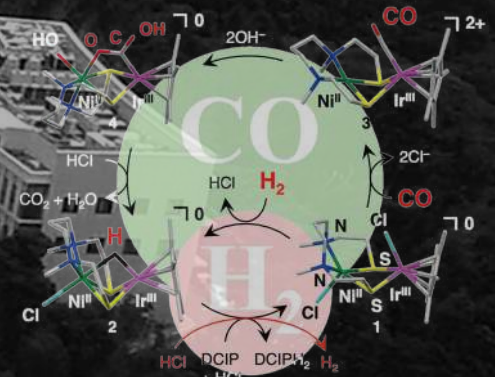
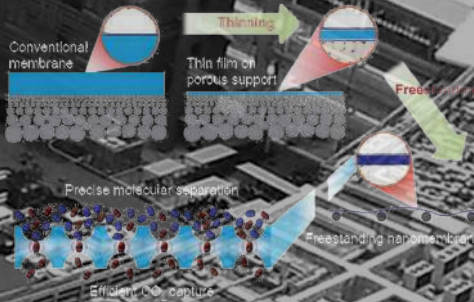
Special Interview Future Energy

George W. Crabtree

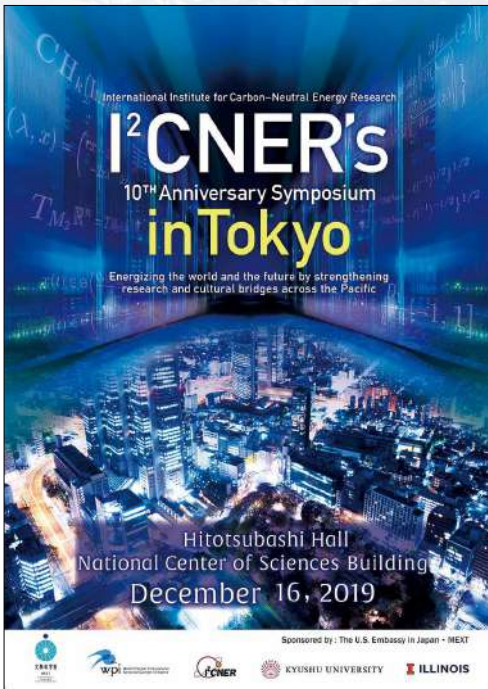
Director, Joint Center for
Energy Storage Research (JCESR)
Argonne National Laboratory

James Stubbins

Professor, University of
Illinois at Urbana – Champaign
I²CNER, Kyushu University



I²CNER's 10th Anniversary Symposium in Tokyo



In December 2019, I²CNER's 10th Anniversary Symposium in Tokyo was held at Hitotsubashi Hall in Tokyo, away from Kyushu, to present and promote I²CNER's research outcomes that has been focused and developed as part of the World Premier International Research Center Initiatives (WPI) over the last 10 years.

It was attended by academics, researchers from industries and members of the public. The theme of the symposium was *Energizing the world and the future by strengthening research and cultural bridges across the Pacific*.

The symposium started with a greeting from the President of Kyushu University, Dr. Chiharu Kubo, followed by the researchers from each division, who presented their research development, implementation and achievements.

In the following session, session II, the topic was about energy transition in the United States, Japan and the world, and the presentations reviewed about current energy trends, such as electric vehicle and hydrogen powered vehicle. Lastly in session III, the researchers from Japan and across the world presented the future energy and its development.



Chiharu Kubo
President, Kyushu University



Yoshio Yamawaki
Senior Deputy Minister, MEXT



Akira Ukawa
Program Director, WPI



Nicholas M. Hill
Deputy Chief of Mission,
The U.S. Embassy in Japan



Petros Sofronis
Director, I²CNER



Masanobu Kubota
Principal Investigator, I²CNER



Akihide Nagao
WPI Visiting Scholar, I²CNER



Miho Yamauchi
Principal Investigator, I²CNER



Tatsumi Ishihara, Nicola Perry
Lead Principal Investigator, I²CNER
University of Illinois at Urbana-Champaign, I²CNER



Shigenori Fujikawa
Lead Principal Investigator,
I²CNER



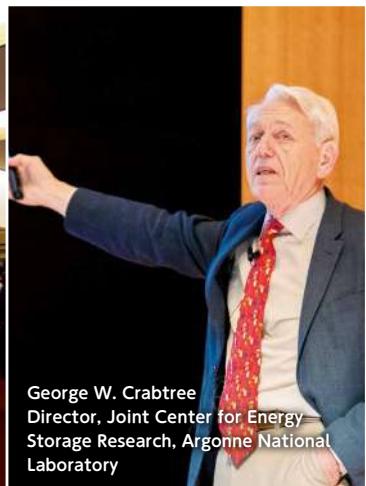
Takeshi Tsuji
Lead Principal Investigator,
I²CNER



Seiji Ogo
Lead Principal Investigator,
I²CNER



Michael Celia
Director, Princeton Environmental
Institute, Princeton University



George W. Crabtree
Director, Joint Center for Energy
Storage Research, Argonne National
Laboratory



Ross Matzkin-Bridger
Energy Attaché, DOE Director,
U.S. Embassy Tokyo



Katsuhiko Hirose
CEO, HyWealth Co



Ken Okazaki
Leader, Global Hydrogen Energy Unit,
Tokyo Institute of Technology



Toyoki Kunitake
University Professor, Institute for
Advanced Study, Kyushu University



During the panel discussion, researchers of the energy systems and the thermal science and engineering joined the discussion, and debated the several technologies to solve the issue of CO₂ emissions. The invited speaker, Dr Crabtree from the Joint Center of Energy Storage Research (JCESR), talked about the importance of communicating with the community, government agencies and private companies together to decarbonize society for energy need. Participants heard the discussion concerning the state-of-the-art technologies such as the batteries for energy storage or hydrogen energy that the scientists are researching on, and the societal issues that may be the cause of climate change, and their effects on the people of the earth.



James Stubbins
University of Illinois
at Urbana-Champaign



Kathryn Huff
University of Illinois
at Urbana-Champaign



Yukihiro Higashi
NEXT-RP, I²CNER



Andrew Chapman
I²CNER



Rashid Bashir
Dean, Grainger College of
Engineering, University of
Illinois at Urbana-Champaign

Special Interview

Future Energy

Putting our energy into the fight against climate change

As the climate change crisis worsens, scientists are searching for ways to reduce the amount of CO₂ being emitted into the atmosphere. In this effort, energy storage technology is crucial. One promising solution is hydrogen power, which researchers at I²CNER have been working to develop. Another is new types of long-discharge batteries, which can even out the intermittent power supply from renewable resources like wind and solar.

