FY 2010 WPI Project Progress Report
World Premier International Research Center Initiative (WPI)

Host Institution	Kyushu University	Host Institution Head	Setsuo Arikawa
Research Center	International Institute for Carbon-Neutral Energy Research	Center Director	Petros Sofronis

* Prepare this report based on the current (31 March 2011) situation of the WPI Center.
* Amounts of money are to be noted in yen in this report. When necessary to convert other currencies into yen, please give the exchange rate used.

Summary of center project progress

The Institute was launched on December 1, 2010 and the Kick-off Symposium was held at Kyushu on February 1, 2011. The Symposium brought together researchers from Kyushu University, the University of Illinois, other participating US institutions (Sandia National Laboratory, University of California, Berkeley, MIT), and a number of collaborating institutions from Europe (e.g., University of Gottingen, Germany; the Swiss Federal Institute of Technology, Switzerland; and Imperial College; London). The objective was to initiate communication among I^2CNER researchers and to foster a collaborative environment. Already the list of foreign WPI Principal Investigators includes 11 internationally-recognized authorities in their fields of expertise. The research thematic areas (divisions) and the individual research groups of I^2CNER have been formed and plans for cross division communication and exchange have been developed. The Institute is administered through the Science Steering Committee and its progress is monitored by the External Advisory Committee (EAC) whose members include distinguished scientist from Europe, Japan, and the United States. On March 23, a booklet containing detailed outlines of research projects was sent to the EAC for review and input. The rules for the regular recruiting process by a Faculty Recruiting Committee (FRC) have been developed and implemented as well as the rules for several other functions of the Institute such as the recruitment of talented young graduate students, an I^2CNER seminar series with invited speakers, and a seminar series for I^2CNER's young faculty. Several assistant professors have been hired and a new faculty search is underway. Also, a "Faculty Excellence Program" has been instituted to recruit leaders who will bring transformational change across I^2CNER. The Director of the Institute worked to finalize and complete the agreement between Kyushu and the University of Illinois to establish the satellite institute. The agreement was entered into on December 1, 2010. Establishing the satellite is underway, with a down-select of proposals that complement and extend the activities of the center completed. The selected efforts have been invited to submit a full proposal for possible inclusion in the center.

In summary, progress has been made on building the Institute, on attracting faculty, on the research front in all thematic research areas, and marketing/advertising the Institute across the U.S. and the world. It can be reported that the I^2CNER concept is being well received and the transformational change to the Japanese University culture is on track. The Institute's future near-term activities include summer schools and outreach programs, organizing international conferences and workshops, as well as coordinating between Kyushu and the Satellite Institution for proposal submissions to obtain funds through JSPS and NSF for faculty, post-doctoral, graduate, and undergraduate student exchanges between Japan and the U.S. The Director is scheduled to visit the Max Planck Institute in Germany and the Royal Institute of Technology of Sweden later this year to explore opportunities for establishing similar exchange programs within Europe.

Lastly, in light of the recent earthquake-caused calamities, I^2CNER plans to contribute to the national debate for the creation of a new energy policy of Japan though social outreach fora and by publicizing research results on i) carbon capture and storage given that fossil fuels are now expected to play a significant role in the country's energy portfolio as part of a short-term solution; ii) fundamental science that will enable the technology for a hydrogen-powered society; iii) the importance of hydrogen as a long term solution relative to other renewable energy sources.

1. Summary of center project

<Initial plan>
<Center Project>

- For green energy innovations, alternate fuels to petroleum-based energy sources are required to provide reliable and sustainable energy sources for future generations. The alternate energy carriers must be produced and consumed without leaving an imprint on the environment. One potential energy carrier is hydrogen gas. However, the transition to a hydrogen-based economy faces many challenges in terms of production, storage, delivery to end-user stations, and energy generation. A grand challenge amongst the many in this transition is the management of the CO_2 accompanying hydrogen production from promising technologies such as natural gas or carbon reformation. In order to realize a complete carbon-neutral energy fueled society based on a hydrogen economy, major advances in technologies of CO_2 capture and sequestration (CCS) are required. An international effort centered at Kyushu University will be mounted to overcome the challenges. The research effort will be focused on the fundamental science underlying development of technologies for CO_2 capture and sequestration and the realization of the hydrogen economy. In particular the Kyushu effort will focus on the problems associated with carbon-free hydrogen production, development of hydrogen storage materials, hydrogen embrittlement resistant materials, fuel cells, material transformation; CO_2 separation and concentration; and geological storage and ocean sequestration of CO_2. Understanding the fundamentals of these problems will enable the development of solutions against global warming through a carbon-neutral hydrogen economy.

- There is no more opportune time for such an international research project to be undertaken if one considers the future international energy landscape. The FutureGen project in the US for electricity and hydrogen production through efficient coal burning and CCS and the ongoing industrial efforts on CCS and photoelectrochemical hydrogen production funded by the US Department of Energy are key science and technology strategies for energy independence and sustainability. The fundamental science objectives of the Kyushu Research Institute will address similar technological challenges and will serve as a platform for coordinated research between Japanese and US institutions. We

<Results/progress/alternations from initial plan>
<Center Project>

- The International Institute for Carbon-Neutral Energy Research, (I^2CNER) officially began on December 1, 2010.

- Upon the official launching of the Institute, the director in consultation with the Vice-director contacted senior authorities in the fields of renewable energy and carbon capture and storage as well as members of the US Department of Energy to establish the External Advisory Committee (EAC). To date the constitution of the EAC is as follows:

  - Members of the External Advisory Committee
    - Professor Ronald J. Adrian, Arizona State University, USA
    - Dr. Robert J. Finley, Illinois State Geological Survey, USA
    - Dr. Deborah Myers, Argonne National Laboratory, USA
    - Professor Tetsuo Shoji, Tohoku University, Japan
    - Dr. George Thomas, Sandia National Laboratory, Retired, (Sandia National Laboratories and EERE office of US DOE, USA
    - Professor Reiner Kirchheim, University of Gottingen, Germany

- Dr. Robert Finley, an expert in the area of CO_2 geological storage at the University of Illinois and director of the Midwest Geological Sequestration Consortium at Illinois, has agreed to help the Institute in developing research plans in the area of CO_2 Storage as it pertains to the geological and sub-sea bed geological formations of Japan.

- At the Director's request, each I^2CNER Principal Investigator (PI) compiled a white paper describing her/his research plans which included her/his grand challenge, technical barriers, goals, technical approach, near-term objectives, and long-term impact. After reviewing the papers, the Director then met with each PI to discuss her/his plan in more detail. The papers were then combined into a book and were sent to the External Advisory Committee (EAC) for review. Plans will be finalized based upon the EAC's comments.

- The Science Steering Committee (SSC) has been set in place upon the

aspire to establish a "Carbon-Neutral Energy Research Institute" as a center of excellence in which top-level researchers collaborate, cooperate, share knowledge and exchange ideas, and discuss and debate the science issues and their impact on society.

- From a fundamental science viewpoint, a pervading theme in all areas of the proposed research is the lack of understanding of a range of phenomena occurring at the interface between materials/rocks/ocean turbulence-eddies and gasses such as hydrogen, oxygen, and CO_2. By way of example we do not understand i) the mechanisms by which hydrogen is adsorbed in materials making it difficult to design alloys resistant to hydrogen degradation of mechanical properties or how to design a light-weight on board storage medium with the desired hydrogenation/de-hydrogenation properties; ii) the properties and behavior of hydrogen and CO_2 under extreme pressures, iii) the triple-phase rocks/water/CO_2 interactions and the

  stability of geological traps; iv) the interaction of supercritical CO_2 with ocean turbulence in order to predict how ocean weather affects the efficiency of CO_2 sequestration at the bottom of the ocean. From this abbreviated list, it can readily be surmised that the phenomena to be addressed involve disparate length and time scales ranging from nanometers to thousands of kilometers and from nanoseconds to centuries. The proposed research will address the issues as they pertain to all time and length scales, from atomic to the global scale, i.e., from the atom and molecule, to meso/macro-scale crystalline materials, to devices, up to geological formations and oceanic systems. The phenomena, although occurring at different media and disparate time and length scales, often evolve on the basis of the same processes (e.g., species adsorption, absorption, dissolution, diffusion, reaction, conduction) and are characterized by similar scientific principles. Thus, the Kyushu approach will cross-cut disciplinary boundaries through a judicious integration of information from atomistic/microscopic/macroscopic time and length scales for phenomena occurring at the interface of chemistry, physics, materials science, mechanics, geo-science, oceanic science, and biomimetics.

- The administration and management of our project will involve a constant peer evaluation and review of the research activities and outcomes in terms of efficiency and feasibility of each individual

launching of the Institute. Members of this committee are the director, vice-director, associate director, and the lead PIs of the thematic research areas (divisions).

- Also, upon the launching of the Institute, the director, in consultation with the SSC, instituted the Faculty Recruiting Committee (FRC). The committee is chaired by the Vice-director and its members include members of the SSC and any other faculty that can provide input for cases of targeted hiring.

- I^2CNER received 136 applicants from an open international recruitment call that was initiated after the Institute was awarded and before its launching. The successful candidates (1 associate professor, 7 assistant professors, and 1 postdoctoral research associate) from both Japan and overseas, will join the Institute on or after April 1, 2011. Our recruitment policy at the junior level is to hire researchers who hold promise for the future and only world-class researchers at the senior level. A second recruitment campaign began at the end of March 2011.

- To attract senior faculty who are internationally recognized authorities and capable of bringing about transformation change in I^2CNER across divisions, the director instituted the "Faculty Excellence Program."

- The "I^2CNER Seminar Series" was launched in March 2011. This regular seminar series features distinguished internationally-recognized researchers and actively engages I^2CNER's researchers in an open exchange of views in a varied range of interdisciplinary research areas while enhancing I^2CNER's global visibility.

- I^2CNER is also planning for an "Institute Interest Seminar Series" in April 2011. This series will serve as a forum with the express purpose of promoting cross-disciplinary exchange and furthering our young researchers' abilities to present and defend their viewpoints and scientific methods before an audience of experts.

- I^2CNER is also planning to institute a program of recruiting and supporting excellent graduate students to carry out PhD thesis work by joining the various divisions of the Institute as graduate research assistants.

research project area as well their progress toward attaining the overall project objectives, that is, the realization of a hydrogen economy and the elimination of the CO_2 footprint. We will adopt a rigorous approach as we assess our research progress that will be predicated on how our science advances technology development and how we impact the removal of roadblocks to a carbon-neutral energy society, such as the lack of a mechanism-based understanding of fatigue of materials or the stability issues associated with supercritical CO_2 at the bottom of the oceans. Lastly, the Kyushu project will pay serious attention to the dissemination of the research results and its scientific culture in the society over several fronts. Tapping on the Illinois academic expertise we will institute societal educational outreach programs. We will leverage the expertise of the HYDROGENIUS Institute at Kyushu in organizing international development to engage the scientific community of the industry and national laboratories through specialized workshops. We plan to inform the society at large through the development of web-based learning tools for all age levels, museum exhibits, as well as other strategies. This effort will pave the way for enriching public understanding of scientific achievements and at the same time teach our scientists the needed communication skills • In summary, the Kyushu effort will carry out research on fundamental science issues underscoring the removal of roadblocks toward a hydrogen economy with zero carbon emissions through carbon capture and sequestration.	
<Research Organization> • The research effort will be organized around high profile research teams of faculty of the University of Kyushu. The Institute will also rely on top level domestic and internationally recognized researchers in the fields of chemistry, physics, materials science, mechanics, geo-science, oceanic science and biomimetics. An important component of the organization will be the Satellite Institute at the University of Illinois which will promulgate and administer the research activities in the US.	<Research Organization> • Effective January 1, 2011, Professor Kyuro Sasaki, resigned his post as Lead PI of I^2CNER's CO_2 Geological Storage division for personal reasons. Both Dr. Larter and Prof. Babadagli, who were collaborative researchers, also resigned. • Following the resignations, the SSC decided to consolidate the CO_2 Geological Storage and CO_2 Ocean Sequestration divisions into one comprehensive division titled CO_2 Capture and Storage (CCS). To restructure the division, the director is receiving input and advice from Dr. Robert Finley, EAC member and an expert in this area. In general, the plan is to i) streamline the division's research activities in a way that the geology of Japan and time scales involved will feed
<Project Management> • One of the main goals of the Institute is the restructuring of research	

management at the Kyushu University. This new approach to research administration will rely heavily on the management style, academic experience, and scientific achievements of the Institute director whose duties will include the research team formation, the recruitment of the international research participants, the establishment of international collaborations and interactions with top research Institutions, the administration of the peer evaluation process of the Institute's research output, potential team reorganization and redirection of efforts in response to the feedback from the annual review of the Institute, review of the research personnel, and the observance of the research expenditures.

- The Institute is established as an organization directly under the president of the Kyushu University. The structure of the organization is such that the Institute director has the authority to make decisions regarding the planning and operation of the research activities, the formation and composition of the research clusters, and the budget implementation related to the management of the Institute. On all these matters the director is assisted by the Internal Advisory Committee that is headed by the director and its members will be program area leaders of the Institute although the Director may invite additional members as deemed appropriate.

- A vital component of the Institute is the External Advisory Committee composed of national and international leaders in the field. This Committee will be convened annually or, if deemed necessary by the Director, more frequently at Kyushu University. The Committee will review all aspects of the Institute, including the leadership and management, the research progress being made in each activity, and the plans for any initiatives. The Committee will provide the Director with a written report on their findings and recommendations. The final decision regarding Institute activities and directions will be the responsibility of the Director.

- The Director is assisted by two Science Associate Directors (one in Japan and one in the satellite Institute at the University of Illinois) for the management of the Institute' research activities. The Office of the Director is supported by the Administrative Director, head of the office of the Institute's Management Department whose purpose is to provide administrative support to the research personnel of the Institute. The

back to define basic research requirements, and ii) reinforce the area of fundamental science underlying CCS as considered to be pursued by industry in an industrial scale at various sites of Japan.

- Upon the recommendation of the SSC, the director appointed the following foreign researchers, who are internationally recognized for their research contributions, to the position of "WPI Principal Investigator" in I^2CNER:
    - Prof. John A. Kilner, Imperial College London (UK)
    - Dr. Brian P. Somerday, Sandia National Laboratories (USA)
    - Prof. Robert O. Ritchie, University of California, Berkeley (USA)
    - Prof. Ludwig J. Gauckler, Swiss Federal Institute of Technology (SUI)
    - Prof. Harry L. Tuller, Massachusetts Institute of Technology (USA)
    - Dr. Xing Zhang, Tsinghua University (China)
    - Prof. Louis Schlapbach, Federal Institute of Technology Zurich(ETH) (SUI)
    - Dr. Ping Chen, Dalian Institute of Chemical Physics (China)
    - Prof. Chen-Tung Arthur Chen, National Sun Yat-sen University (Taiwan)

- These investigators are expected to vigorously pursue collaborative research with I^2CNER principal investigators, offer lectures and seminar presentations, and engage with student or post-doctoral research associate supervision as well as with teaching short courses. By participation in I^2CNER, these foreign investigators will contribute to the excellence of our research program.

- Other Principal Investigator personnel changes are:
    - March 31, 2011: Professor Okada of Tohoku University resigned due to his assignment of a principal of a higher professional school.