In conjunction with I²CNER's 10th anniversary symposium in Tokyo in December 2019, Dr. James Stubbins of University of Illinois at Urbana-Champaign, and also a professor at I²CNER, sat down for an interview with Dr. George Crabtree, Director of the Joint Center for Energy Storage Research (JCESR), Argonne National Laboratory, in the U.S. Dr. Crabtree shared JCESR's research on energy storage, several ways to solve decarbonization problems and what scientists can offer to society.

The latest trends in battery research

James Stubbins: Thank you for coming today. First, can you tell us about the Center's goals and accomplishments?

George Crabtree: We're trying to promote energy storage for many reasons – the coming transition in the grid, as well as in electric vehicles and in aviation. Each of these applications requires different kinds of batteries. The most popular and the best battery we have now, lithium-ion, is an excellent battery, but is not capable of doing all of those jobs. So, our mission is to invent a diversity of batteries for a diversity of uses.

Stubbins: Where does this stand in terms of where JCESR is going?

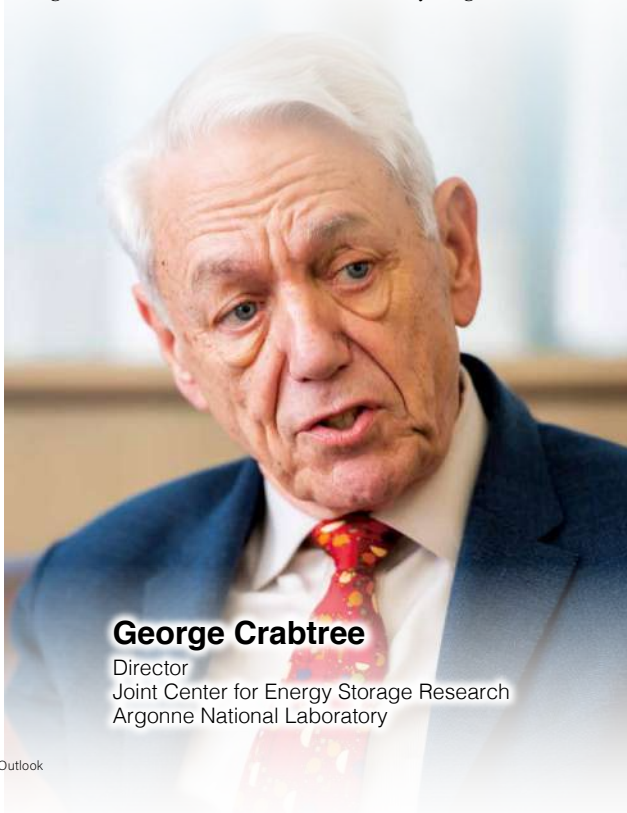
Crabtree: We have started work on specific batteries, such as lithium sulfur, as well as magnesium batteries, which are similar to lithium-ion, except that magnesium has two chargers instead of the usual one, and you get twice the

energy stored or released whenever a chemical reaction occurs.

One very interesting battery is called the aqueous air-breathing sulfur battery, which has two positive things going for it. Firstly, the material cost is the lowest of any of the proposed batteries because it uses sulfur, water as the electrolyte and oxygen from the air as the cathode. Nothing could be cheaper, more abundant or more environment-friendly. And secondly, it is capable of long-duration storage, and able to discharge for 50 or even 100 hours, which lithium-ion cannot do.

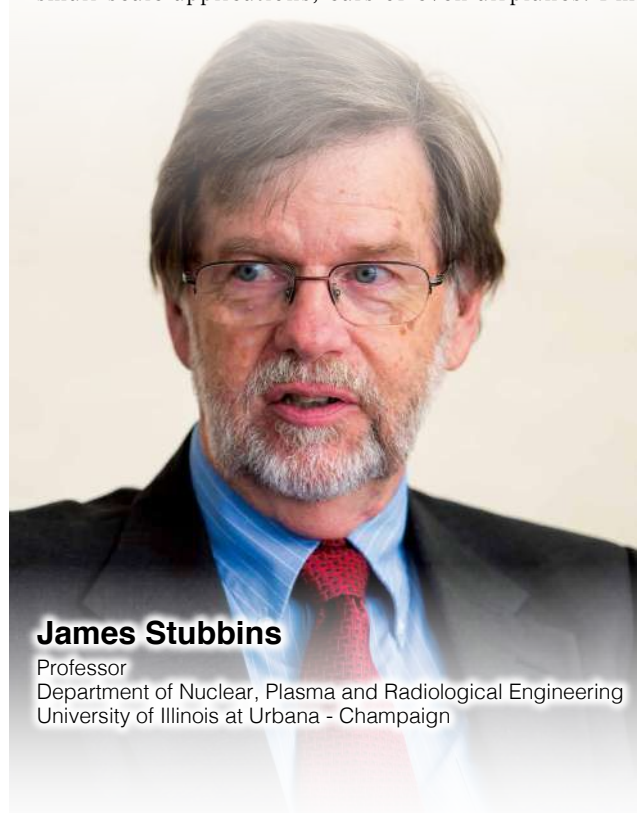
As the transition to a more advanced grid progresses, we will have more wind and solar, which do not produce energy when it is overcast or calm, so we need something to back them up, and one possibility is batteries. These are some of the things we have been doing.

Stubbins: Most people think of batteries as appropriate for small-scale applications, cars or even airplanes. I'm



George Crabtree

Director
Joint Center for Energy Storage Research
Argonne National Laboratory



James Stubbins

Professor
Department of Nuclear, Plasma and Radiological Engineering
University of Illinois at Urbana - Champaign

wondering where you see the battery technology having an impact on large-scale, centralized power production.

Crabtree: When the lithium-ion battery was born, nobody foresaw that it would be the king of personal electronics, and now it is moving on to other applications – electric vehicles (EVs) are the most notable and will become the fastest and biggest in the next five years. To store that much energy, the grid needs a thousand times more battery than an EV. Although there are plenty of lithium-ion deployments on the grid and in the pipeline, the batteries are not suitable for such large-scale use.

There is another battery called the flow battery which, instead of a solid electrode for the anode and cathode, has a tank of liquid. All the chemical reactions take place in the liquid, and redox (reduction–oxidation) active materials release electrons into the solution. Because energy is stored in the electrolyte, the storage capacity can be scaled linearly. If you want 10 times more energy, you just make the tank 10 times bigger.

This is the way the grid is going as a large-scale application. However, the challenge is that the cost is too high. JCESR, along with scientists elsewhere, is working on organically active materials, such as hydrogen, oxygen and nitrogen, which are plentiful, cheap and usually environment-friendly, instead of vanadium, which is used in the flow battery. You can design organic molecules to perform much better than either lithium or vanadium.

Stubbins: You mentioned renewables, which are an intermittent power supply. What about leveling out the demand cycles for large-scale systems like nuclear or coal, which are not good at load-following but could be operated at a regularly steady rate with the right amount of storage?

Crabtree: With renewables you need storage to take care of their intermittency. Nuclear doesn't emit any carbon, so it might be a good candidate for decarbonizing the grid, since it does not need storage the way renewables do. This is getting more attention.

Working toward a decarbonized energy future

Stubbins: What about industrial activities? High-temperature processes seem to be a major part of the carbon footprint of most industrial processes. Do you see batteries playing a role?

Crabtree: Decarbonization in the industrial sector is probably the most difficult, because high temperatures – 1,000°C to 1,400°C – are required, and CO₂ is released

during production of feedstock materials, such as with cement production. This CO₂ does not come from simply producing heat; it is an inherent part of the process. So, batteries will have to play a role. They can be applied on the electrical cycle to retrofit industrial processes when you have low-temperature heat. You can do that with resistive heating. At a bit higher temperatures you can do it with electric arc heating, and these require controlling in accordance with the process. The batteries can help to modulate that up and down as required.

The other side is how to replace and decarbonize the inherent carbon emissions from processes themselves. Carbon capture and sequestration and, even better, using CO₂ to make useful, high-value chemicals would be some of the solutions.

Stubbins: How will the carbon footprint of all these energy sources evolve in the next decade or two?

Crabtree: Some areas are easy to imagine decarbonizing. One is the electrical grid: people talk about having 85-90% driven by wind and solar, and that is only possible with batteries. Although we are far from that stage, we have the technology to do it, in principle. The second big area is electric vehicles. That will blossom enormously and will not only ease the carbon problem but could be an economic solution as well, as they achieve cost parity with gasoline engines.

However, for long-haul trucking or shipping, it's hard to imagine batteries supplying power to do that without lots of inconvenience, namely lots of recharging. That could mean hours of downtime for trucks. And aviation uses a lot of jet fuel, which also emits carbon. What do we do about that?

There is a solution, and that is hydrogen. It is produced electrolytically by splitting water, is completely carbon-free, and can be used as a combustible fuel. Hydrogen can be used for example in the industrial sector, burned to produce high temperatures or in conjunction with fuel cells to make electricity, or to fuel long-distance freight trucks and ships.

That is an opportunity to further decarbonize most of the economy. The Intergovernmental Panel on Climate Change (IPCC) says we need to do it by 2050, so there is still time to develop the technology. This is one of the most promising areas.

Transition to a future energy system

Stubbins: This is one of the things that I²CNER has been heavily concentrating on. Japan in particular has been leading a lot of the effort into fuel cell vehicles and other hydrogen applications, as well as home applications for





heating and electricity generation. How can these be made complementary rather than competing technologies?

Crabtree: Hydrogen can take that model to new heights. It could be completely connected to the electrical system. If you had excess electricity, you could split water to produce hydrogen; if you needed more electricity, you could turn hydrogen back into electricity through fuel cells, or simply by burning it in combustion turbines that use hydrogen to replace natural gas to generate electricity. This is a very flexible system and could be a huge benefit to the entire energy system.

Stubbins: This is certainly something that could happen in the U.S. and Japan, and some other places in the world, but the biggest impact on fossil fuels will be in China, India and other big economies where there is a similar kind of grid system.

Things you are working on are leading-edge technology. What will be their international impact?

Crabtree: A United Nations report in 2019 says that carbon emissions in the electricity sector in the European Union and the U.S. have gone down significantly because they both have begun to phase out coal, but not in Asia, which still relies on coal. We need to find a way to deal with the need for more energy, especially in developing countries without pumping out more carbon emissions. For example, India only has a basic grid, which needs to be upgraded with wind, solar and batteries to solve decarbonizing problems. These countries do not need to repeat the path that the EU and U.S. have followed. Instead of legacy grids and their problems, let's go straight to tomorrow's grid.

A solution for climate change issues

Stubbins: You have been very active in the scientific community. How effective is our community in helping people understand the carbon issue and climate change? Have we done enough? What else should we be doing?

Crabtree: I think a lot of this is communication. Scientists need to communicate much more effectively and simply to policy makers, to countries' decision makers and to the general public. The other thing that scientists can offer is technological solutions, such as hydrogen power, batteries, fuel cells and long-duration discharge storage.

The cost of solar energy and wind power has gone down dramatically in the last 10 years, because of the learning curve. However, the learning curve has not happened yet in

hydrogen or fuel cells. We need technologists and scientists to work with policy makers to make them aware of this possibility.

Stubbins: Do you think investment in these technologies is at the right level? Should we be doing more?

Crabtree: We should do much more. JCESR has developed a long-discharge battery that is inexpensive and environment-friendly, but many technologies of this kind are not yet commercially mature. If we want to make that happen, we need to promote them and make them attractive to the private sector.

Stubbins: Do you think we have done enough in the battery area and hydrogen area?

These large infrastructure investments don't necessarily pay off and require government support until they can have an impact.

Crabtree: We do need to be more persistent and more deliberate. We need to devise new, more specific and financial incentives for hydrogen and long-duration storage.

In the West, it's the private sector that brings technology to society.

We should be looking at developing countries. That's where the biggest impact is going to be. Developing countries can put in advanced grids, and that is something we have experience in. We can certainly innovate to make them even more resilient, such as by digitizing them and putting energy management systems in place that automatically shift power around as needed and deal with emergencies much more efficiently.

Stubbins: Since we have had such a good conversation about the impact of carbon, how about geoengineering solutions, such as carbon capture and storage, sulfur aerosols and mirrors in space?

Crabtree: People were talking about geoengineering 10 years ago, but in those days, it was looked on rather suspiciously. Not because it wouldn't work, but because there could be serious unintended consequences, and carbon might continue to be released at high levels. Countries all over the globe would have to cooperate.