    - Professor Yukitaka Murakami, former Trustee, Vice President of Kyushu University, and chief center project officer, was appointed as I^2CNER Vice Director and PI.

official language of the Institute's Management Department is English. To ensure efficiency and expediency of operations in the Management Department, we will opt for post-doctoral researcher employees so that carrying out of the operations is done by personnel that understand the research activities of the Institute	o April 1, 2011: Professor Reiner Kirchheim and Professor Takaki were appointed as PIs in the Hydrogen Structural Materials Division.
<Collaboration with Other Institutions> • To carry out its mission, the Institute will seek to establish collaborations with internationally recognized research centers, universities, and national and international laboratories. These collaborations will involve and promote research interactions and researcher exchanges and visits between the institutions. The framework will be in the form of a satellite Institute in the case of the University of Illinois and collaborating institutions for the all other cases. o Satellite Institute, University of Illinois at Urbana-Champaign, USA ▪ The Director of the WPI Institute, Professor Petros Sofronis, is a faculty member at the University of Illinois at Urbana-Champaign, Illinois, and is an internationally recognized expert on the effects of hydrogen on the mechanical properties of materials. Other research activities at Illinois mirror parts of the proposed program. Therefore a satellite office will be established at Illinois to facilitate cooperative research activities as well as personnel exchanges. In addition to conducting Institute related research, the satellite office will serve as the base for identifying and engaging key research programs and faculty at Universities and Institutions nationally and internationally. As Director of the WPI Institute, Professor Sofronis will serve as the Director of the satellite institute. In this latter capacity he will report directly to the Dean of the College of Engineering at the University of Illinois. Appropriate agreements between Kyushu University and the University of Illinois, other than an exchange of students which is already in place, will be negotiated if the Institute is funded. Both parties have expressed interest and support for establishing this satellite institute at the University of Illinois.	<Collaboration with Other Institutions> • The agreement between Kyushu University and the University of Illinois was entered into on December 1, 2010 and the Satellite Institute at the University of Illinois Urbana-Champaign has commenced activities A request was sent out on March 15, 2011 to invite Illinois faculty to submit letters of intent for proposal submission. These letters were reviewed and a request for proposal submissions were sent to the faculty members whose research proposals, as described in the letters of intent, are complementary to the research carried out at Kyushu. • Cooperative research activities and personnel exchanges between Kyushu and Illinois universities have also begun. By way of example, graduate research assistants are visiting I^2CNER at Kyushu this summer to carry out experiments jointly with Japanese researchers. • Negotiations between I^2CNER and the Sandia National Laboratories are ongoing for Dr. Somerday to join as lead PI of the structural-materials/hydrogen-compatibility division. In addition, plans are developed for a broad I^2CNER engagement in the Livermore Valley Open Campus project. This project launched jointly between the Sandia National Laboratories and the Lawrence Livermore National Laboratory aims at fostering an environment of international collaboration and exchange amongst US and foreign researchers. • The director and the vice director are making contacts in the US and Japan to promote a network of interaction and exchange on research and energy policy between government, industry, and national laboratories. The objective is to ensure that I^2CNER's mission and research agenda remains informed on the latest technology and societal developments. By way of example, I^2CNER researchers already collaborate with researchers from the ExxonMobil Research and Engineering Company, I^2CNER will work in concert with Mohawk

- Collaborating Institutions
  - We envision engaging in collaborative research with distinguished scientists from internationally recognized institutions. This includes site visits to facilitate research capabilities.

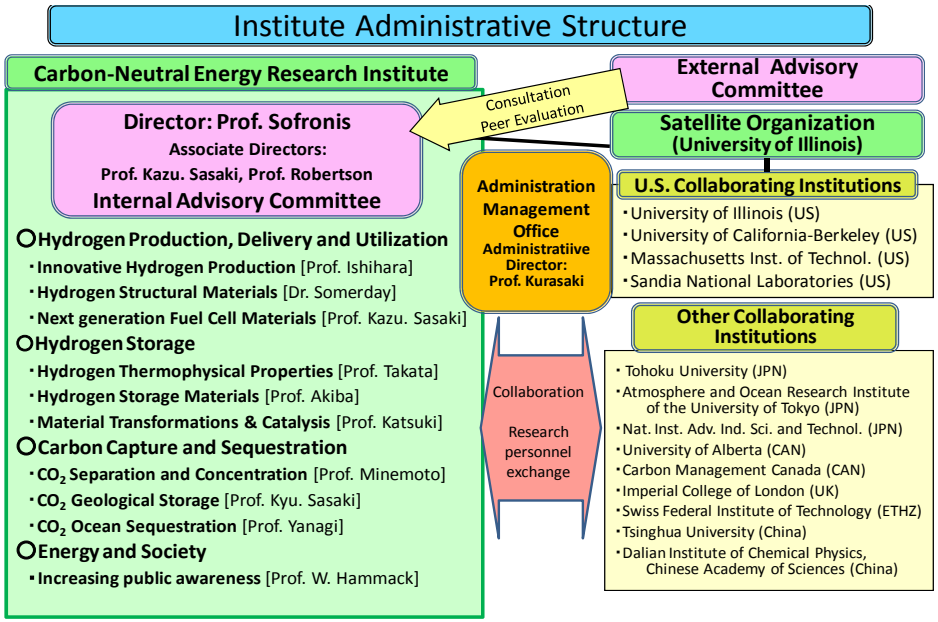

Fig. Administrative structure of the Institute

Innovative Technology to coordinate material selection for future hydrogen compressor concepts, and Toyota Motor Corporation on fuel cells.

2. Research fields

<Initial plan>

Research Field

- Fundamental science for an economy based on carbon-neutral energy
- Multi/interdisciplinary science integrating Chemistry, Physics, Materials Science, Mechanics. Geoscience, Oceanic Science, and Biomimetics

Significance of the Proposed Project

- There is a vital need to develop sustainable sources of energy without CO_2 emissions, and to establish safe and reliable carbon capture and storage (CCS) systems for the realization of a carbon-neutral society.

- From the viewpoint of limited fossil fuel resources energy security, capital outflow, and the economic instability due to increasing oil prices, there is an urgent need for the establishment of a flexible energy system which integrates a diverse range of energy sources, with no dependence on fossil fuels.

- In particular, due to the unique properties of hydrogen energy to be described below, there are increasing expectations for hydrogen fuel to play a very important role, not only as a leading and ultimate choice for an alternative energy source for the establishment of sustainable development and a carbon neutral energy society, but also as a promising energy carrier that can be produced from a diverse range of energy sources. The benefits of a hydrogen-fueled economy used in conjunction with CCS systems are summarized as follows:
  - Hydrogen does not produce any CO_2 when it is utilized (burnt).
  - Hydrogen fuel cells are significantly more efficient when compared to the ordinary/existing energy generation systems based on the combustion of fossil fuels—the chemical energy stored in fossil fuels has to be converted to heat to obtain the useful electrical energy, a process which produce waste heat energy, i.e., not all of the energy stored in fossil fuels can be utilized.
  - Hydrogen can be produced by using a diverse range of

<Results/progress/alternations from initial plan>

- The social situation caused by the Tohoku Region Pacific Coast Earthquake, has brought to fore the energy independence and national security issues in Japan. Certainly, I^2CNER will be called to engage in the national energy discussion and as such its mission and goals are now even more important than ever.

- The director and the vice director of the Institute are working on establishing plans for I^2CNER to address:
  a. A comparative study assessing the energy options of Japan in light of the recent earthquake-caused calamities.
  b. How I^2CNER can keep its research objectives in perspective relative to other potential technologies toward a carbon-neutral energy society.

  In establishing these plans, the director is consulting with the US Department of Energy and the Vice Director is consulting with corresponding agencies of Japan.

- Research is being conducted in the fields proposed at the time of application. There has been little, if any, alternation from the initial plan.

- A detailed report of each division's research progress over the past few months is presented in section 3. To identify and study issues related to the cohesion of the research activities in I^2CNER's across research groups and division boundaries
  a. Director Sofronis requested and reviewed white papers submitted by each PI, which give a detailed description of her/his research plan. The white papers were sent to the External Advisory Committee for input.
  b. The I^2CNER Kick-Off Symposium was held on February 1, 2011 and was followed by workshops given by each division on February 3rd to promote active exchanges amongst researchers from diverse research areas

technologies, such as electrolysis, nuclear heat utilization, reforming of fossil fuels, photocatalytic water splitting. Especially, the energy in natural recourses, which is stored at low densities, can be converted to a concentrated chemical form in hydrogen energy systems.

- Hydrogen energy (i.e., chemical energy) can be efficiently converted to electrical energy, and vice versa, by using technologies such as electrolysis and fuel cells.

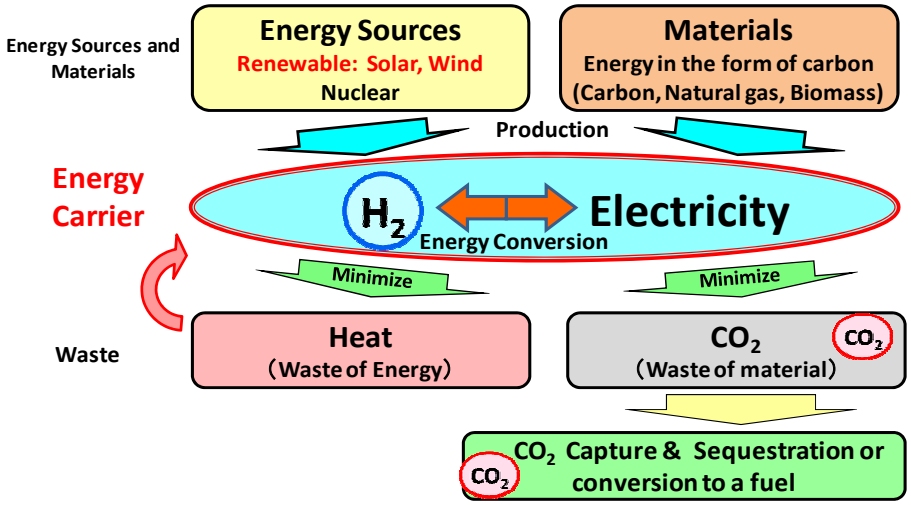

Fig. A Carbon-Neutral Energy Fueled System

- The production of hydrogen and the CCS process require energy inputs. It will defeat the purpose of a clean/sustainable energy system, if the energy input (e.g., the energy generated from fossil fuels) exceeds the chemical energy extracted from hydrogen, or if the CO_2 emission from the energy utilized in a CCS process exceeds the actual CO_2 captured and stored. Moreover, as has been stated above, carbon-based energy sources (e.g., fossil fuels and biomass) require a combustion process to produce useful electrical energy and heat. This process produces waste heat energy and emits CO_2 byproducts. Electrical energy and heat energy are also generated from renewable energy sources, such as solar, wind, and geothermal energy. The

final byproduct of these processes is also waste heat energy due to the inefficiencies in the conversion process. Therefore, it is vital that we develop an optimum/economical holistic energy system which minimizes overall CO_2 emission and waste heat energy, with flexible but appropriate combinations of the following technologies:

  - Highly efficient production of hydrogen from existing energy production systems (thermal electric power generation and nuclear power generation systems) with both fossil fuels and renewable energy sources, in combination with reuse of waste heat energy within the systems.

  - Highly efficient energy conversion between hydrogen (chemical) energy and electrical energy.

  - Highly efficient carbon capture and storage.

- Thus, it is important to approach the research issues underlying the development of hydrogen energy and carbon capture and storage from a holistic viewpoint and a careful examination of the interdependencies between the components and stages of the entire energy system.

- Japan has been one of the world's pioneers in the field of renewable/clean energy technologies such as fuel cells for residential application, fuel cell vehicles, and hydrogen stations, and we, especially the Kyushu University, have a strong research record and cutting-edge research facilities in these fields. For example, the Kyushu University is internationally recognized for its research activities related to hydrogen energy, from fundamental science issues to the assessment and evaluation of actual fuel cells and hydrogen stations. Thus, the existing research foundations and accomplishments of the Kyushu University provide a valuable and advantageous setting for the launching of the proposed international effort. Although the research on carbon capture and storage has been intensively undertaken worldwide, there are still a number of critical issues to be addressed in terms of the long-term safety and reliability of CCS systems. Thus, it is crucial to strengthen the scientific foundation underpinning these technologies for its practical application. In the area of fundamental research for geological

storage, the Kyushu University has ongoing research activities on the effect of SO_x on the CO_2 storage capacity and the physicochemical behavior of CO_2 in shallow ocean beds. In addition, in the area of ocean sequestration, the Kyushu University currently pursues development of ocean circulation models and virtual moorings systems for monitoring.

- To remove the roadblocks to the realization of a carbon-neutral hydrogen economy, the proposed research will focus on: hydrogen production; hydrogen storage materials; hydrogen-induced material degradation; fuel cells; material conversion; carbon capture, ocean sequestration and geological storage. To achieve the breakthroughs needed to develop the required technologies, it is essential to understand the fundamental processes and reactions occurring at the interface between materials and hydrogen, oxygen or CO_2. This project will undertake research across multiple temporal and spatial scales on phenomena characterized by a commonality of challenges, e.g., issues of absorption, adsorption, dissolution, diffusion, reaction, and conduction. Therefore, solving the current energy and environmental problems will necessitate the integration of atomistic to macroscopic approaches.

- To achieve these research goals, it is essential for scientists and engineers from various research fields, such as chemistry, physics, materials science, mechanics, geoscience, oceanic science and biomimetics to conduct research together on the same topics. The synergy generated will consequently result in a positive influence on the overall research outcome, and lead to the development of innovative technologies

3. Research objectives

<Initial plan>

- Our ten-year research goal is to establish innovative, safe, and reliable technologies for the production, storage and utilization of hydrogen (hydrogen production; hydrogen storage materials; hydrogen embrittlement resistant materials; fuel cells; material conversion), as well as for CO_2 separation and concentration, CO_2 geological storage, and ocean sequestration. To attain this goal, our approach will involve multiple disciplines; such as chemistry, physics, materials science, mechanics, geoscience, oceanic science and biomimetics in order to investigate phenomena such as species diffusion taking place at the interface of interactions between materials and hydrogen, oxygen, and CO_2 at all scales, from the atomic to those for oceanic systems and from nanoseconds to decades. We also aspire to contribute to the societal debate by informing and educating the public on ocean sequestration and geological storage through sound scientific data and on the benefits of transitioning to a carbon-neutral energy society. In the following, an outline of our individual research objectives is presented followed by the detailed description of the related research methodologies:

  - Development of high efficiency material conversion processes without any by-products such as waste and CO_2.
  - Development of innovative and sustainable hydrogen production processes, such as photocatalytic water splitting;
  - Development of novel hydrogen storage materials with storage capacity of over 6wt% H_2;
  - Design of hydrogen-embrittlement resistant materials for the development of a safe and reliable material infrastructure;
  - Development of the next generation of fuel cells by the research on novel materials and devices;
  - Development of low-energy carbon separation and concentration processes;

<Results/progress/alternations from initial plan>

- No deviations have been made from the initially proposed plan. In the following, the progress made within each division so far is reported by focusing on i) technical accomplishments since the launching of the Institute; ii) established synergisms and collaborations; iii) future work and near term issues; iv) conclusions; v) publications.

- Development of CO_2 geological storage considering CO_2 behavior and chemical interactions;

- Development of ocean sequestration by understanding CO_2 behavior in ocean;

- Increase public awareness for hydrogen technologies and long-term CO_2 behavior in each earth and ocean.

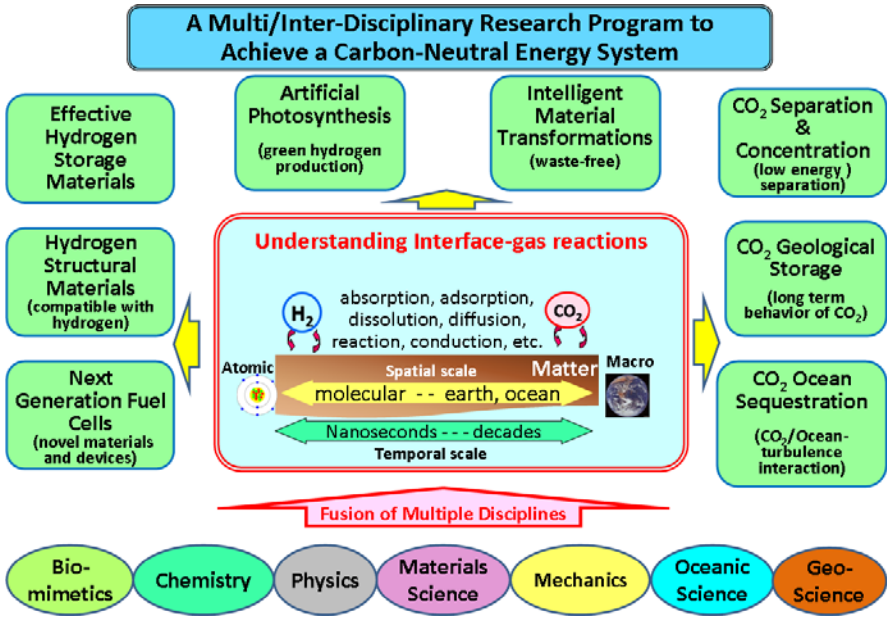

Fig. Interfaces in the multi/inter-disciplinary research program in I^2CNER

(Research Objectives and Methodologies)

1. Artificial photosynthesis through complete photocatalytic water splitting by the Z-scheme type excitation mechanisms (Lead PI: Prof. Tatsumi Ishihara)

- Artificial photosynthesis, specifically photocatalytic water splitting**,** is a promising approach for innovative hydrogen production without CO_2 generation. However, currently, complete water splitting has not been achieved. This is due to the short lifetime of the separated charge which is too short for the process to complete.
- To date, we have developed the double excitation Z-scheme which combines a structure-controlled oxide semiconductor and an organic semiconductor to produce hydrogen and oxygen efficiently. We have also developed the methodology for very fast charge transfer to an organic compound by using certain type of oxides. In the proposed research, we will investigate generation of hydrogen through complete photocatalytic water splitting and apply these principles to i) innovative solar cells development, and ii) conversion of CO_2 to functional compounds in combination with electrolytic techniques mimicking dark reactions.