The climate change issue is serious, and it's not going away. The most important thing is communicating and acting on it. As you mentioned, there are two ways to act: stop emitting carbon and mitigating its effects. There will be some effects of climate change that we have to minimize, but what do we do about them? It seems to be far in the future and it is hard to deal with. We, the citizens of the world, need to change the way we think about these things.



I²CNER 10 Years Accomplishments

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

Tatsumi Ishihara, Molecular Photoconversion Devices Division

Solid Oxide Fuel Cells are highly efficient and reliable power sources already deployed in the markets. However, for increased service life and reduced cost, decrease in operating temperature or further increase in power density are still required and for this, increase in the performance of the air electrode is critically important. Cross divisional team efforts in I²CNER tackled the very difficult problem of understanding the surface properties of multicomponent oxide air electrodes in the complex gaseous environment of ambient air. Air electrodes can typically experience degradation under operation, consequently limiting the commercialization of high temperature electrochemical devices for efficient energy conversion. The evolution of surface composition, surface reactions, and the degradation mechanism shows that the most common materials used as air electrodes are the mixed ionic electronic conducting perovskite oxides with a general formula of $A_{1-x}A'_xBO_3$, where the transition metal B cations such as Co or Fe are thought to be essential to the ORR/OER process and the large A and A' atoms, most usually La and Sr respectively, were both thought to be inert. Under operating conditions, the surface quickly reorganizes to a termination consisting entirely of A type cations and O ions, covering the catalytically active B cations. In addition, there is a rapid segregation of substituted A' cations to produce a majority A'O (e.g. SrO) rich near-surface region. Using this knowledge of the surface composition, we computationally modelled the adsorption and incorporation of molecular oxygen onto these segregated electrode surfaces. Our analysis shows that pristine segregated SrO surfaces are inactive for oxygen adsorption and the surface oxygen vacancies provide a window to access the active B site transition metals. According to these results, we have shown that in related A' free materials, e.g. La_2NiO_4 , the surfaces are again AO dominated and that, in this case, and contrary to conventional understanding, the surface La cations are the active participant in the ORR reaction.

References

- J. Druce, H. Tellez, M. Burriel, M.D. Sharp, L.J. Fawcett, S.N. Cook, D.S. McPhail, T. Ishihara, H.H. Brongersma, J.A. Kilner (2014) Surface termination and subsurface restructuring of perovskite-based solid oxide electrode materials, *Energy & Environmental Science*, 7(11), 3593-3599.
- A. Staykov, H. Tellez, T. Akbay, J. Druce, T. Ishihara, J. Kilner (2015) Oxygen Activation and Dissociation on Transition Metal Free Perovskite Surfaces, *Chemistry of Materials*, 27(24), 8273-8281.

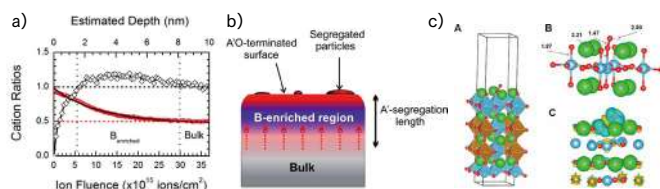


Figure a) Measured compositional profile shows segregation of cations to the surface, **b)** Schematic of measured composition profile. The segregation is closely linked to performance degradation, **c)** Atomistic modelling has unveiled a vacancy-assisted mechanism for surface oxygen exchange involved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

Mitigation of Hydrogen Embrittlement

Brian P. Somerday, Masanobu Kubota, Hydrogen Materials Compatibility Division

One of the safety considerations for hydrogen fuel technology is the phenomenon of hydrogen embrittlement, in which hydrogen permeates into the containment component and degrades its material strength. While many hydrogen embrittlement mitigation strategies focus on modifying material properties, it is also possible to manage this detrimental phenomenon by preventing hydrogen permeation into the material. Conventional approaches to preventing hydrogen permeation involve engineered coatings applied to material surfaces, however their performance can deteriorate as a result of cracking or debonding. Since the inception of I²CNER, researchers have focused on an alternative method of preventing hydrogen permeation, which involves “chemical inhibitors”. The principle of this method is that extremely small concentrations (parts-per-million) of certain species that are typically considered impurities in hydrogen gas can actually interfere with hydrogen permeation. By applying state-of-the-art modeling at the molecular level, I²CNER researchers demonstrated that species such as oxygen and carbon monoxide can restrict the splitting of hydrogen molecules into individual hydrogen atoms on the surface of materials. Since only hydrogen atoms can permeate into the material, the oxygen and carbon monoxide are effectively mitigating hydrogen embrittlement. In addition to advancing the fundamental understanding of how chemical inhibitors function, I²CNER researchers have performed comprehensive material strength experiments and developed physics-informed engineering models to enable the practical application of this method. As a result, I²CNER’s industry partners are now considering deploying this concept of chemical inhibitors to enhance the safety of hydrogen-containment components.

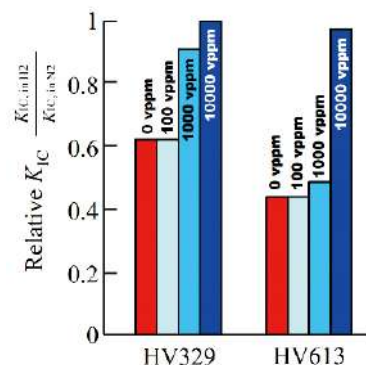


Figure Results from material strength experiments showing that small concentrations of carbon monoxide (100 to 10,000 parts-per-million) improve the fracture resistance of steel in hydrogen gas. The inhibiting effect of carbon monoxide is more pronounced for low-strength steel (HV329) compared to high-strength steel (HV613).

References

- B.P. Somerday, P. Sofronis, K.A. Nibur, C. San Marchi, R. Kirchheim (2013) Elucidating the Variables Affecting Accelerated Fatigue Crack Growth of Steels in Hydrogen Gas with Low Oxygen Concentrations, *Acta Materialia*, 61(16), 6153-6170.
- R. Komoda, M. Kubota, A. Staykov, P. Ginet, F. Barbier, J. Furtado (2019) Inhibitory Effect of Oxygen on Hydrogen-Induced Fracture of A333 Pipe Steel, *Fatigue & Fracture of Engineering Materials & Structures*, 42(6), 1387-1401.

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

Hiroshige Matsumoto, Electrochemical Energy Conversion Division

Steam electrolysis is the most energy-efficient approach of water splitting for hydrogen production that can be used as a storage medium for renewable energy. We newly developed an ideal proton conducting electrolyte BZCY54_{8/9}2 exhibiting high performance at intermediate temperatures (400-600 °C). The conductivities in this temperature region are higher than other state-of-the-art solid electrolytes. This composition was determined to be the best in the series of perovskite-type BaZr_xCe_{1-x-y}Y_yO_{3-δ} (BZCY) electrolyte materials with respect to conductivity and thermodynamic stability. The previously reported BaZr_{0.1}Ce_{0.7}Y_{0.2}O_{3-δ} (9×10^{-3} S/cm at 500 °C), as holding the benchmark conductivity, is disadvantageous due to its low stability in CO₂ and H₂O environments. We discovered that the cerium/zirconium ratio of 5/4 at the B-site of the perovskite exhibits both a higher conductivity and stability than the benchmark. We also succeeded in reducing the operating temperature of electrolysis to 500 °C without compromising the hydrogen production rate. Hydrogen is directly produced at a current density of 0.5 A/cm² at 500 °C and 600 °C with an applied voltage of 1.45 and 1.2 V. In addition, we have established a standard protocol for highly efficient intermediate temperature steam electrolysis, which has been shared with Nippon Shokubai Co., Ltd. through collaborative research initiated in 2013 toward commercialization.

References

K. Leonard, Y. Okuyama, Y. Takamura, Y.-S. Lee, K. Miyazaki, M. E. Ivanova, W. A. Meulenberg, H. Matsumoto, "Efficient intermediate-temperature steam electrolysis with Y:SrZrO₃-SrCeO₃ and Y:BaZrO₃-BaCeO₃ proton conducting perovskites" *J. Mater. Chem. A*, 6, pp19113 (2018)
 K. Leonard, Y. Okuyama, Y. Lee K. Miyazaki, H. Matsumoto, "The Influence of Dopant Levels on the Hydration Properties of SZCY and BZCY Proton Conducting Ceramics for Hydrogen Productions" *Int. J. Hydrogen Energy*, 42, pp3926 (2017)

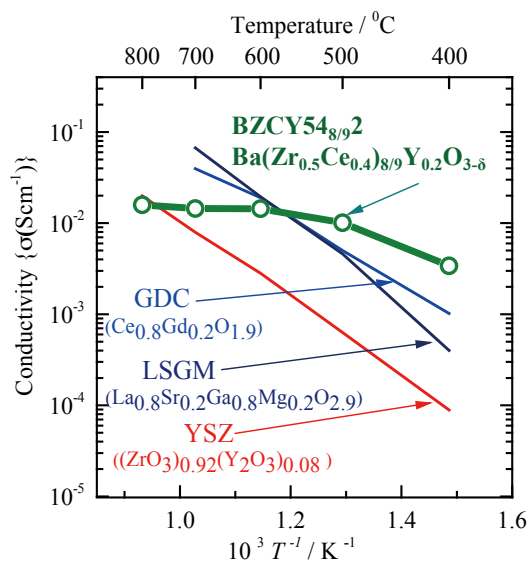


Figure Ionic conductivity of (BZCY54_{8/9}2) compared with existing oxide-ion-conducting electrolyte materials.

Novel electrocatalyst design based on polymer-wrapping of carbon supports:

Tsuyohiko Fujigaya, Electrochemical Energy Conversion Division

To realize polymer electrolyte fuel cells (PEFC) with high durability and high activity, Professors Nakashima and Fujigaya developed a novel electrocatalyst structure, in which the carbon supports are wrapped with polymer prior to the catalyst loading. One of the powerful advantages of this strategy is that various types of carbon materials can be loaded with catalyst nanoparticles, e.g. platinum, homogeneously and uniformly (Advantage 1). The team managed to realize by this approach the most durable PEFC catalyst structure worldwide and for the first time through using unoxidized carbon nanotube (CNT) as a carbon support (Advantage 2). In addition, this new structure enabled the remarkably stable dispersion of the electrocatalyst due to the homogeneous and stable coating of the electrocatalyst surface by the electrolyte based on the polymer-electrolyte interaction (Advantage 3). Due to such a homogeneous coating, a higher Pt utilization efficiency of 20-30% in comparison to that with conventional electrocatalyst approach was achieved, leading the dramatic cost reduction of PEFC (Advantage 4).

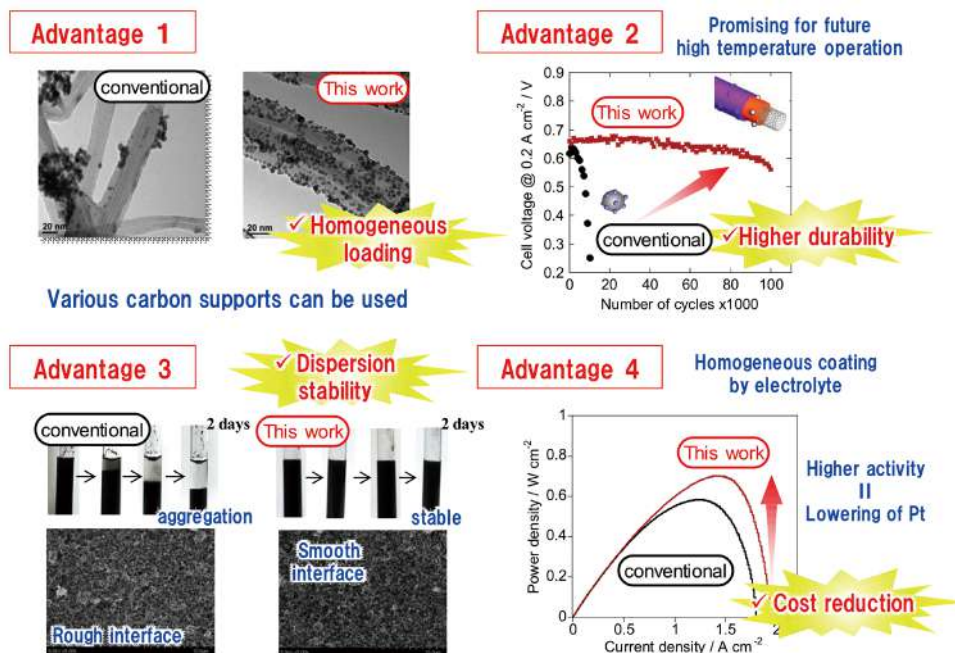


Figure New approach to highly durable electrocatalysts for polymer electrolyte fuel cells based on polymer wrapping, and associated advantages.