- To achieve these goals, we will carry out research on: the biomimetic synthesis of new inorganic-organic semiconductors; the control of dye at material interfaces; the charge transfer process; the structure of the electrodes in solar and electrolytic cells at the atomic level; and the separation efficiency of photo-excited charges. Ultimately our research will contribute to the development of a hydrogen production technology without CO_2 emission and the conversion of CO_2 to functional compounds using sunlight, through the integration of molecular chemistry, biomimetics, green chemistry, and surface chemistry.

Reference

[1] H. Hagiwara, T. Inoue, K. Kaneko, and T. Ishihara, "Charge-Transfer Mechanism in Pt/KTa(Zr)O_3 Photocatalysts Modified with Porphyrinoids for Water Splitting", *Chem. Europe. J.*, **15**, 12862 (2009).

(Research Objectives and Methodologies)

1. Artificial Photosynthesis for Hydrogen Production

A) Technical Accomplishments and Progress

- Using visible light up to 450 nm with oxynitrate of Ga(Zn)ON, we successfully created H_2 and O_2 (Fig. 1b)

- We tested the power generation property of the cell through using hetero bulk junction of C60 donor and thiophene base organic semiconductor acceptor. We found that a mixing ratio of 6:4 shows the highest power density and conversion efficiency of 1.3%.

- Studying electrodes for steam electrolyzer, we found that a combination of Ni-oxide ion conductor is effective on improving the electrolysis activity. The H_2 formation rate was doubled in comparison to our previous electrode usage.

B) Collaborations/Synergism

- The division consists of four groups (Ishihara (Photocatalyst), Adachi (Solar Light), Takahara (Interface), and Kilner (Electrolyzer)) working in concert toward the overall objective of hydrogen production.

C) Future Work/Near-Term Issues

- Optimize of organic dye for Ga(Zn)ON semiconductor, in particular focusing on hexaphyline.

  Synthesize a new organic semiconductor, thiophene base, to be applied for bulk junction layer in solar cell.

  Measure the surface activity of doped La_2NiO_4 base oxide for anode in electrolyzer by using 18O isotope. We will investigate the activity of fluorite oxide.

D) Conclusions

We successfully developed a new photocatalyst to achieve complete water splitting in response to visible light

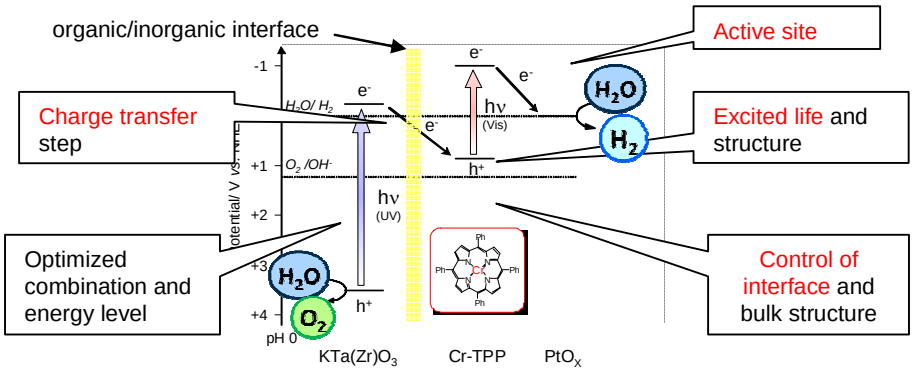

Fig. 1a. Artificial photosynthesis through complete photocatalytic water splitting

E) Publications

[1] S. Ida, K. Yamada, T. Matsunaga, H. Hagiwara, Y. Matsumoto, and T. Ishihara, *J. Am. Chem. Soc.*, 132 (49), pp 17343 (2010)

[2] K. Harada, T. Edura, and C. Adachi , Appl. Phys. Exp. 3, 121602 (2010)

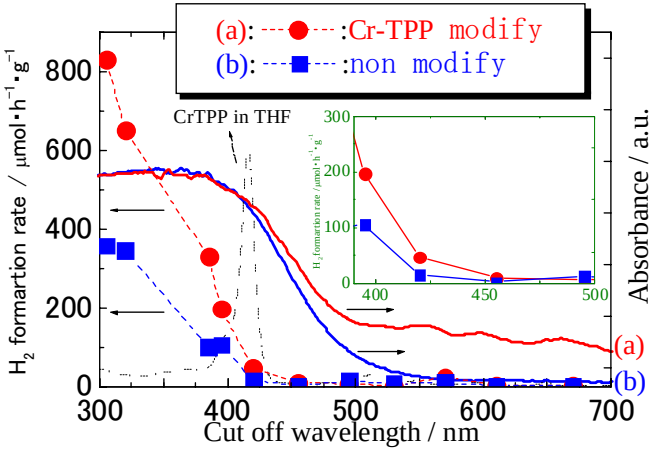

Fig.1b. H_2 formation rate on RhOx,NiOx/CrTPP/IrOx-GaN:ZnO as a f unction of wave length and absorption spectra of the catalyst. TPP: organic dye: tetraphenyl prophine

2. Hydrogen materials compatibility: mitigation/remediation strategies against hydrogen embrittlement (Lead Investigator: Dr. Brian P. Somerday)

- Hydrogen embrittlement is a severe environmental type of failure that can cause a sudden and catastrophic failure under normally safe working loads in almost all materials. Although the phenomenon of hydrogen-induced degradation of metals is well documented and significant progress has been made in the discovery of the fundamental mechanisms for particular loading conditions (cf. work of Murakami, Kondo, Matsuoka, Robertson, and Sofronis), there remains a paucity of information about the wide spectrum of pathways through which hydrogen degrades the material properties and how these depend on the in-service conditions. A few examples should suffice to demonstrate the magnitude of the challenge: In hydrogen-accelerated fatigue failure, we do not understand how relatively low pressures of hydrogen degrade the material resistance by orders of magnitude. At a more fundamental level, we do not understand how relatively low pressures of hydrogen degrade the material resistance by orders of magnitude. At a more fundamental level, we do not know if vacancy stabilization by hydrogen is a potential fracture mechanism, let alone the operation and loading conditions under which vacancy formation can potentially bring about failure. Further, we do not know whether gaseous hydrogen serves as a lubricant in dry sliding seals or whether it couples with wear mechanisms to hasten failure. The systems that will be used in production, delivery, storage, and dispensing will contain non-metallic components. For example, polyethylene may be used as the liner in the pressurized tanks envisioned for use in automotive applications, and elastomers will be used in seals. In comparison to metallic systems, our knowledge base for hydrogen effects on the structural properties of non-metallic systems is, at best, rudimentary.

- In summary, assessing component lifetime, developing mitigation or remediation strategies, or designing smart structural materials for employment in a hydrogen environment are not yet feasible. The proposed effort seeks to fulfill this challenge by devising a program that employs synergistically experimental and computational methodologies over multiple spatial and temporal scales. Efforts at each scale will inform the design and interpretation of efforts at the next higher scale. For example, first principle density functional

2. Structural Material Compatibility with Hydrogen

A) Technical Accomplishments and Progress

- For the first time, we discovered that chemisorbed hydrogen lubricated iron surfaces in almost pure hydrogen gas (Fig. 2b on next page). This interaction between hydrogen and iron surfaces has significant implications for material damage at tribo-interfaces.

- Hydrogen-accelerated fatigue crack growth is mitigated in ferritic steels with carbide-forming elements and refined grains. Establishing such structure-property relationships enables understanding of the basic mechanisms governing hydrogen-induced material degradation.

- We found that hydrogen-assisted fatigue crack growth in steels is a strong function of load-cycle frequency, but this sensitivity depends on the steel crystallographic structure, i.e., BCC or FCC. Defining the optimum load-cycle frequency is critical for improving fatigue measurements in H_2 gas.

- Two novel austenitic stainless steels were fabricated: ultra-fine grained steel and high-nitrogen steel having yield strengths of 0.9 GPa and 0.8GPa, respectively. These high-strength steels represent candidates for next-generation hydrogen-compatible materials.

B) Collaborations

- Universities: University of Illinois at Urbana-Champaign, University of California, Berkeley, University of Gottingen.

- Research Laboratories: Sandia National Laboratories, AIST, National Institute of Materials Science.

- Industry: Mohawk Innovative Technology, Inc., ExxonMobil Research and Engineering Company.

C) Future Work/Near-Term Issues

- Characterize hydrogen-affected tribo-interfaces as a function of the component metals.

calculations coupled with experimental measurements of the local hydrogen concentration will determine the dependence of the electronic structure, and consequently the cohesive energy, on the hydrogen concentration. Knowledge of the hydrogen effect on the cohesion of internal material interfaces is a key input to the development of constitutive relations integrated in micromechanical models for property prediction and life assessment at the macroscale. The proposed effort requires assembling an international research team comprised of experts in state-of-the art computational and experimental methods and such a team has been assembled. In particular, we plan to:

- Study the interaction of hydrogen with metallic surfaces. Understanding how molecular hydrogen interacts with the surface atoms, dissociates to atomic hydrogen and enters the metal is an essential prerequisite to the understanding of how the degradation mechanisms depend on the modes of hydrogen uptake. We will study and explore the physics and chemistry of hydrogen adsorption on free surfaces and internal material interfaces in the presence of other possibly embrittlement mitigating species.

- Develop experiments for the study of formation and interaction of regenerative coatings (e.g. oxides) with hydrogen adsorption at crack tips under static and cyclic loading.

- Measure, for the first time, local-concentrations of hydrogen and its effect on the local electronic structure, lattice cohesive strength, and strength of internal interfaces such as grain boundaries in fcc structures. We will employ first principles density functional theory and molecular dynamic simulations to characterize the interaction of hydrogen with defects such as vacancies and dislocation cores.

- Develop experiments to measure interfacial cohesion and plastic flow activation along individual slip systems as affected by hydrogen at the nanoscale and measure the intensity of the degradation at the macroscale in terms of macroscopic parameters through fracture mechanics specimens under conditions, for the first time, of environmental transferability.

- Determine relationship between hydrogen-affected tribo-interfaces and crack nucleation under fretting fatigue conditions
- Measure fatigue and fracture properties of new high-strength stainless steels in high-pressure H_2 gas.
- Apply state-of-the-art focused ion beam-transmission electron microscopy (FIB-TEM) techniques to fatigue test specimens to identify the basic mechanisms of material degradation.

D) Conclusions

- The recent technical accomplishments demonstrate progress toward improving fatigue and fracture property measurements in H_2 gas, better understanding basic hydrogen-surface interactions and material degradation mechanisms, as well as developing next-generation materials having improved resistance to hydrogen embrittlement at higher strength levels.

E) Publications

[1] K. Fukuda, M. Hashimoto, J. Sugimura, Friction and Wear of Ferrous Materials in a Hydrogen Gas Environment, Tribology Online, Vol.6, No.2, pp.142-147 (2011).

[2] T. Awane, Y. Fukushima, T. Matsuo, S. Matsuoka, Y. Murakami and S. Miwa, Highly sensitive detection of net hydrogen charged into austenitic stainless steel with secondary ion mass spectrometry, Analytical Chemistry, 83, pp. 2667-2676 (2011).

- Develop models for the constitutive response of materials that account for the interaction of hydrogen with the crystal structure of the material. Such models which are essential for understanding and modeling fatigue from a mechanistic perspective are completely lacking.

- Employ finite element analysis and simulation to synthesize the results from the micro/nano scale with those from the macroscale in order to come up with tools of material performance prognosis that can be used toward the development of science-based codes and standards.

- In summary, the objective of the proposed research is to: i) remediate the problem of hydrogen embrittlement in existing materials by developing mitigation strategies and possibly suppressing it altogether; ii) design intelligently through employment of experimental/computational methodologies materials that are not susceptible to hydrogen embrittlement over a wide range of operating conditions.

References

[1] B. P. Somerday, D. K. Balch, M. Dadfarnia, K. A. Nibur, C. H. Cadden, and P. Sofronis, "Hydrogen Assisted Crack Propagation in Austenitic Stainless Steel Fusion Welds," *Metallurgical and Materials Transactions A*, **40**, 2350-, 2362, (2009).

[2] M. Dadfarnia, P. Novak, D. C. Ahn, J. B. Liu, P. Sofronis, D. D Johnson, and I. M. Robertson, "Recent Advances in the Study of Structural Materials Compatibility with Hydrogen", *Advanced Materials*, **22**, 1128-1135 (2010).

[3] I. M. Robertson, P. Sofronis, and H. K. Birnbaum, "Hydrogen Effects on Plasticity", In: J. P. Hirth and L. Kubin, Editors: *Dislocations in Solids*, Vol. **15**, pp. 249-293, Elsevier, The Netherlands: North Holland, 2009.

[4] P. Novak, R. Yuan, B. P. Somerday, P. Sofronis, R. O. Ritchie, "A statistical, physical-based, micro-mechanical model of hydrogen-induced intergranular fracture in steel, *J. Mech. Physics*

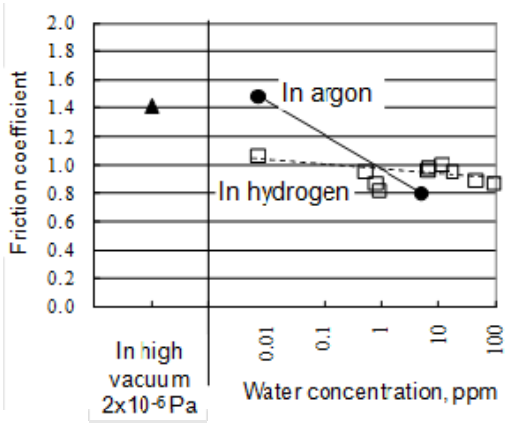

Fig. 2b. Variation of friction coefficient (pure iron vs pure iron) as a function of water concentration. Data from pin-on-disk tests in ambient pressure gas (except for data in vacuum) with a novel technique of controlling trace impurities.

Solids, **58**, 206-226 (2010).

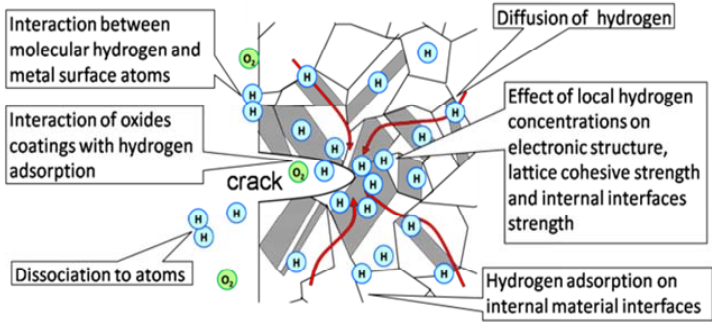

Fig. 2a. Fundamental processes around a crack in the presence of hydrogen

3. Materials for the next generation fuel cells: fundamentals of high efficiency energy conversion systems and development of novel devices: (Lead PI: Prof. Kazunari Sasaki)

- Fuel cells can efficiently convert chemical fuels, such as hydrogen, to electricity, and are the core technology in a hydrogen energy society. However, there has been no practical application of such fuel cells due to the restricted operational conditions of the fuel cell materials. Therefore, a breakthrough in the development of innovative materials for fuel cells is crucial. Leading the field of fuel cell research in Japan, e.g. the Expert representing Japan to an Annex Meeting of International Energy Agency (IEA) on polymer electrolyte fuel cells, Prof. K. Sasaki has a strong research record in the area of the state and concentration of electrons and ions in solids at temperatures of interest, and has been actively undertaking the study of material devices at cell levels.

- In this project area, the goal is to develop innovative electrolyte materials, electrode materials, and new devices for fuel cells, based not only on established research methodologies, but by resorting to the fundamental studies of the chemistry and electrochemistry of solids at material interfaces and in nano-regions.

- In particular, we will carry out research on the development of electrolyte materials (inorganic and organic systems) and electrode materials (novel metal and inorganic systems) for the next generation of fuel cell devices. These materials researches are based on fundamental investigations: (i) nano-electrochemical measurements of parameters such as electrical, electrochemical and catalytic properties of nanostructures materials (nanocomposite, thin films, low-dimensional materials, and catalysts with strong meta-support interactions), (ii) computational science to calculate microscopic processes such as surface adsorption and diffusion, and macroscopic processes such as ionic and electronic conduction, mass and heat transport and (iii) molecular chemistry, surface science, and materials research to understand surface and interfacial transport phenomena in model surfaces and interfaces. Our objective is to elucidate the nano-level reaction mechanisms of electrons, atoms, and molecules in fuel cells, and ultimately design innovative material microstructures and devices which will allow major breakthroughs in the field of fuel cells within the next 10 years.

3. Fuel Cells

A) Technical Accomplishments and Progress

- We achieved high durability of 60,000 voltage cycles, on stimulating practical Fuel Cell (FC) vehicles, through Pt/SnO_2 catalysts. The fact that a ceramic material for high temperature FC has been successfully applied/used to low temperature FC will impact future electrochemistry developments (Fig.3b).