References

T. Fujigaya et al., *Sci. Rep.* 5, art. no. 16711 (2015).
 T. Fujigaya et al., *Electrochimica Acta*. 312, 349-357 (2019).

Surface engineering for enhanced heat transfer in power generation

Yasuyuki Takata, Nenad Miljkovic, Thermal Science and Engineering Division

Dropwise condensation of steam on metallic surfaces coated with hydrophobic films has the potential to achieve remarkable heat transfer coefficients resulting in 4% efficiency enhancement on 85% of the baseload power-generating infrastructure globally. However, the main challenge of using these coatings for the past century is their lack of long-term durability. The Miljkovic and Takata team has developed the world's first fundamental understanding of degradation of hydrophobic thin films during condensation. They quantitatively elucidated the fundamental failure mechanisms governed by the mechanics of blister formation beneath hydrophobic thin-films due to nanoscale pinholes. They used their understanding to develop, for the first time, scalable and durable hydrophobic coating approaches, in collaboration with the biggest coatings and paints companies in the world (PPG and Chemours), that can be applied to a variety of industrial energy systems.

Another grand challenge in the energy field is the inability to develop engineered surfaces that can enhance the condensation heat transfer with low surface tension working fluids (refrigerants). The Miljkovic group has overcome this challenge for the first time ever through utilizing liquid infused surfaces (LIS). They rigorously investigated lubricant-condensate pairs to develop rational design guidelines for LIS with low surface tension fluids to develop, for the first time in the world, an engineered surface coating that can achieve stable dropwise condensation of an alkane, attaining a 200% enhancement in condensation heat transfer coefficient for both fluids compared to filmwise condensation on hydrophobic surfaces.

Condensation and boiling on smooth and engineered surfaces have received much attention in the past century due to its inherently high heat transfer efficiency. Although widely used in a plethora of industries, the fundamental mechanisms governing the physics of phase change heat transfer are poorly understood. The Takata group, working with international collaborators, have challenged this by observing water confined in open hydrophilized CNTs with diameter of tens of nanometers using transmission electron microscopy. The stability of these water phases could not be explained by existing thermodynamics-based theories. The results advance the understanding of water behavior at the nanoscale and open the door for new applications of phase-change heat transfer.

References

- Ma, J., Cha, H., Kim, M.-K., Cahill, D. G., and Miljkovic, N., Condensation Induced Delamination of Nanoscale Hydrophobic Films. *Advanced Functional Materials* 2019, 29 (43), 195222.
- Sett, S., Sokalski, P., Boyina, K., Li, L., Rabbi, K. F., Auby, H., Foulkes, T., Mahvi, A., Barac, G., Bolton, L. W. and Miljkovic, N. Stable Dropwise Condensation of Ethanol and Hexane on Rationally Designed Ultrascale Nanostructured Lubricant-Infused Surfaces. *Nano Letters* 2019, 19 (8), 5287-5296.
- Tomoo, Y., Askounis, A., Ikuta, T., Takata, Y., Sefiane, K. and Takahashi, Superstable Ultrathin Water Film Confined in a Hydrophilized Carbon Nanotube. *Nano Letters* 2018, 18 (3), 1869-1874.

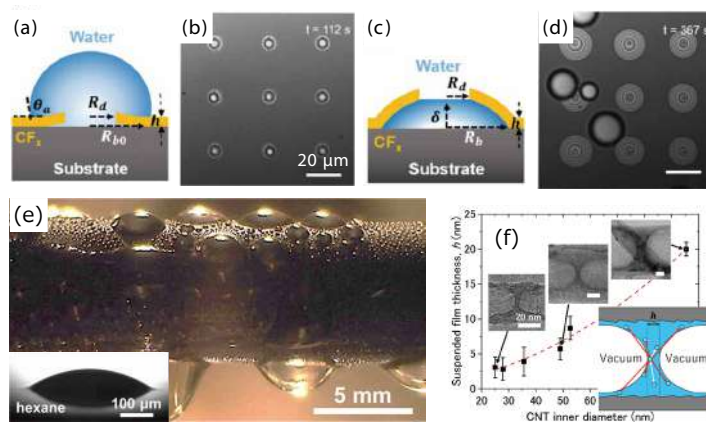


Figure (a-b) Droplet growth and (c-d) blistering on a hydrophobic thin film. (e) Dropwise condensation of a low surface tension fluid (hexane). (f) TEM images of a suspended water film in a CNT under high vacuum conditions.

Biomimetic activation of hydrogen and carbon monoxide for future fuel cell technology

Seiji Ogo, Catalytic Materials Transformations Division

Professor Ogo and his group have invented the first catalyst that can oxidize both hydrogen and carbon monoxide. Carbon monoxide is a common pollutant in commercially available hydrogen gas and it significantly reduces the catalytic activity in today's fuel cells by poisoning the platinum catalyst. However, the new I^2CNER catalyst, based on a nickel-iridium complex, was designed to act as mid-point between two naturally occurring enzymes: hydrogenase which oxidizes hydrogen and carbon monoxide dehydrogenase which oxidizes carbon monoxide. Instead of approaching the issue from the conventional standpoint of protecting the catalyst from the carbon monoxide, the Ogo group designed a catalyst that facilitates the use of carbon monoxide as a fuel (electron source) in the same manner as hydrogen. Indeed, *the group managed to showcase a proof-of-concept for a fuel cell that uses poisonous carbon monoxide as a fuel to generate energy from a 50:50 mixture of the two gases.* Significantly, since this system can operate in water, it is also environmentally friendly.

References

- S. Ogo, Y. Mori, T. Ando, T. Matsumoto T. Yatabe, K-S Yoon, H. Hayashi, M. Asano. One Model, Two Enzymes: Activation of Hydrogen and Carbon Monoxide. *Angew. Chem. Int. Ed.* 2017, 56(33), 9723-9726.

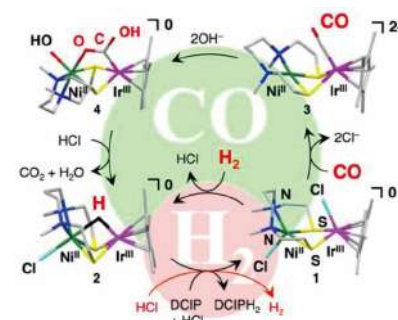
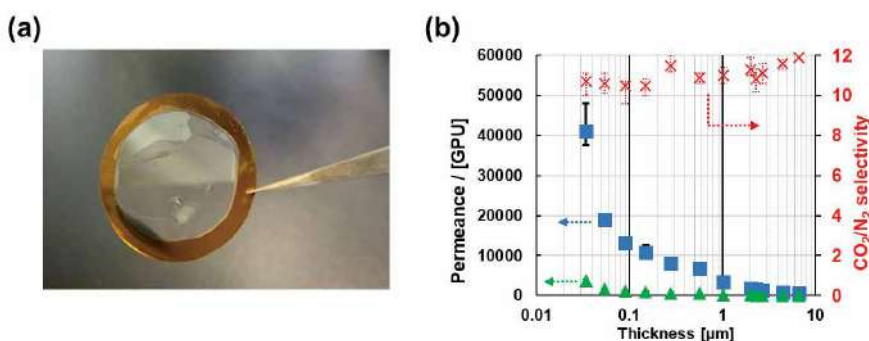


Figure The anode of a fuel cell that uses a 50:50 mixture of hydrogen and carbon monoxide gases as fuel.

Nano membrane for CO₂ separation in power generation and industrial processes

Shigenori Fujikawa, CO₂ Capture and Utilization Division

Efficient CO₂ capture technologies are indispensable and urgently needed for carbon-neutral energy systems. CO₂ capture by permselective membranes is a new promising technology that involves smaller and simpler set-ups, but the associated permeation throughput is not yet satisfactory for operation under economically-feasible conditions. Improvement of the gas permeance toward reducing the cost of CO₂ capture from flue gas in power plants is more important than enhancing selectivity. Industrial requirements for membranes for CO₂ separation over nitrogen require that the CO₂ permeance exceeds 4,000 GPU, which is the I²CNER target. Professor Fujikawa and his group developed well-defined, free-standing polydimethylsiloxane (PDMS) nanomembranes with thickness of 34 to 6700 nm for the systematic investigation of the thickness effect on the gas permeance. Generally, the gas permeability of polymeric materials is inversely proportional to the membrane thickness, since gas permeability is essentially determined by the diffusion process within the polymer matrix. However, the CO₂ permeability of thinner nanomembranes, i.e. with thickness less than 1 μm, decreases with decreasing thickness. Apparently, the overall rate of the gas permeation is determined by the surface adsorption process and the gas selectivity may be mainly controlled by the surface adsorption process. Professor Fujikawa's group succeeded in manufacturing free-standing membranes with thickness of 34nm and associated CO₂ permeance of more than 40,000 GPU, which is the world's highest, better than the current benchmark of 2,000 GPU held by MTR Inc., USA, and with a moderate 10 to 11 CO₂/N₂ selectivity. Additionally, when tested under atmospheric pressure conditions, the membranes captured CO₂ from CO₂/N₂ mixture with a CO₂ concentration of 1000 ppm. This finding expands the relevance of our research goals beyond capturing CO₂ from fire-powered plants to the entirely new area of CO₂ capture directly from the atmosphere.



References

S. Fujikawa, M. Ariyoshi, R. Selyanchyn, T. Kunitake (2019) Ultra-fast, selective CO₂ permeation by free-standing siloxane nanomembranes, *Chemistry Letters*, 48(11), 1351-1354.

Figure CO₂ separation nanomembrane and its gas separation performance: (a) a free-standing and 150-nm thick PDMS nanomembrane (orange O-ring is a frame); (b) gas permeance of CO₂ (blue squares), N₂ (green triangles), and CO₂/N₂ selectivity (red crosses) as a function of thickness.

Co-electrolysis of CO₂ and waste glycerol to enhance economic viability of CO₂ valorization

Paul Kenis, CO₂ Capture and Utilization Division

Professor Kenis' research focuses on ways to reduce the energy required to convert carbon dioxide to value-added chemicals. Surplus industrial carbon dioxide creates an opportunity to convert waste into a valuable commodity. Excess CO₂ can be a feedstock for chemicals typically derived from fossil fuels, but the process is energy-intensive and expensive. The I²CNER team has assessed the economic feasibility of a new co-electrolysis approach that uses the oxidation of a cheap biofuel byproduct, glycerol, to reduce the energy consumption of the overall waste-to-value process by 50 percent. Conversion of CO₂ to chemicals like ethylene for plastics is possible through a process called electrochemical reduction. Typically, a stream of CO₂ gas and a fluid electrolyte move through an electrolysis cell that breaks the CO₂ down into molecules like ethylene on the cathode, but it also produces oxygen from water on the anode. However, about 90 percent of the energy required in conventional CO₂ reduction is used up by the oxygen-producing anode side of an electrolysis cell. But since there is no big market for the excess oxygen, 90 percent of the energy is essentially wasted.

Professor Kenis' new approach uses the anodic oxidation of glycerol – a byproduct of sugar cane biofuel production – as an alternative to the energy-intensive oxygen-producing step. Life-cycle analysis reveals that this co-electrolysis approach has the potential to push the full CO₂ conversion process to be close to carbon neutral, whereas the current thermo-chemical processes used to convert fossil fuels into the same products are heavily carbon positive. The analysis includes best- and worst-case CO₂ emissions and energy consumption scenarios and concludes that the prospects of CO₂ reduction, in terms of CO₂ emissions and economics, can drastically improve by replacing conventional anode reactions (oxygen evolution) with oxidation of organic waste materials. Looking beyond oxygen evolution at the anode seems like a win-win situation, as this not only reduces the processes' energy consumption by 40-50%, but it also has the potential to produce a second valuable product stream.