B) Collaborations

- The division researchers are meeting regularly (There was one meeting in December, 2010 and three more this year. Participants in the meetings are representatives from i) Industry: Kyocera, MHI, Tokyo Gas, TOTO, Mitsubishi Materials, Kansai Electric (NEDO project); ii) Academia: Dr. Tsuchiya of Harvard University; iii) National Laboratories: Prof. Traversa and Dr. Rupp from NIMS-(MANA); and iv) over 20 professors from I^2CNER including WPI principal investigators, Prof. T. Ishihara and Prof. J. A. Kilner. In addition, Associate Prof. A. Hayashi, WPI Assistant Prof. M. Nishihara have joined our division since last April and WPI Assistant Profs. S. Bishop and S. Lyth will join the division in June.

  The division's research work is administered by the four group leaders, i.e., Profs. K. Sasaki, H. L. Tuller, L. J. Gauckler, and N. Nakashima, who are specialists on oxide/carbon electrocatalysts and Solid Oxide Fuel Cell (SOFC) materials/processing, and two collaborating Principal Investigators (PIs), Profs. Ishihara and Kilner, who are experts addressing electrolyte issues of FCs from low to high temperature operation range.

C) Future Work/Near-Term Issues

We plan to focus on new materials and alternative functions for those materials under various running conditions for FCs.

D) Conclusions

We started our research on "unification" of FC electrochemistry through interdisciplinary studies of electrolyte/electrode materials, device processes, and FCs at various operating

References

[1] A. Masao, Z. Noda, F. Takasaki, K. Ito and K. Sasaki, “Carbon-Free Pt Electrocatalysts Supported on SnO2 for Polymer Electrolyte Fuel Cells.”, Electrochemical and Solid-State Letters, 12, 9, B119-B122 (2009).

[2] K. Sasaki and Y. Teraoka, “Equilibria in Fuel Cell Gases,” J. Electrochem. Soc., 150, 7, A878-A888 (2003).

[3] K. Sasaki and J. Maier, “Low Temperature Defect Chemistry of Oxides”, J. Appl. Phys., 86, 10, 5422-43 (1999).

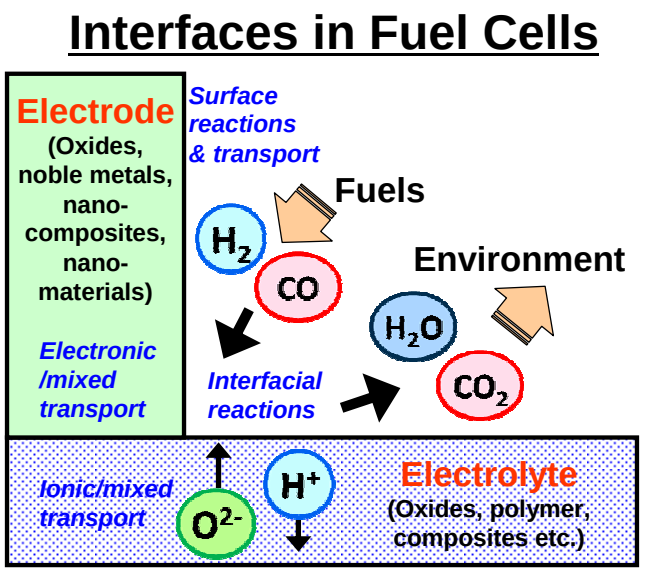

Fig. 3a. Transport and reaction processes around the electrode/electrolyte interfaces

conditions. We also initiated our work on effectively using materials for high temperatures and devices to low temperature FCs.

E) Publications

[1] K. Sasaki et al. “Impurity Poisoning of SOFCs.” ECS Trans., 35 (1), 2805-2814 (2011).

[2] H.L. Tuller et al. “Point Defects in Oxides: Tailoring Materials Through Defect Engineering.” Annual Review of Mater. Sci., (2011), in press.

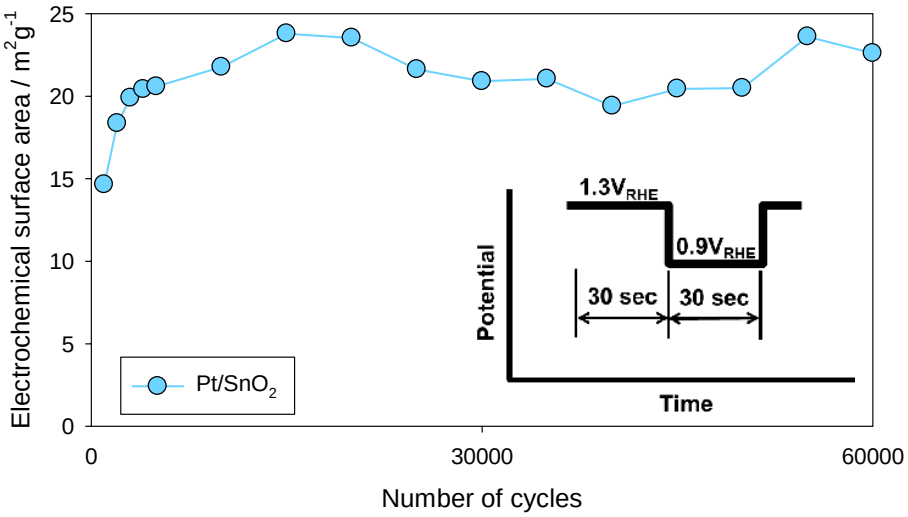

Fig. 3b. Electrochemical surface area of Pt/SnO_2 electrocatalysts with durability up to 60,000 cycles corresponding to 20-year life time.

4. Thermal and flow properties of hydrogen and CO_2 under extreme pressures (Lead PI: Prof. Yasuyuki Takata)

- Development of hydrogen and CO_2 storage technologies requires the knowledge of fundamental thermophysical properties of hydrogen and carbon dioxide under extreme pressure conditions, e.g. 100MPa. Properties, such as PVT-relations, specific heat capacity, thermal conductivity, and heat transfer characteristics are not available at high pressures, and values extrapolated from low pressure measurements are currently used. Prof. Takata's research group at Kyushu University will focus on understanding such issues as the conversion rates between orthohydrogen and parahydrogen, the thermal properties and heat transfer characteristics of supercritical carbon dioxide, and the adsorption and desorption properties of carbon dioxide The objective is to develop accurate thermophysical property database for a wide range of temperatures and pressures.

References

[1] E. Yusibani, P. L. Woodfield, M. Fujii, K. Shinzato, X. Zhang, and Y. Takata, "Application of the Three-Omega Method to Measurement of Thermal Conductivity and Thermal Diffusivity of Hydrogen Gass," *Int. J. Thermophysics*, **30** (2), 397-415 (2009).

[2] P.L. Woodfield, S. Moroe, J. Fukai, M. Fujii, K. Shinzato, M. Kohno, and Y. Takata, "Techniques for Accurate Resistance Measurement in the Transient Short-Hot-Wire Method Applied to High Thermal-Diffusivity Gas," *Int. J. Thermophysics*, **30** (6), 1748-1772 (2009).

4. Thermophysical Properties

A) Technical Accomplishments and Progress

- Developed PVT apparatus for hydrogen up to 100MPa and 500°C.
- Measured thermal conductivity of hydrogen up to 100MPa & 500°C.
- Developed new prediction correlation for thermal conductivity of hydrogen (Fig. 4 on next page).
- Measured viscosity of hydrogen up to 100MPa and 200°C.
- Extended thermophysical properties database for hydrogen.
- Developed a thermodynamic analysis for hydrogen leakage through a crack in a high pressure tank.
- Measured adsorption isotherms of methane onto activated carbons at temperatures from 5 to 75°C & pressure up to 2.5 MPa.

B) Collaborations

- P. L. Woodfield, Griffith University, Australia, on Thermal Conductivity and Viscosity of Hydrogen.
- M. J. Assael, Aristotle University of Thessaloniki, Greece, on Thermal Conductivity of Hydrogen.
- K. C. Ng, National University of Singapore, on Adsorbed Natural Gas Storage System.

C) Future Work/Near-Term Issues

- Develop hydrogen PVT data up to 100MPa and 500°C.
- Thermal analysis of hydrogen storage systems (refill/discharge/leakage to/from pressure tank and metal hydride system).

- Measure of orho-para conversion rate under various temperature and pressure conditions.

- Develop experimental apparatus for CO_2 adsorption study.

- Study the effect of surface wettability for liquid-vapor phase change.

D) Conclusions

New correlation equation for hydrogen thermal conductivity was developed for the range up to 100MPa and 500°C based on measurements through the transient short-hot wire method. The equation predicts measured experimental data within an uncertainty of 2%. A relevant paper has been submitted to the International *Journal of Thermophysics*.

E) Publications

[1] B. B. Saha, S. Jribi, S. Koyama, and I.I. El-Sharkawy, "Carbon dioxide adsorption isotherms on activated carbons", *Journal of Chemical & Engineering Data*, dx.doi.org/10.1021/je100973t (available online)

[2] S. Moroe, P.L. Woodfield, J. Fukai, K. Shinzato, M. Kohno, M. Fujii and Y. Takata, "Thermal Conductivity Measurement of Gases by the Transient Short-Hot-Wire Method", *Experimental Heat Transfer*, Vol. 24, Issue 2, pp.168-178, 2011

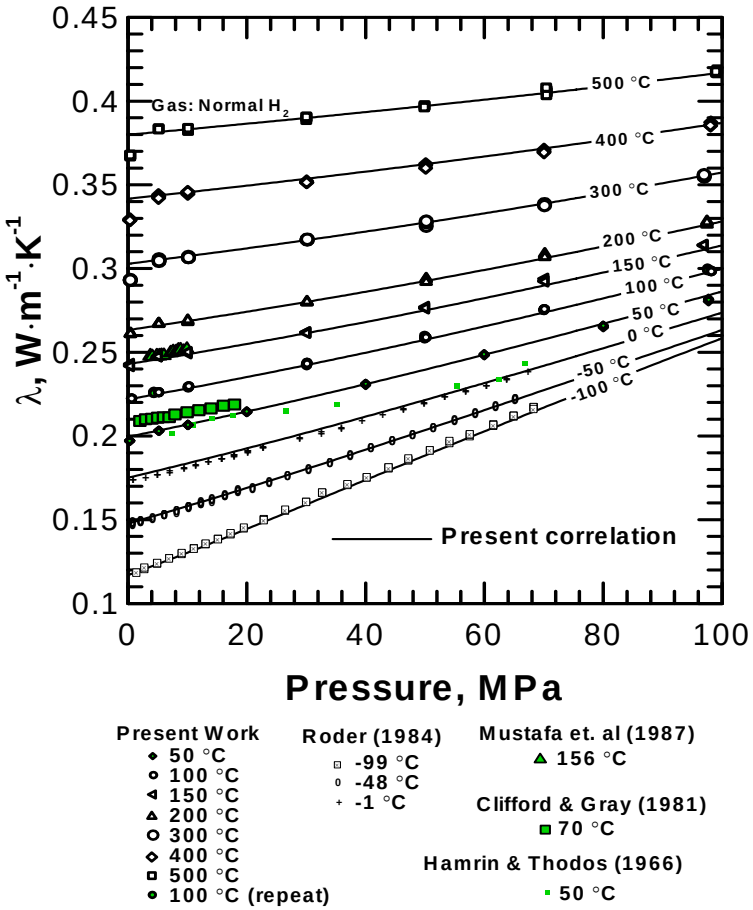

Fig. 4. Isotherms of normal hydrogen thermal conductivity (Solid lines according to our new correlation equation)

5. Hydrogen storage materials: a new pathway under extreme pressures? (Lead PI: Prof. Etsuo Akiba)

- Development of a compact, safe, inexpensive, and highly energy efficient hydrogen storage technology is required, since the volumetric energy density of hydrogen gas is significantly small for gaseous storage to be considered as an efficient means. In addition, hydrogen storage materials provide higher storage capacities than storage in liquefied form. The hydrogen storage capacity of 3wt% H_2 achieved in the study by Prof. Akiba is so far the highest in the world. However, we maintain that improvement in mass energy density of hydrogen storage is still possible.

- By applying diverse ranges of approaches of molecular chemistry, surface science, solid mechanics, solid-state physics, and materials science, we will investigate Mg-based materials and complex hydrides as promising candidate materials for hydrogen storage. We plan to investigate i) the bond property between hydrogen and storage materials for the control of the reaction temperatures; ii) the position of hydrogen in the storage materials that is potentially associated with the highest hydrogen storage capacity; and iii) the transport properties of hydrogen we aim at developing materials with the storage capacity of over 6wt% H_2.

Reference

[1] H. Iba and E. Akiba, "Hydrogen absorption by Laves phase related BCC solid solution", Intermetallics, 6, 461 (1998).

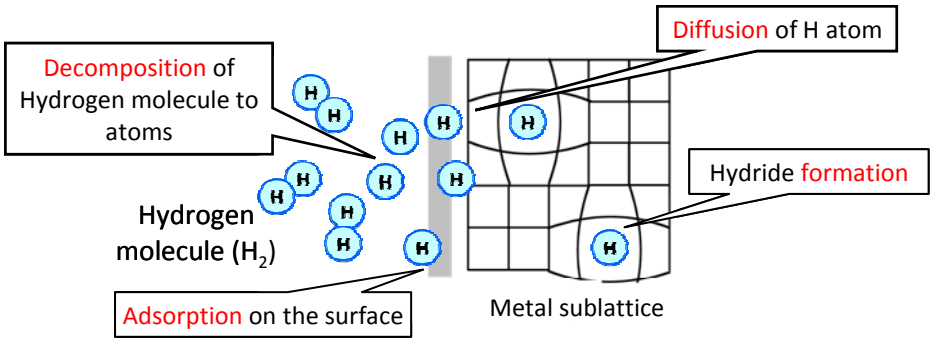

Fig. 5a. Fundamental processes at the surface of hydrogen storage materials

5. Hydrogen Storage Materials

A) *Technical Accomplishments and Progress*

- A single hydrogen atom has been observed using transmission electron microscopy (TEM) as shown in Fig. 5b. This observation of a single hydrogen atoms is the first worldwide. The relevant technique and observation are also extremely useful for the investigation of the hydrogen effect on structural materials.

B) *Collaborations*

- National Institute of Advanced Industrial Science and Technology (AIST)

- I^2CNER Division of Thermophysical Properties to understand and improve the heat management of hydride reactors

- Toyota Motor Corporation with discussions on future research and development

C) *Future Work/Near-Term Issues*

- Using various techniques including TEM, X-ray and neutron diffractions, and Raman, we will investigate the mechanism and structure of hydrogen storage materials in close collaboration with the I^2CNER Division on Thermophysical Properties.

D) *Conclusions*

- Through TEM, a single hydrogen atom in metal sublattice was observed for the first time. Along with research on materials/hydrogen storage issues, research has begun on the relevant heat management problems.

E) *Publications*

[1] J. Matsuda, Y. Nakamura, E. Akiba, *J. Alloys Comp.*, **509**, 4652-4356 (2011).

[2] J. Matsuda, Y. Nakamura, E. Akiba, *J. Alloys Comp.*, JALCOM-D-10-06054

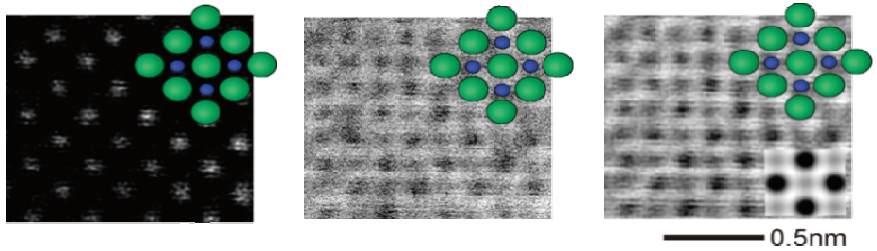

Fig. 5b. Direct observation for the first time of a single hydrogen atom using transmission electron microscope: **(**a) The annular dark field (ADF) image of a crystal of VH_2 viewed along [001] and filtered by the radial difference filter20 released by HREM Research and a low pass filter to reduce the periodic scan noise. (b) The raw annular bright field (ABF) image recorded simultaneously with (a). (c) The ABF image from (b) filtered by the radial difference filter and a low pass filter. The projected structure is superposed on all images. A simulated ABF image assuming a specimen thickness of 5 nm is superposed on (c). The images are shown on nonlinear intensity scales to improve visual clarity.

6. Asymmetric oxidation for material transformation: toward discovery of a catalyst process for a "zero-waste/no-carbon" reaction (Lead PI: Prof. Tsutomu Katsuki)

- A large number of functional material substances used in everyday life are derived by chemical transformations from fossil fuels. These chemical reactions require substantial energy expenditures and usually result in the creation of huge amounts of waste and emission of unwanted CO_2. Therefore, development of new and efficient approaches to chemical reaction for material transformation will help in the direction of diminishing the society's carbon footprint and assist in energy sustainability given the limited availability of fossil fuels. Prof. Katsuki who has a long and profusely cited research record in this area of organic chemistry will undertake this task of "greening" chemical reactions for material conversion by focusing on the development of asymmetric oxidation through employing atom-efficient oxidants. The effort will focus on devising an approach to producing target materials without waste generation, emission of CO_2, and energy loss through using molecular oxygen as an oxidizing agent. The approach can be tied to artificial photosynthesis processes thus providing an effective utilization of the generated oxygen.