Figure Flow electrolyzer for the co-electrolysis of CO₂ to CO or ethylene on the cathode, and glycerol to lactate and/or formate on the anode

References

S. Verma, S. Lu, P.J.A. Kenis (2019) Co-electrolysis of CO₂ and glycerol as a pathway to carbon chemicals with improved technoeconomics due to low electricity consumption, *Nature Energy*. (DOI: 10.1038/s41560-019-0374-6)

Continuous and accurate monitoring system for injected CO₂:

Takeshi Tsuji, CO₂ Storage Division

In carbon capture and storage (CCS), the monitoring of injected CO₂ is crucial for i) predicting the risk of CO₂ leakage from reservoirs, ii) increasing the efficiency of CO₂ injection and reducing the cost, and iii) reducing the risk of injection-induced seismicity. To date time-lapse seismic surveys have been used to monitor injected CO₂ distribution. However, the interval of the time-lapse monitoring surveys is long due to their high cost and it is difficult to continuously monitor the injected CO₂. In addition, continuous monitoring of the dynamic CO₂ behavior is crucial for detecting accidental incidents, such as CO₂ leakage. To address these issues, we first developed a continuous monitoring approach to estimate spatio-temporal variation of seismic velocity using ambient noise (or microtremor). Since this method constructs virtual seismic data from noise, we can extract subsurface information using only passive seismometer data. However, the disadvantage of this monitoring system that relies on ambient noise is that the temporal variation of ambient noise would decrease the monitoring accuracy. To overcome this problem, we have developed a new novel monitoring method for injected CO₂ using a continuous and controlled seismic source. This new monitoring system generating controlled seismic signal is cost-effective, with high temporal resolution and accuracy. By using this system to the ongoing CCS project in Canada, we successfully identified spatial and temporal variation in the shallow subsurface. To further reduce the cost of seismometers, we deployed fiber-optic type seismometers (i.e., distributed acoustic sensor (DAS)) in a geothermal field in the Kyushu Island. By recording the signal of continuous seismic source system by DAS, we successfully monitored geothermal reservoirs with high accuracy. High spatial resolution of our approach makes it possible to identify leaked CO₂. Also, the system's low cost and high temporal resolution are particularly attractive for long-term monitoring of sequestered CO₂.

References

- T. Tsuji, T. Ikeda, T.A. Johansen, B.O. Ruud (2016) Using seismic noise derived from fluid injection well for continuous reservoir monitoring, *Interpretation*, 4(4), SQ1-SQ11.
(DOI: 10.1190/INT-2016-0019.1)
- H. Nimiya, T. Ikeda, T. Tsuji (2017) Spatial and temporal seismic velocity changes on Kyushu Island during the 2016 Kumamoto earthquake, *Science Advances*, 3(11), e1700813.
- T. Ikeda, T. Tsuji, M. Nakatsukasa, H. Ban, A. Kato, K. Worth, D. White, B. Roberts (2018) Imaging and monitoring of the shallow subsurface using spatially windowed surface-wave analysis with a single permanent seismic source, *Geophysics*, 83(6), EN23-EN38.

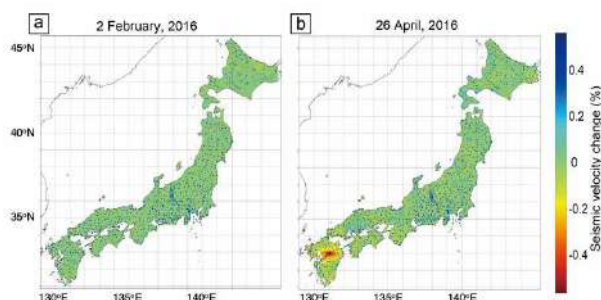


Figure Results from our continuous monitoring system of seismic velocity for all Japanese Islands on (a) 2 February 2016, (b) 26 April 2016. Warm colors indicate regions where the seismic velocity was decreased (materials weakening). Seismic velocity in Kyushu Island was decreased in panel (b) due to subsurface stress changes caused by the Kumamoto earthquakes (Mw7) on April 16.

Hydrogen station deployment for fuel cell vehicles:

Kenshi Itaoka, Andrew Chapman, Energy Analysis Division

Deployment of FCV (fuel cell vehicles) as well as BEV (battery electric vehicles) is essential for the energy transition in the transportation sector. FCV deployment relies on the efficient location of hydrogen refueling stations. The objective of this study was to develop an effective model for domestic hydrogen station deployment and identify prospective areas for hydrogen station locations to meet the future refueling demands of FCVs. A deployment model employing location allocation theory using GIS (geographic information systems) was used to consider user convenience and FCV penetration phases.

Based on our model results, we concluded that the most effective approach was to locate the hydrogen stations in a way that minimizes average distance between potential customers and the nearest hydrogen station. The study also identified gaps between existing and planned stations, and the suggested station sites. This gap analysis identified certain cities, particularly prefectural capital cities, in need of coverage. The results were directly reported to the Ministry of Economy, Trade and Industry and shared with hydrogen station stakeholders to support hydrogen deployment policy and planning in Japan. Also, the model results of follow-up analyses are currently used by JHyM (the Japan Hydrogen Station Network Joint Company), created by major car companies and energy companies to develop future hydrogen refueling infrastructure. In addition to this study, The energy analysis team of I²CNER is also pursuing a global hydrogen penetration model, which has identified a strong future potential for FCV deployment, up to 50% of the future passenger vehicle fleet by 2050[2]. Of particular interest is the consistently strong end use case for FCVs under a number of 'Hydrogen Society' scenarios, extolling the value of this hydrogen station deployment research.

References

- K. Itaoka, S. Kimura, K. Hirose (2019) Methodology Development to Locate Hydrogen Stations for the Initial Deployment Stage, *E3S Web of Conferences*, 83(01014), 18.
(DOI: 10.1051/e3sconf/20198301014)
- A. Chapman, K. Itaoka, H. Farabi-Asl, Y. Fujii, M. Nakahara (2020) Societal Penetration of Hydrogen into the Future Energy System: Impacts of Policy, Technology and Carbon Targets. *International Journal of Hydrogen Energy*.

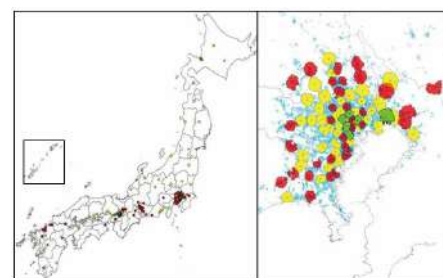


Figure Red dots and red areas show existing/planned station sites and their 10 minute driving radii. The additional stations that will be created, bringing the total of initial stations to 100, are indicated by green dots (10 minute driving radii indicated by green areas). The additional stations (initial 100 to 200 stations) and their 10 minute driving radii are indicated by yellow dots and yellow areas. The initial 5000 customers are represented by blue areas. The additional 15000 customers, which will bring the total to 20000 early customers, are represented by light blue areas. Lastly, the additional 30000 customers, which will bring the total to 50000 early customers, are represented by pale blue areas.