- It is well known that traditional "biological" type of oxidation includes several steps and it is catalyzed by a combination of various enzymes. However, most enzymes are unstable, difficult-to-handle, and they are not necessarily ideal catalysts especially for mass production. Thus, there is a strong demand for development of efficient oxidation catalysts that exhibit efficiency in oxidation catalysis comparable to enzyme catalysis. Also it is known that many weak bond interactions participate in enzyme catalysis. However, lack of sufficient information for the active site of oxidizing enzyme and its catalysis make the construction of a desired high performance molecular catalyst difficult. This is a critical problem that needs to be resolved for the development of asymmetric oxidation catalysis.

- In particular, we aim to capture the intermediate chemical products in the oxygen activation process in order to understand their reaction properties by integrating various fields such as green chemistry, molecular chemistry, surface chemistry, charge-mass-thermal conversion, and biomimetics. Further, we plan to i) create an

6. Materials Transformation

A) Technical Accomplishments and Progress

- Our research is closely related to the catalysis of hydrogenasese, photosynthetase and oxygenase, the mechanisms of which are still only poorly understood.
  - o Proposed mechanism for inhibition of [NiFe] hydrogenase by CO which is modified with respect to previous studies
  - o Developed porphyrin dimer catalysts, which are chemically attached to metal oxide-surfaced electrodes, as a Mn cluster mimic in photosynthesis, and realized highly efficient water oxidation process
  - o Developed asymmetric aerobic oxidation under non-irradiated conditions including a hydrogen-bonding coupled electron transfer process.

B) Collaborations

- The division PIs (see Fig. 6b) and experts (synthetic, bioinorganic and bio-chemists) work toward enabling efficient material transformations by trying to understand the mechanisms of the corresponding biological and related chemical reactions through the exchange of opinions and proposals on new methodologies for simple and efficient material transformations based on small molecular chemistry. In particular:
  - o Katsuki is collaboration with Nissan Chemical Industries Ltd. on atom-efficient asymmetric oxidation
  - o Naruta is collaboration i) with the inorganic materials group at Chubu University and the Toyota Motor, Co. Ltd. on the elemental strategy and technology project; and ii) with Dr. Akihiro Furube of AIST on rapid spectroscopic analysis of charge transfer systems.
  - o Ogo plans to collaborate with Prof. Thomas B. Rauchfuss at the Department of Chemistry at the University of Illinois at Urbana-Champaign on activation of hydrogen in water.

oxygen activation system without proton-electron transfer through identifying the electron transfer mechanism associated with oxygen activation; and ii) develop fine oxygen oxidation catalysts using molecular oxygen as an oxidizing agent at room temperature. This development will result in an oxygen activation process radically different from those operating in biological oxidation reactions.

- Our research will impact the fundamental science for the construction of conformationally flexible catalysts that exhibit multi-catalysis. Our goal is to demonstrate that multi-step asymmetric aerobic oxidation can be catalyzed by a complex, if its conformation can be appropriately controlled along the oxidation pathway and each conformer can exert a suitable catalysis in each step.

References

[1] H. Egami and T. Katsuki, "Iron-Catalyzed Asymmetric Aerobic Oxidation: Oxidative Coupling of 2-Naphthols", *J. Am. Chem. Soc.*, **131**, 6082-6083 (2009).

[2] H. Shimizu, S. Onitsuka, H. Egami, and T. Katsuki, "Ruthenium(salen)-Catalyzed Aerobic Oxidative Desymmetrization of meso-Diols and Its Kinetics", *J. Am. Chem. Soc.,* **127**, 5396-5413 (2005).

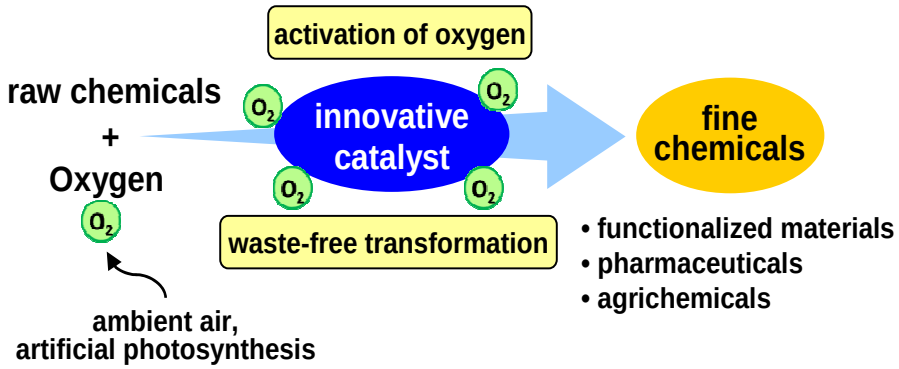

Fig. 6a. Concept of a catalyst process for a "zero-waste/no-carbon" reaction

C) Future Work/Near-Term Issues

- Through understanding the mechanisms for key steps such as electron transfer and oxygen activation in photosynthesis and oxygen atom transfer, we will construct new catalysts that show high catalytic performances equivalent to each enzyme. In addition, we will explore the mechanism for a fuel cell based on [NiFe] hydrogenase mimic.

D) Conclusions

- We are working on new methodologies for dihydrogen activation, dioxygen reduction, artificial photosynthesis (see Fig. 6c), and waste-free aerobic oxidative chemical transformation.

E) Publications

[1] J. Fujisaki, K. Matsumoto, K. Matsumoto, and T. Katsuki, Catalytic Asymmetric Oxidation of Cyclic Dithioacetals. Highly Diastereo- and Enantioselective Synthesis of the S-Oxides by a Chiral Aluminum(salalen) Complex, *J. Am. Chem. Soc.*, *133*, 56-61 (2011)

[2] Jin-Gang Liu and Y. Naruta ((Invited review)) Probing dioxygen activation mechanisms in heme-containing enzymes by heme models, *Ind. J. Chem.*, *50A*, 369-373, 2011.

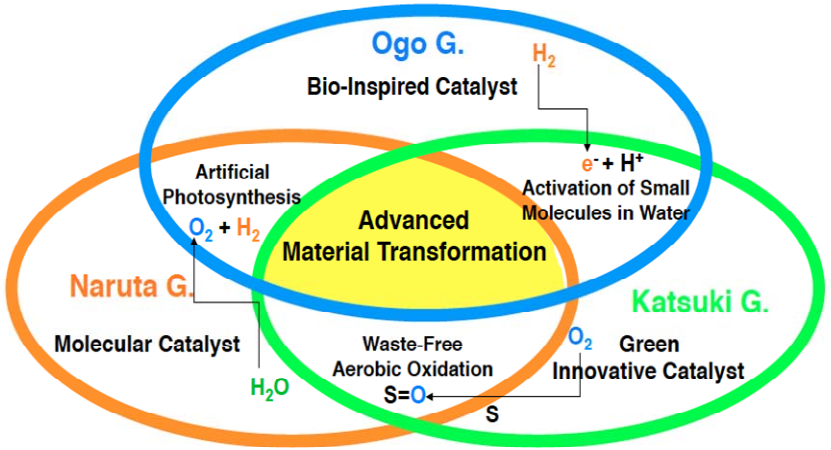

Fig. 6b. The structure of the Materials Transformation Division

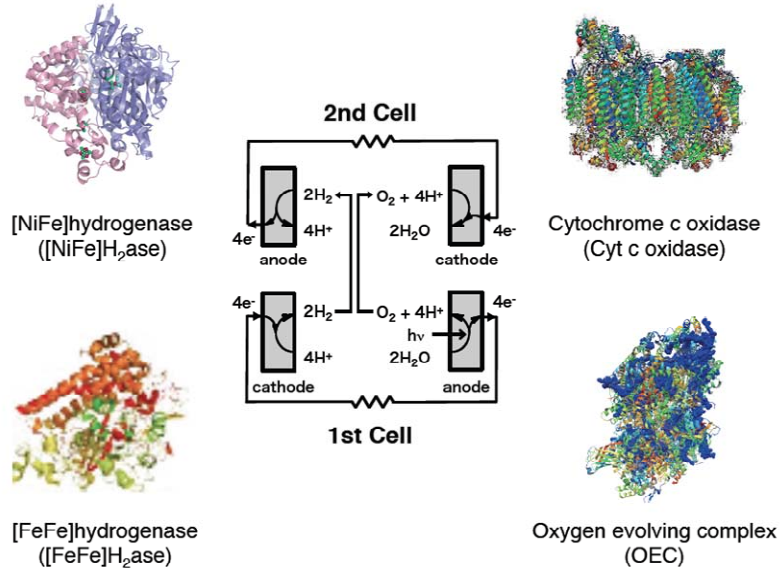

Fig. 6c. Molecular solar cell (the 1st cell) and molecular fuel cell (the 2nd cell) based on phototrophic bacteria and oxidoreductases or their models.

7. Fundamentals of advanced CO_2 separation and concentration systems: toward an efficient and low cost CO_2 separation and concentration technology (Lead PI: Prof. Masaki Minemoto)

- There are currently many methods for the separation of CO_2 produced in the combustion of fossil fuels. However, none of them has yet found practical application due to the large amount of energy required for the separation processes. In this project area, we will carry out fundamental research in order to improve adsorption and absorption of CO_2 in membranes and to develop an electrochemical CO_2 separation process which is highly efficient and can be operated at low cost.

- Specifically, we propose a CO_2 absorption process to be used in conjunction with water electrolysis through ion exchange membranes, where CO_2 is absorbed by the alkaline solution produced from the process and the produced hydrogen can be captured to be utilized. Our objective is to i) develop a novel material (membrane and absorbent) for a most efficient CO_2 separation process through understanding the fundamental mechanisms of the process, and ii) develop and evaluate high efficiency catalysis and solution processes and membrane properties by using a molecular dynamics approach. Further, for the absorption and adsorption processes, we plan to investigate an optimum structure of adsorbent as a novel and unique adsorptive material which can easily desorb the absorbed CO_2.

- The research will be carried out by integrating approaches from various disciplines such as fluid mechanics, surface science, charge-mass-heat transfer theory, and electrochemistry. In addition we will collaborate with the other research groups of the Institute, e.g. the hydrogen production, fuel cells, and CO_2 storage groups.

- Ultimately we seek to develop a novel CO_2 separation system which requires less than one fourth of the energy requirements of an ordinary system.

7. CO_2 Separation and Concentration

A) Technical Accomplishments and Progress

- We proposed six types for CO_2 absorption processes based on the mechanism of water electrolysis. We evaluated the consumption energy of each system in order to find the optimal operating conditions. Although the simulation results were obtained under ideal conditions, we can infer that the required energy for the processes will be substantially reduced when the CO_2 is absorbed through a condensed alkaline solution.

- We examined through Scanning Electron Microscopy (SEM) needle-shaped and amorphous powders of synthesized crystalline compounds (Metal Organic Frameworks (MOF-2); designations 2 and 5 are used to denote the most prominent structures). BET theory for the specific surface area of MOF-2 indicated a relatively high value, though less than the values reported in the open literature. This indicates that the synthesized MOF-2 is a mixture of crystal MOF-2 and amorphous impurities. We tried to improve the quality of the MOF-2 crystal by changing the fabrication conditions. Simulation of CO_2 adsorption on MOF-5 indicates that CO_2 is randomly adsorbed in the space formed in MOF-5 structure. We extended this approach to investigate mixture adsorption of CO_2/N_2 or various MOFs. (Figs. 7b, 7c)

B) Collaborations

- I^2CNER divisions: hydrogen production, fuel cell and CO_2 storage groups.

- Universities: Prof. Fujioka (Fukuoka Women's University) on electrochemical CO_2 absorption and MOF synthesis; Prof. Guan (Hirosaki University) on MOF membrane preparation.

C) Future Work/Near-Term Issues

- Feasibility study of the electrochemical method to separate CO_2. This involves experiments for water electrolysis and electrochemical concentration of water solutions, and experiment for CO_2 absorption and desorption by alkali solution.

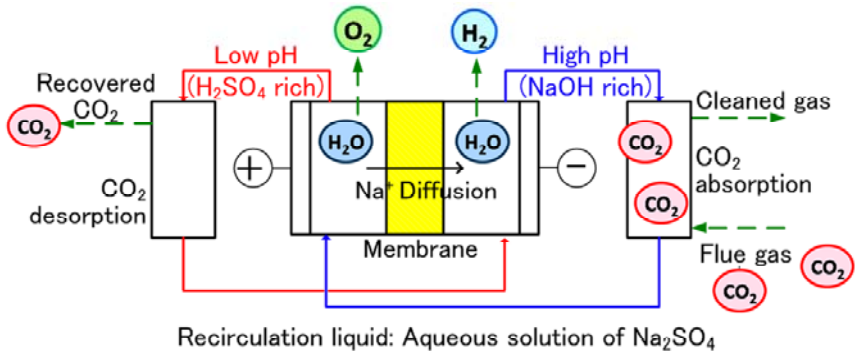

Fig. 6a. An advanced CO_2 separation and concentration system

- Preparation of MOF membrane on a porous plate support. Development of permeation test apparatus

D) Conclusions

- We started basic experiments and developed preliminary inspections methods to obtain data within our scope of reducing the consumption energy of the proposed separation method

E) Publications

[1] M. Minemoto and Y. Matsukuma (2011) Optimization of CO_2 recovery using honeycomb adsorbent, *Novel Carbon Resource Sciences Newsletter*, 4, 5-8, 2011.

[2] M. Minemoto, Y. Matsukuma et al. (2011) Study on CO_2 Recovery Systems by Pressure Swing Adsorption under High Pressure Conditions, *J. Novel Carbon Resource Sciences*, 3, 6-10, 2011

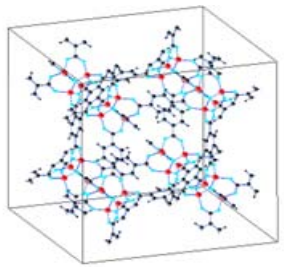

Fig. 7b. Molecular dynamic simulation of the crystal structure of MOF-5

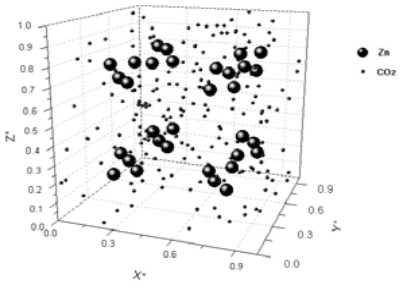

Fig. 7c Molecular dynamic simulation of CO_2 adsorption state in MOF-5

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8. CO_2 geological storage: understanding of the CO_2 behavior in underground reservoirs and development of numerical prediction models (Lead Investigator: Prof. Kyuro Sasaki)

- CO_2 geological storage is carried out in underground reservoirs over around one thousand meters below the surface. There has been a limited number of studies on the long-term safety and reliability of CO_2 geological storage, and as a consequence issues related to the adsorption, dissolution and trapping of CO_2 in highly pressurized porous layers, and CO_2 gas diffusion through faults near the ground surfaces remain poorly understood.

- Our research approach is to integrate a diverse range of disciplines such as molecular chemistry, surface science, green chemistry, solid mechanics, physics, biomimetics, and geoscience to understand dissolution, transformation, and mineralization of CO_2 at the triple phase boundary of rocks and water and in micropores under high pressure. We will also investigate the microbial CH_4 conversion mechanisms. The ultimate goal is to develop a numerical simulation tool for CO_2 diffusion, by testing and evaluating the diffusion behavior of CO_2 from the underground reservoirs to the ground surface including both saturated and unsaturated layers.

- Prof. Kyuro Sasaki has a notable research record on the study of the effect of SO_x on the CO_2 storage capacity and CO_2 phase behavior.

References

[1] P. Q. Huy, K. Sasaki, Y. Sugai, T. Kiga, M. Fujikowa, T. Adachi, "Effects of SO_2 and pH Concentration on CO_2 Adsorption Capacity in Coal Seams for CO_2 Sequestration With Considerations for Flue Gas From Coal-Fired Power Plants", *JCPT(SPE)*, **48** (10), 58-63 (2009).

[2] T. Yasunami, K. Sasaki, Y. Sugai, "CO_2 Temperature Prediction System in Injection Tubing Considering Supercritical Condition at Yubari ECBM Pilot-Test", *JCPT (SPE)*, **49** (4), 44-50 (2010).

8. CO_2 Geological Storage

- Due to Professor Sasaki's resignation, the decision was made to consolidate CO_2 Geological Storage and CO_2 sub-sea bed sequestration into one division: CO_2 Capture and Storage.

- In the new division, the research objectives on geological CCS are to i) characterize reservoir seal properties and the condition of supercritical CO_2 and displaced brine through understanding the integrated geochemical/geomechanical processes that result from CO_2 injection; and ii) develop predictive models of site integrity over extended periods of time.

- The technical approach in the area of geological storage involves: i) assessment of the geology of Japan and time scales involved to feed back and define basic research requirements; ii) Constitutive models for chemistry and fracture of porous rock will be developed to capture the coupling between CO_2 reaction, transport, and mechanics in order to inform models of site integrity with predictive capabilities.

- Interactions between I^2CNER and the Midwest Geological Sequestration Consortium are ongoing and communication for future collaborations between some researchers at Research Institute for Innovative Technology for the Earth (RITE), Kyoto University and National Institute of Advanced Industrial Science and Technology (AIST) has been established. Dr. K. Kitamura of RITE has been offered a position of an Assistant Professor and will join I^2CNER this summer.

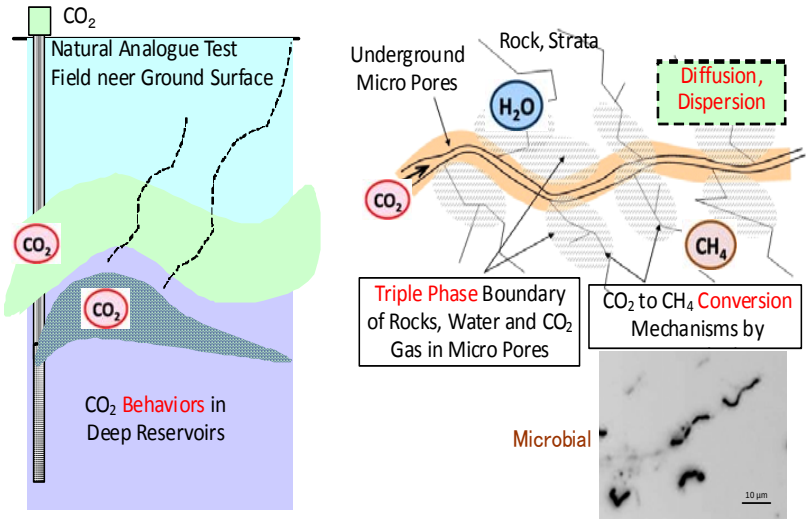

Fig. 8a. CO_2 geological storage

9. CO_2 ocean sequestration: informing the public on ocean sequestration (Lead PI: Prof. Tetsuo Yanagi)

- Ocean absorption helps to naturally remove CO_2 from the atmosphere. However, due to the ever increasing rate of CO_2 emission into the atmosphere, we are at a stage that the rate of CO_2 emission exceeds the removal rate. In order to meet CO_2 emission reduction targets, CO_2 ocean sequestration is expected to play an important role. However, there are still many unresolved issues that need to be addressed, e.g., the stability of the ocean/CO_2 system in the presence of meso-scale eddies and the upwelling and environmental and biological impact of acidification of the oceans.

- This project area will evaluate the stability of CO_2 and the impact on the oceanic and global environments. Further we will analyze and determine the risks of CO_2 injection and monitoring systems in order to increase our understanding and inform the public on the advantages or disadvantages of ocean sequestration.

- In particular, we will investigate the behavior of CO_2 in the presence of meso-scale eddies and the upwelling and environmental and biological impact of acidification of the ocean by using the tools of fluid mechanics and oceanic science. For the analysis, the ocean current model developed by Prof. Yanagi and co-workers at Kyushu University will be used in conjunction with a carbon circulation model that accounts for the carbon flux between the atmosphere and the ocean, the change in oceanic pH, and bio-pumping of CO_2.

- Lastly an outcome of this project-area's research activities will be the construction of monitoring systems on the basis of the virtual moorings systems developed at Kyushu University.

References

[1] T. Yanagi, "Great water temperature changes of 1.5^{o}C per decade in Tokyo Bay, Japan - its causes and consequences", *J. Disaster Research*, **3**, 113-118 (2008).

[2] G. Onitsuka, I. Uno, T. Yanagi and J. H. Yoon, "Modeling the effects of atmospheric nitrogen input on biological production in the Japan Sea", *J. Oceanography.*, **65**, 433-438 (2009).

9. Carbon Capture and Storage (Combined geological and sub-sea bed sequestration division

A) Technical Accomplishments and Progress

- We started our work on the development of the pipe system for the injection of CO_2 in a sea-bed hole of depth of more than 3000m.

- We started simulations of the CO_2 flux through the CO_2 hydrate between the liquid CO_2 and sea water by accounting for the effect of meso-scale eddies through two-dimensional numerical model;

- We started work on the development of a monitoring system of CO_2 partial pressure and pH through using underwater remotely operated vehicles (ROV) (Fig. 9b on next page).

- We started work on geo-sequestration (see Fig. 9c on next page) by measuring compressional and shear wave velocities of core samples under in-situ conditions of deep reservoir (10-15 MPa and 40 C).

B) Collaborations

- Sub-sea bed CCS and Geological CCS teams have been interacting on setting future research directions.

- We are in contact and exchange views with many experts of Geological CCS in Kyoto University, AIST and RITE.

- Collaboration on rock physics studies and CCS with the Midwest geological Sequestration Consortium (MGSC).

- Collaboration with many researchers in the Geo-reactor sequestration project of Japan.

C) Future Work/Near-Term Issues

- We will estimate distribution patterns of geo-sequestered CO_2 by measuring electrical impedance changes. These data from geophysical monitoring will provide important information to assess CO_2 behavior in deep reservoirs.

[3] G. Onitsuka, T. Yanagi and J. H. Yoon, “A numerical study on nutrient sources in the surface layer of the Japan Sea using a coupled physical-ecosystem model”, *J. Geograph. Research*, **112**, C05042 (2007).

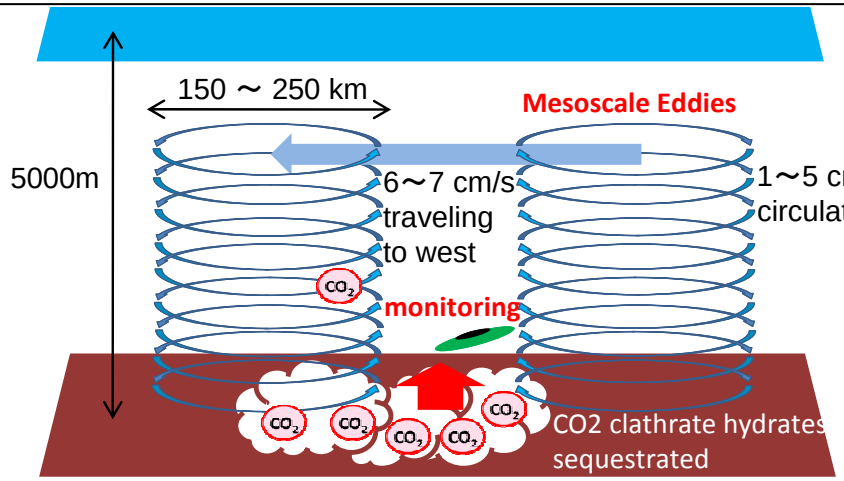

Fig. 9a. CO_2 ocean sequestration

- We will carry out simulations of CO_2 behavior by expanding the present so called TOUGH2 model (a 2-D model) to build a more realistic 3-D model based on the data we will obtain from geophysical monitoring.

- Design the most suitable pipe system for the injection of CO_2 to a deep sea-hole.

- Develop the numerical model for the simulation of CO_2 flux through the CO_2 hydrate.

- Develop the monitoring system of CO_2 pressure and pH in the deep sea water.

- Sub-sea bed CO_2 sequestration project
  - Development of monitoring system of CO_2 behavior in sub-ocean bottom reservoir by using geodesic methods (gravity, deformation).
  - Monitoring of leakage of CO_2 from reservoir to ocean floor by physical, chemical and biological methods.

D) Future Work/Long-Term Issues

- Specialization of CCS project to Kyushu area.

- Kyushu is a well-known geothermal field of Japan. It is the best site for a Geo-reactor project. The concept of Geo-reactor involves utilizing geothermal heat to enhance the chemical reactions that increase mineral trapped CO_2 as calcite.

E) Conclusions

- We have begun work on both ocean and geological sequestration research and the development of the required systems for experimental and simulation analyses.

F) Publications

[1] Kitamura, K., Xue, Z. and Nishizawa, O. (2010) Simultaneous measurement of Vp and Vs of Tako sandstone, Proceedings of the 123rd SEGJ Conference, The Society of Exploration Geophysicist of Japan, 229-230 (in Japanese with English abstract).

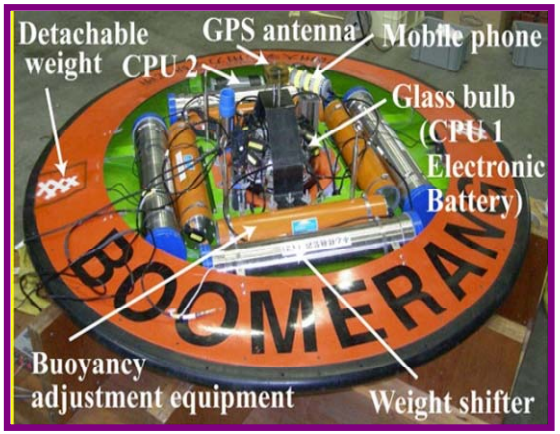

Fig. 9b. Underwater vehicle for CO_2 monitoring in the deep ocean

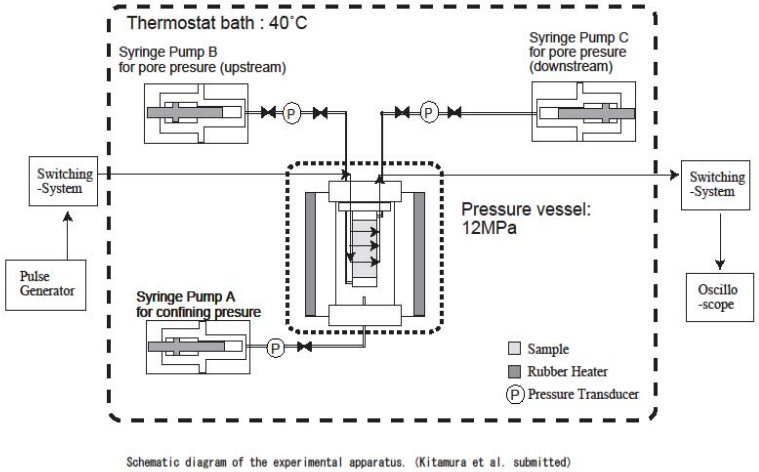

Fig. 9c. Schematic diagram of the experimental apparatus for for geological CCS.

4. Management

<Initial plan>

1) Composition of administrative staff

- In order to efficiently respond to the requests from the Institute Director and researchers, and also to provide an ideal research environment, there will be an Administrative Department (Management Department) specially set up for this Institute. The department will consist of 1) general affairs and human recourses section; 2) accounting and contracting group; 3) research support and international affairs; and 4) public relations.

- The administrative officers in the Management Department of the Institute will get support from other administrative officers in the Kyushu University who have competent English language skills. Personnel outside the Kyushu University with competent technical knowledge, experience, and English language skills will also be employed in the management department. The official language in the Management Department will be English.

- Further, it is vital that the personnel in the administration office has some technical knowledge in its support role for the international activities of the Institute, such as the preparation of grant application documents, presentation of research findings, project designs and agreement for collaborative research work, and application for and management of patents. For such an efficient and competent research support system, we are to appoint postdoctoral fellows as research administrators (RAs). These fellows will help in the formation of a research environment such that researchers in the Institute will be able to concentrate on their research activities. This will also help establish the RA concept, which is fairly uncommon in Japan, as a new attractive career path for postdoctoral fellows.

- The Institute will offer support to international researchers for their research activities as well as other services both within and outside the University, in close cooperation with the existing International Student and Researcher Support Center of the Kyushu University. The Institute will offer full-time support including visa applications, accommodations, airport pickups, administrative procedures at the University, alien registrations, paper work and processes required for

<Results/progress/alternations from initial plan>

1) Composition of administrative staff

- The Administrative Office is composed of four groups; 1) General Affairs and Human Resources; 2) Accounting and Contracting; 3) Research Support and International Affairs; and 4) Public Relations. The 18 staff members (as of April 1, 2011) have established support systems under the supervision of both Administrative Director and Associate Administrative Director.

- Kyushu University staff members have technical knowledge of general affairs and human resources and those in the accounting and budget section are also highly experienced. A member in the research support and international affairs group is a PhD degree holder which enables him to better communicate with I^2CNER researchers.

- New staff members have a good command of English, which allows for smooth English communication between the Institute Director and others foreign PIs and researchers, especially in daily correspondence.

- The Administrative Office is in close communication with the existing International Student and Researchers Support Center at Kyushu University. At I^2CNER, we offer full-time support to international researchers in the areas of invitation procedures including visa application processing.

banking, school attendance, etc., and the purchasing of essential items such as mobile phones, and related payments. • Below are the main tasks allocated to each department: o General Affairs and Human Resources (8 officers) ▪ General management of the Institute, preparation of meetings, management of the Institute policy, human resource management such as employment, salary and business trips, safety management, and support services for international researchers. o Accounting and Contracting (3 officers) ▪ Compiling of budget, resourcing of Institute facilities, equipment and other goods, payments for goods, salary, business trips etc., and general accounting. o Research Support and International Affairs (5 officers) ▪ Preparation of grant application documents, presentation of research findings, project designs and agreement for collaborative research work, application for and management of patents (in conjunction with the office for Intellectual Property), etc. o Public Relations (3 officers) ▪ Public relations advertisement, management of home page, support of international visitors, organization of international conferences, etc.	
2) Decision-making system • It is vital to provide the Institute Director with sufficient authority to work toward restructuring of the university system and management based on his multi-year experience and interactions within the US academic community. Examples of areas in which such authority is needed are: researcher recruitment, joint-research with top-class research institutes, rigorous evaluation processes of research findings and plans, research expenditures, and personnel salary compensation.	2) Decision-making system • The Director's decision-making authority has been established by preparing <u>relative regulations and rules</u> to apply a top-down approach, in consultation with the science steering committee that consists of the Institute Director, Vice Director, Associate Director and division leaders: o Faculty employment based upon "Regulation on Faculty Recruiting Committee of Carbon Neutral Energy Research of Kyushu University"

• The Institute will be established as an organization under the direct management of the president of the Kyushu University. The system will be set up for the Institute Director to be able to make decisions on research plans, research framework, and budget implementation in consultation with the Internal Science Committee that consists of the Institute Director and program area leaders (science advisors) and any other additional members that the Director may invite as deemed appropriate. • The Director will be assisted by two Science Associate Directors, one in Japan and one in the US. An External Advisory Committee composed of national and international figures in the field will review the Institute annually and provide input and recommendations.	o Science Steering Committee (formerly Steering Committee) o External Advisory Committee o Program Review Committee o Compensation considerations based upon "Special Regulation on Employment of International Institute for Carbon-Neutral Energy Research of Kyushu University" • The Director is assisted by Vice Director; Yukitaka Murakami and Associate Director Kazunari Sasaki; Dr. Ian Robertson serves as Chief Science Advisor. An External Advisory Committee comprised of national and international researchers in related fields provide recommendations.
3) Allocation of authority between center director and host institution • The appointment/dismissal of the Institute Director and authorization for employment of the Principal Investigators has to be authorized by the head of the host institution, the president of Kyushu University. The Institute Director has the authority for the other administrative operations such as the human resource management and the implementation of budget.	3) Allocation of authority between center director and host institution • Institute regulations and rules give most of the authority for the administrative operations to the Institute director and the appointment/dismissal of the Institute director is authorized by the President of the host institution.

5. Researchers and center staffs

i) “Core” to be established within host institution

Principal investigators

	At beginning	Planned for end of FY 2010	Final goal (Date: month, year)	Results at end of FY 2010	Results at end of April 2011
Researchers from within host institution	16	16	16 (March, 2011)	17	18
Foreign researchers invited from abroad	11	11	11 (March, 2011)	10	11
Researchers invited from other Japanese institutions	3	3	3 (March, 2011)	2	1
Total principal investigators	30	30	30 (March, 2011)	29	30

All members

	At beginning	Planned for end of FY 2010	Final goal (Date: month, year)	Results at end of FY 2010	Results at end of April 2011
Researchers <Number of foreign researchers among them and their percentage> [Number of female researchers among them and their percentage]	71 <21, 30%>	92 <36, 39%>	130 <54, 42%> (March, 2014)	61 <17, 28%> [2, 3%]	73 <21, 29%> [3, 4%]
Principal investigators <Number of foreign researchers among them and their percentage> [Number of female researchers among them and their percentage]	30 <11, 37%>	30 <11, 37%>	30 <11, 37%> (March, 2011)	29 <10, 34%> [1, 3%]	30 <11, 37%> [1, 3%]
Other researchers <Number of foreign researchers among them and their percentage> [Number of female researchers among them and their percentage]	41 <10, 24%>	62 <25, 40%>	100 <43, 43%> (March, 2014)	32 <7, 22%> [1, 3%]	43 <10, 23%> [2, 5%]
Research support staffs	32	37	51 (March, 2013)	28	30
Administrative staffs	23	23	23 (March, 2011)	16	18
Total	126	152	204	105	121

ii) Satellites <Initial plan> <u>Institution (1)</u> • Role o University of Illinois at Urbana-Champaign, USA: The University of Illinois at Urbana-Champaign is a top-world institution in the field of hydrogen energy and materials research in the USA. In addition to conducting Institute related research, the satellite office will serve as the base for identifying and engaging key research programs and faculty at Universities and Institutions nationally and internationally. • Personnel composition and structure o As Director of the Institute, Professor Sofronis will serve as the Director of the satellite institute. In this latter capacity he will report directly to the Dean of the College of Engineering at the University of Illinois. Appropriate agreements between Kyushu University and the University of Illinois, other than an exchange of students which is already in place, will be negotiated if the Institute is funded. Both parties have expressed interest and support for establishing this satellite institute at the University of Illinois. • Collaborative framework	<Results/progress/alternations from initial plan> <u>Institution (1)</u> Plans on the role of the Satellite institute remain the same and are as described in the left column.
iii) Partner institutions <Initial plan> We envision engaging in collaborative research with distinguished scientists from internationally recognized institutions. This includes site visits to facilitate research by leveraging research capabilities. Key institutions are the following: • Tohoku University (JPN) • Atmosphere and Ocean Research Institute of the University of Tokyo (JPN) • National Institute of Advanced Industrial Science and Technology (JPN) • University of California, Berkeley (USA) • Massachusetts Institute of Technology (USA) • Sandia National Laboratories (USA)	<Results/progress/alternations from initial plan> 1. TOHOKU UNIVERSITY (JPN) • Although joint research with the Hydrogen Storage Material Division was initially planned, it was cancelled due to Prof. Okada's resignation from Tohoku University. 2. ATMOSPHERE & OCEAN RESEARCH INSTITUTE, UNIVERSITY OF TOKYO (JPN) • Role o Joint research with the CO_2 Capture and Storage division

- University of Alberta (CAN)
- Carbon Management Canada (CAN)
- Imperial College of London (UK)
- Swiss Federal Institute of Technology Zurich (SUI)
- Tsinghua University (China)
- Dalian Institute of Chemical Physics, Chinese Academy of Sciences (China)

- Personnel Composition and Structure
  - Dr. Yoshihisa Shirayama
- Collaboration Framework
  - Promotion of joint research with the CO_2 capture and Storage division

3. NATIONAL INSTITUTE OF ADVANCED INDUSTRIAL SCIENCE & TECHNOLOGY (JPN)
   - Role
     - Joint research with the Hydrogen Structural Material and the Thermophysical Properties divisions
   - Personnel Composition and Structure
     - Prof. Matsuoka, Prof. Sugimura, and Prof. Takata
   - Collaboration Framework
     - Promotion of joint research with the Hydrogen Structural Materials and the Thermophysical Properties divisions

4. UNIVERSITY OF CALIFORNIA, BERKELEY (USA)
   - Role
     - PI in the Hydrogen Structural Materials division
   - Personnel Composition and Structure
     - Prof. Robert Ritchie (Head of the Materials Science Department)
   - Collaboration Framework
     - Collaborative research on hydrogen-induced fatigue of materials

5. MASSACHUSETTS INSTITUTE OF TECHNOLOGY (USA)
   - Role
     - Dispatch of PI to the Fuel Cell division
   - Personnel Composition and Structure
     - Prof. Harry Tuller
   - Collaboration Framework
     - Joint research with the Fuel Cell division

6. SANDIA NATIONAL LABORATORIES (USA)
   - Role
     - Lead PI in the Hydrogen Structural Material division
   - Personnel Composition and Structure
     - Dr. Brian Somerday (senior research scientist in the hydrogen/materials group in the Sandia National Laboratories)
   - Collaboration Framework
     - Direct and guide research in the Hydrogen Structural Material division
     - The collaborative research agreement is currently being negotiated.

7. IMPERIAL COLLEGE OF LONDON (UK)
   - Role
     - PI in the Hydrogen Production division
   - Personnel Composition and Structure
     - Prof. John Kilner
   - Collaboration Framework
     - Promotion of joint research with the Hydrogen Production

division

8. SWISS FEDERAL INSTITUTE OF TECHNOLOGY, ZURICH (ETH)
   - Role
     - PI in the Fuel Cell division
   - Personnel Composition and Structure
     - Prof. Ludwig Gauckler
   - Collaboration Framework
     - Joint research

9. TSINGHUA UNIVERSITY (CHINA)
   - Role
     - PI in the Thermophysical Properties division
   - Personnel Composition and Structure
     - Prof. Xing Zhang
   - Collaboration Framework
     - Joint research

10. DALIAN INSTITUTE OF CHEMICAL PHYSICS, CHINESE ACADEMY OF SCIENCES (CHINA)
   - Role
     - PI in the Hydrogen Storage Materials division
   - Personnel Composition and Structure
     - Prof. Ping Chen
   - Collaboration Framework
     - Joint research

6. Summary of center's research environment

<Initial plan>

1) Environment in which researchers can devote themselves to their research

- In order for the Institute researchers to focus exclusively on their research, we will employ an efficient and competent administrative department to execute the all required administrative work needed for a world-class Institute. This will involve planning of the Institute's budget, purchasing of equipment and goods, procurement procedures, business trips procedures and preparation support, grant application preparation and submission processes, support for presentations, assistance for joint research projects and launching of new initiatives, handling of contracts, patent applications, publications processes, and facilitating visitors. We are determined to build a strong support infrastructure so that the Institute can pursue its mission with no hindrances whatsoever.

- In addition, we will constantly work toward improving the skills of the technical staff employed in the support of research operations and maintenance of facilities and equipment.

- Furthermore, we plan to decrease the teaching academic load for the Institute researchers and set up a system rewards for teaching substitutes.

2) Startup research funding

- In order to facilitate Institute researchers and invited researchers from external institutions to focus on their research—with no need for immediate engagement on grant application preparation for research funding—we will provide the necessary research facilities and equipment as possible so that the researchers can start and/or continue their research. We are also planning to set a system such that the Institute Director can decide and provide initial research funding to the researchers as deemed appropriate.

3) Postdoctoral positions through open international solicitations

- To recruit well qualified post-doctoral research associates,

<Results/progress/alternations from initial plan>

1) Environment in which researchers can devote themselves to their research

- The Administrative Office was established to allow I^2CNER researchers to focus on their research. Currently, there are 4 groups in the office who report to the Administrative Director and Associate Administrative Director. The General Affairs and Human Resources group has 8 members; the Research Support and International Affairs group has 2 members, one possess a doctoral degree and the technical background necessary to successfully administer this office; the Public Relations and Accounting and Contracting groups each have 3 members.

- When it was founded in December 2010, the Institute had 29 technical support staff members. We are studying our structure and exploring whether further expansion in personnel number is needed.

2) Startup research funding

- The Hydrogen Storage Materials division is currently receiving budgetary priority to build its personnel base, because a PI from the outside of Kyushu University has been newly assigned to this division.

3) Postdoctoral positions through open international solicitations

- From October to December 2010, the first open international

advertisements for the positions will be placed on the web site of the Kyushu University, the Kyushu University Offices overseas in Great Britain, California, Washington D.C., Munich, Korea, Beijing, etc., at the Satellite Institute's web site in Illinois, and major international academic magazines and related magazines in Japan. The recruitment process will be supervised by the Institute Director in consultation with the Internal Advisory Committee. The corresponding recruitment practices at the University of Illinois will be used on all Institute research personnel hiring. • The Kyushu University has already carried out a recruitment campaign for its projects on "Young Researcher's Independent Research Environment Maintenance and Promotion Program" and "Next Generation Research Training Program." • The number of recruits will be 21 researchers and 5 research assistants in 2010; 23 researchers and 9 research assistants in 2011; 9 researchers and 5 research assistants in 2012; and 6 researchers in 2013, with the objective being to reach a net number of 204 researchers by the end of 2013. • We also plan to recruit an international research assistant or a research administrator (RA) for the Institute's administration management department.	recruiting call was conducted. Advertisements were published in international academic magazines such as Nature World, and Science and yielded 61 faculty applicants and 75 postdoctoral applicants. The Faculty Recruiting Committee reviewed the applications and identified candidates for an on-site interview. Finally, 8 faculty members and 3 post-doctoral research associates received offer letters. One post-doctoral research associate declined due to being offered a position in a research theme other than the one applied for; another postdoctoral research associate declined due to his expectation that he qualified for an assistant professorship which, was contrary to the assessment of the Institute's FRC. • The decision was made to not simply fill positions, but to carefully choose amongst those faculty candidates who hold promise in building an internationally visible research program. • I2CNER's second international open recruiting call will be in March 2011. Additional researchers will be sought through the Faculty Excellence Program through which the Director can administer the hiring process of exceptionally qualified candidates without going through the standard recruiting process.
4) Administrative personnel who can facilitate the use of English in the work process • We will adopt English as the primary language for work-related communications. • In order to foster an English speaking environment in the Institute, we will employ in the administration department personnel from the Kyushu University who are fluent in English. • We also plan periodically to provide training opportunities for the administration work force. • The administration department will oversee the translation from	4) Administrative personnel who can facilitate the use of English in the work process • Newly hired administrative staff members have an excellent command of English. Drawing on this experience, the Administrative Office has been organized in such a way that will enable the development of a research environment where researchers will be able to concentrate on research activities. We have introduced English versions of various applications or other forms, and been developing a system that enables international researchers to engage and interact with I^2CNER with no difficulties. • In cooperation with the International Affairs Division at Kyushu University English versions of various applications and other forms

English of the expenditure supporting documents for business trips, purchasing goods, salary compensation, and daily life activities in order to make the daily life of non-Japanese people at the Institute as easy as possible.	have been introduced. Additional training and workshop opportunities are offered to assist in the transition international researchers experience while conducting research at I^2CNER.
5) Rigorous system for evaluating research and system of merit-based compensation • As stated in the document delineating the Institute Director's vision all aspects of the Institute shall be evaluated on an annual basis, or if deemed more frequently by the Director, by the External Advisory Committee. The Committee will review all aspects of the Institute, including the leadership and management, the research progress being made in each activity, and the plans for new initiatives. The Committee will provide the Director with a written report on their findings and recommendations. • Based on the recommendations of the External Advisory Committee and input from the Internal Advisor Committee, the Institute Director will plan the allocation of research funds and salary adjustments to cultivate and foster a productive research environment by rewarding success. • In the Kyushu University, there is already a system in place that sets salary ranges based on the individual researcher's contributions to the interests of the University. As the Institute needs and activities begin to arise, the University's salary system will be re-examined.	5) Rigorous system for evaluating research and system of merit-based compensation • The Institute established a new salary system (Special Regulation on Employment of the International Institute for Carbon-Neutral Energy Research of Kyushu University) which deviates from the established salary ranges. The Institute also provides an "institute allowance" for existing employees. Individual faculty and researcher salaries are determined based on individual accomplishments and contributions to the interests of the Institute and also on input provided by the Program Review Meeting and External Advisory Committee.
6) Equipment and facilities, including laboratory space, appropriate to a top world-level research center • The Kyushu University is relocating its campus to Ito on the western part of the City of Fukuoka. This relocation decision was made to serve our new strategic goal for an open university at the forefront of cutting edge research in an educational Institution. • Currently, the Ito Campus houses the International Research Center for Hydrogen Energy, the Research Center for Hydrogen Industrial Use and Storage (HYDROGENIUS), and the Inamori Frontier Research	6) Equipment and facilities, including laboratory space, appropriate to a top world-level research center • In order to develop a research environment befitting a top world-level research institute, a new research facility is being designed and will be completed in autumn 2012. • Shared, common-use laboratories (5) have been secured and are shared by researchers from various fields. • Video-conferencing equipment is utilized for meetings and seminars

Center. The Ito Campus is indeed a unique place with the largest Hydrogen Research Institute in the world for hydrogen related cutting edge research and facilities.

- In order to continue developing its research environment and visibility toward becoming a world renowned Institution, the Kyushu University, under an initiative by the president, plans to build a research facility with cutting edge equipment specifically for this WPI program in the Ito Campus. While building the facility, we shall still be able to provide the accommodations or laboratories for the WPI Institute's national and international researchers.

- We will ensure sharing of open space and laboratories amongst researchers from various fields to encourage open meetings, discussion, and debate.

- We also plan to promote exchange and discussion among Kyushu University, the satellite institute, and the collaborating institutes through the TV teleconference system.

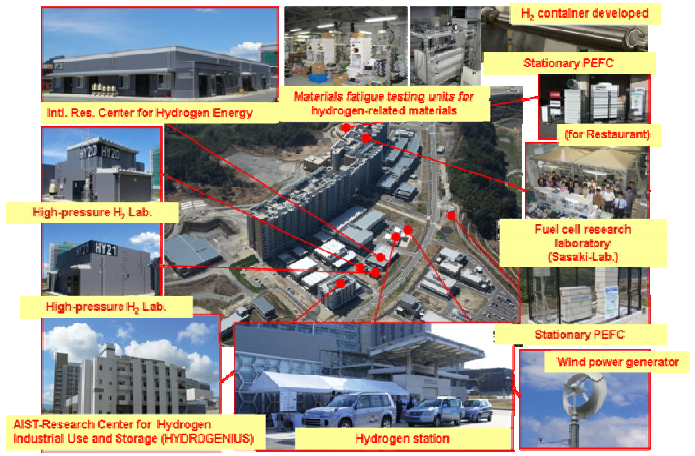

Fig. Overview of the Hydrogen Energy Research Facility in the ITO-Campus of Kyushu University, with ca. 100 research staffs and 100 students in >5000m^2 laboratory area.

at Kyushu University, the satellite institute, and other collaborating institutions.

- New equipment has been introduced in laboratories on campus to update.

7) International research conferences or symposiums held regularly to bring world's leading researchers together

- We host the "International Hydrogen Energy Development Forum" once a year at Kyushu University in collaboration with the city of Fukuoka for the last four years. At this annual hydrogen forum, the top-level researchers from overseas in their fields of expertise present their work and actively interact with not only local but global scientific and industrial communities.

- By capitalizing on the experiences we gained from organizing this Global Forum, we are confident that we will easily organize and host international conferences and specialized workshops with active participation from world famous researchers and institutions on a regular basis and on all aspects of the research activities of the Institute. Examples of conference and symposia themes are hydrogen energy and fuel cells, hydrogen production by photocatalytic water splitting, sustainable material conversion systems, innovative CO_2 capture, CO_2 geological storage and ocean sequestration, and system economic analysis and evaluation.

- The conference and workshop presentations by fostering information exchange, vigorous debate, and exploration of new initiatives and collaborations will assist the Institute in its mission to contribute to the society' efforts on countermeasures for global warming.

7) International research conferences or symposiums held regularly to bring world's leading researchers together

a) International Symposia

- I^2CNER Opening Ceremony
  - Date: December 9, 2010
  - Attendance: 128 national/international attendees
  - Description: Director Sofronis presented the newly-established Institute's future perspective, research plans, and divisions.
    - The relevant YouTube video has been viewed over 500 times to date.

- I^2CNER Kick-off Symposium
  - Date: February 1, 2011
  - Attendance: 160 national/international attendees
  - Description: I^2CNER's first international symposium with 8 invited lecturers from overseas including I^2CNER's foreign PIs. The Institute plans to host an annual international symposium of similar quality and scale.

- HYDROGENIUS & I^2CNER Workshop
  - Date: February 3, 2011
  - Attendance: 266 national/international attendees
  - Description: Held in conjunction with the 2011 International Hydrogen Energy Development Forum held on February 2, 2011 in Fukuoka Japan. Four symposia with a focus on individual research fields were held at Kyushu University, Ito Campus:
    i. Hydrogen Fatigue and Fracture/ Hydrogen Polymers
    ii. Hydrogen Tribology
    iii. Hydrogen Thermophysical Properties
    iv. Fuel cells

b) International Seminars

The I^2CNER Seminar Series was launched in March 2010 with the intention of not only becoming a landmark of the Institute, but a platform in which to foster engagement between I^2CNER, Kyushu University, Japan, and the rest of the world, enhancing I^2CNER's global visibility. Seminars are being held regularly.

- 1st I^2CNER Seminar Series
  - Speaker: Dr. Toyoki Kunitake

	o Date: March 11, 2011 o Title: “Why is nanomembrane so interesting?” o Attendance: 142 participants • 2nd I^2CNER Seminar Series o Speaker: Dr. Darrell Socie o Date: March 18, 2011 o Title: “Multiaxial Deformation and Fatigue Under Discriminating Strain Paths” o Attendance: 97 participants • I^2CNER PIs have also assumed leadership roles in organizing international conferences: o International Conference on Hydrogen/Materials Compatibility at the Grant Teton National Park, September 2012. This conference series is the main event in the area of hydrogen/materials interactions worldwide and takes place every four years.
8) Other measures, if any • We have four university facilities to accommodate invited national and international researchers. We have also arranged for private apartments designated for university use. We will provide comfortable and fully-furnished accommodations for the invited researchers so that they will be able to concentrate on their research activities.	8) Other measures, if any • Currently, we have introduced university facilities to accommodate for invited national and international researchers, or have made arrangements for fully-furnished private apartments with easy-access to Kyushu University.

7. Criteria and methods used to evaluate center's global standing

<Initial plan>

- As stated in the Director's vision statement, indicators and metrics for evaluating the Institute's standing and visibility are: i) the quality and impact of the Journal publications, ii) the extent of joint publications as demonstration of the enabling value of the Institute, iii) invited keynote and plenary lectures; iv) symposia organization in international conferences by Institute researchers; v) trend setting workshops that attract participation of national agencies such as MEXT, JSPS, US NSF, US DOE, European Commission; vi) organization of international conferences and participation of the Institute's researchers in international conferences; vii) invitations to the Institute's researchers for participation in government panels and national laboratory efforts; viii) patents and technology accomplishments. Lastly, the numbers of visitors to the Institute, especially, the visitors from overseas is a key indicator of the Institute's visibility.

- The Director in consultation with the Internal and External Advisory Committees will coordinate the actions to be taken for the Institute to achieve and maintain excellence. This includes prompting the principal investigators to enhance their visibility and hence the Institute's visibility by taking action on all Institute standing indicators listed above. In particular, international awards for the Institute researchers and the number of article citations the Institute's work receives will be used as a metric to evaluate overall standing and visibility. In this regard, a particularly revealing index of the Institute's quality will be considered the degree of citation of the work of young faculty and researchers—it is well known that it usually takes some time for young faculty to get their work recognized. Lastly, funding for program areas will be commensurate to the individual area's level of participation in the Institute's activities to meet its goals and visibility as a world premier institution.

- The primary goal by the time of the interim evaluation (5 years from the Institute inception) is that the Institute has established its reputation as an international center of excellence for fundamental research toward meeting its mission for a carbon-neutral energy

<Current assessment>

- There is has been no deviation from the initial criteria and methods for self-evaluation.

- Using the indicators on the left, we assessed our activities from December 2010 to March 2011 as noted below:

1) Quality & Impact of Journal Publications: 26 papers published

- H. Kitagishi, M. Tamaki, T. Ueda, S. Hirota, T. Ohta, Y. Naruta, and K. Kano, "Formation of ROO–Ferric Porphyrin Complexes (R = alkyl and H) in a Hydrophobic Cage Formed in Aqueous Solution." *Journal of American Chemical Societ*y, 2010, 132, 16730-16732.

- S. Ida, K. Yamada, T. Matsunga, H. Hagiwara, Y. Matsumoto, and T. Ishihara, "Preparation of p-Type CaFe2O4 Photocathodes for Producing Hydrogen from Water," *J. Am. Chem. Soc.*, 2010, 132 (49), pp. 17343-17345.

- S. Matsuoka, H. Tanaka, N. Homma, Y. Murakami, "Influence of hydrogen and frequency on fatigue crack growth behavior of Cr-Mo steel," *Int. J. Fracture* (2011) 168:101–112.

- K. Edalati, A. Yamamoto, Z. Horita and T. Ishihara, "High-Pressure Torsion of Pure Magnesium: Evolution of Mechanical Properties, Microstructures and Hydrogen Storage Capacity with Equivalent Strain," *Scripta Materialia*, 64, 880-883, (2011).

- El-Sayed R. Negeed, S. Hidaka, M. Kohno, Y. Takata, "Experimental and Analytical Investigation of Liquid Sheet Breakup Characteristics," *International Journal of Heat and Fluid Flow*," **(32)** 1, pp. 95-106, 2011.

- K. Fukuda, M. Hashimoto, J. Sugimura, "Friction and Wear of Ferrous Materials in a Hydrogen Gas Environment," *Tribology Online*, **(6)** 2, pp.142-147.

- T. Koga, Y. Matsukuma, G. Inoue, M. Minemoto, "Study on CO_2 Recovery Systems by Pressure Swing Adsorption Under High

society. Indicators for meeting this goal shall be well recognized breakthroughs in fundamental research (e.g., discovery of how hydrogen promotes fatigue of materials or discovery of new catalysts for material transformation through asymmetric oxidation). Such breakthroughs on fundamental science will allow the Institute to expand its second term mission objectives (6th to 10th year) to include directions addressing technology development.

- The 10 year overarching goal is the completion of fundamental research for technology development. By way of example, specific goals include design of new alloy for hydrogen resistant materials, new alloys for on-board hydrogen storage, technologically viable production of hydrogen through artificial photosynthesis, new low-cost catalysts for fuel cells, and demonstration projects for ocean- and geo-sequestration of carbon.

Pressure Conditions, *J. of Novel Carbon Resource Science*, 3, 6-10 (2011).

2) Joint Publications as Demonstration of the Enabling Value of I^2CNER

- Through international cooperative research with institutes such as MEXT, JSPS, US NSF, US DOE, and the European Commission, 11 joint publications were published in academic journals.
  - K. Edalati, A. Yamamoto, Z. Horita and T. Ishihara, "High-Pressure Torsion of Pure Magnesium: Evolution of Mechanical Properties, Microstructures and Hydrogen Storage Capacity with Equivalent Strain, "*Scripta Materialia*, 64, 880-883, (2011).
  - H. Nobukuni, H. Uno, Y. Shimazaki, T. Kamimura, Y. Naruta, and F. Tani," Both 'End-On' and 'Side-On' Orientations of C70 Included by Cyclic Nickel Porphyrin Dimer in Crystalline State," *Chem. Commun*. (Submitted)
  - H. J. Kim, J. Nakamura, H. Y. Shao, Y. Nakamura, E. Akiba, K. Chapman, P. Chupas, and T. Proffen, "Local structure evolution of mechanically alloyed Mg50Co50 from the atomic pair distribution function analysis", *J. Chem. Phys. C.*, Publication Date (Web): March 28, 2011 (Article), DOI: 10.1021/jp111711c.
  - M. J. Assael, J. A. M. Assael, M. L. Huber, A. Perkins, and Y. Takata, "Correlation of the Thermal Conductivity of Normal and Parahydrogen over a Wide Range of Temperatures and Pressures," *J. of Physical and Chemical Reference Data*. (Submitted)

3) Invited Keynote & Plenary Lectures: 12 Lectures

- Prof. E. Akiba et al., "Mg-TM (TM = Ti and Co) alloys: Preparation, hydrogenation, and characterization," (PACIFICHEM-2010), Honolulu, USA, Dec. 17, 2010.
- Prof. E. Akiba, "Synthesis and characterization of novel metal hydrides," IEA Hydrogen Implementing Agreement Task 22,

Fremantle, Australia Jan. 20, 2011.

- Prof. Yoshinori Naruta, “Activation and Catalytic Reduction of Dioxygen: Lessons from Heme Enzyme Chemical Models”, 2010 International Chemical Congress of Pacific Basin Societies (PACIFICHEM-2010), Honolulu, USA, Dec. 19, 2010.

- Prof. Saburo Matsuoka, “Global Strategies for Realization of a Hydrogen Energy Society”, International Hydrogen Energy, Fukuoka, Japan, Feb. 2, 2011.

4) Symposia Organization in International Conferences by I^2CNER Researchers

- Four symposia were/are to be held:
  - Organizer of S3: 8th International Symposium on Solid Oxide Fuel Cells, 35th International Conference and Expo on Advanced Ceramics and Composites, January 24-28, 2011, American Ceramic Society
  - 2011 HYDROGENIUS Tribology Symposium, February 3, 2011
  - Scientific Committee Members of Symposium X, Fuel Cells Energy Conversion, E-MRS, Bilateral Energy Conference, May 9-13, Nice, France, E-MRS
  - The International Symposium on Metal-Hydrogen Systems to be held in October 2012. (Prof. E. Akiba: Vice Chair of the Organizing Committee)

5) Trend-setting Workshops that Attract the Participation of National Agencies such as MEXT, JSPS, US NSF, US DOE, and the European Commission

- Two workshops were held.
  - Prof. E. Akiba, Hydrogen Storage Material Forum 2011, Tokyo, Jan. 20, 2011.

- Prof. Yoshinori Naruta, 1st International Conference on MEXT Project of Integrated Research on Chemical Synthesis, Jan. 24-25, 2011.

- Director Sofronis was invited by the US DOE and NSF to present the Illinois/Japan project on March 7-8 2011. During his visit to Washington D.C., he gave a webinar for DOE's Fuel Cell Technologies Program. Over 200 people attended his webinar titled "I^2CNER: An International Collaboration to Enable a Carbon-Neutral, Energy Economy." Director Sofronis made a similar presentation at NSF on March 8 and discussed details for joint proposal submissions between I^2CNER and US Institutions to NSF in the US and to JSPS in Japan.

6) Organization of International Conferences & Participation of I^2CNER Researchers in International Conferences.
   - I^2CNER researchers participated in a total of 21 conferences and one PI serves on the organizing committee of the 8th ASME/JSME Thermal Engineering Joint Conference in Honolulu, Hawaii on March 13-17, 2011.

7) Invitations Extended to I^2CNER researchers for Participation in Government Panels & National Laboratory Efforts
   - Saburo Matsuoka, Venus Orbiter "Akatsuki" Accident Investigation Committee (Dec. 17, 2010, Dec. 27, 2010)
   - Yoshinori Naruta, Member of Science Council of Japan (2000-present)
   - Kazunari, Sasaki, International advisor of the European Fuel Cell Forum
   - Director Sofronis continues to serve as a member in the Hydrogen Pipeline Working Group (PWG) of the US DOE.

8) Patents & Technology Accomplishments

- Two patents were obtained.
  - H. Takadama, S. Yamaguchi, T. Kokubo, T. Matsushita, y.

	Naruta, Manufacturing methods of electrode components, JP2011-046627. o Direct H_20_2 synthesis method from H_2 on Pd-Au/Brookite TiO_2 (Kokaitokkyo kouho) 9) Number of visitors to I^2CNER; especially those from overseas: o 20 international visitors traveled to I^2CNER. Among them, 19 were from abroad.

8. Securing competitive research funding

<Initial plan>	<Results/progress/alternations from initial plan>
A. Past Record • Research funding acquired by Japanese PIs in the past 5 years is as follows: o Fiscal 2005: 3.7 million dollars o Fiscal 2006: 21.7 million dollars o Fiscal 2007: 24.6 million dollars o Fiscal 2008: 29.2 million dollars o Fiscal 2009: 28.5 million dollars	A. Past Record • (Exchange rate: JPY/USD = 100) • The total amount of research funding acquired by Japanese principal investigators and researchers of I^2CNER in FY 2010 is 11.86 million US dollars.
B. Prospects after establishment of the center • The total amount of research funding acquired by main Japanese Principal Investigators in the past five years is over 21.5 million dollars per annum on average. The goal is to leverage the Institute for more funding to be secured in the coming years.	B. Prospects after establishment of the center

9. Other important measures taken to create a world premier international research center

<Initial plan>

- The activity of this research Institute will continue after the end of the grant period. The research in the Institute will be continued to be promoted since we expect that the scientific breakthroughs over the next 10 years will open new research pathways associated with the impact from technologies developed by the Institute's research contributions.

- The concept and project of this research Institute will be promoted as an example of the internationalization of research and education mission of the Kyushu University as described by the present-year mid-term goals and strategic plans of the Kyushu University. The research environment of this Institute in which world-leading researchers collaborate will remain and similar research activities which serve national and social needs will spread through the entire Kyushu University.

- This Institute is the first example of a foreign researcher to be selected as the Institute Director. It is expected that other units and organizations of the Kyushu University will benefit from the academic administration system of this Institute, which will be morphed according to the academic stature of the Institute Director. We expect that the Institute mode of operation will serve for the entire Kyushu University as a role model for recruiting researchers, establishing and promoting international collaborations with top-class research institutions, vigorous peer evaluation of research and faculty productivity, allocation of research resources and personnel financial compensation according to academic qualifications, scientific visibility, and established research record, etc.

<Results/progress/alternations from initial plan>

- I^2CNER has been positioned as a permanent institution just as other research institutes have been established in Kyushu University.

- The Institute Director has the authority to make decisions regarding international recruitment of researchers and allocation of research resources in response to research proposals (white papers) submitted by I^2CNER researchers.

10. Host institution's commitment

<Initial plan>

-Provision in host institution's mid-to-long-term plan

- Details of the mid-term goal and strategy plans for Kyushu University from 2010 are as follows:
  - Mid-term goal: "Kyushu University will undertake research activity as a global research and education center, and reflect the results to the social development. We will have our academic environment in a high-quality and attractive condition, where excellent researchers will gather and share/grow their knowledge. The university contributes to the development and creation of a new research area of integrated sciences."
  - Mid-term strategy plans for this goal are: "To promote the research and development activities on the subjects which are in national and social demands, and to attain creative and advanced research results by taking advantage of feature of a university."; "To undertake interdisciplinary and world leading researches in a wide range of subjects, from humanities and social sciences to natural sciences and engineering, for attainment of outstanding achievement."; and "To establish a research organization which can promptly, flexibly, and appropriately respond to the social needs of the times."
- The concept of Carbon-Neutral Energy Research Institute is in close line with this new mid-term goal and plans of Kyushu University. The Institute is organized directly under the president of Kyushu University, and the support to the Institute Director Prof. Sofronis from the University President and from the whole departments of Kyushu University will be guaranteed.

- Concrete Measures

(1) Competitive grants obtained by researchers participating in the project and in-kind contributions, etc.

- In order to acquire large competitive research grants, the Office for Strategic Research Planning and other related offices of Kyushu

<Results/progress/alternations from initial plan>

-Provision in host institution's mid-to-long-term plan

- No modification

-Concrete Measures

(1) Competitive grants obtained by researchers participating in the project and in-kind contributions, etc.

- I^2CNER's Administrative Director is also a professor of the Office for Strategic Research Planning and is actively engaging in gathering

University will proactively support researchers, such as on information gathering and strategic advice on grant applications. In addition, university funding will be effectively used to provide financial support to researchers. • For the provision of the world's top-level research environment, a new research building for the WPI project with advanced equipment and facilities will be constructed in the new ITO campus, under initiative of the university president. Prior to the completion of the construction of this new building, research rooms and spaces will be arranged for invited or newly-employed researchers from external organizations. • The institute will proactively act on the attainment of financial supports from the local government and industries in related areas.	information regarding research grants, providing strategic advice on grant applications, etc. In addition, an administrative staff member with a doctoral degree has been given charge of research support and international affairs. This staff member provides support and assistance, including applications, for substantial competitive research grants. • The Institute's permanent facility will be built in the ITO Campus and will open around October 2012. We are currently working on the budget and design. o We are proactively pursuing outside support for the construction and management of the new facility. • Until the completion of the new facility, the Institute has secured temporary arrangements for the Director's office, the Administrative Office, 5 rooms for researchers, 5 rooms for laboratories, and one meeting room. All of these rooms are situated in existing buildings on ITO campus.
(2) System under which the center's director is able to make substantive personnel and budget allocation decisions • The Institute will be established as an organization directly under the president of Kyushu University. The system will be set up for the Institute Director to be able to make decisions on research plans, research frameworks, budget implementation, that are related to the Institute management, with the exceptions for the appointment/dismissal of the Institute Director and authorization for employment of the Principal Investigators.	(2) System under which the center's director is able to make substantive personnel and budget allocation decisions • The Institute is, under the rule of Kyushu University, positioned as a permanent international research institute. Governing documents have been developed to enable the Institute Director to be able to make decisions on research plans, research frameworks, budget implementation, and other issues related to Institute management, in consultation with the Science Steering Committee, etc. • New faculty recruitment is carried out through open international calls. The Director makes the final hiring decisions in consideration of recommendations from the Faculty Recruiting Committee based on application screening and interviews.
(3) Support for the center director in coordinating with other departments at host institution when recruiting researchers, while giving reasonable regard to the educational and research activities of those departments • In regards to the researchers in Kyushu University contributing to the	(3) Support for the center director in coordinating with other departments at host institution when recruiting researchers, while giving reasonable regard to the educational and research activities of those departments • Active support is provided to Kyushu University researchers to facilitate

project, the university will work in coordination with the parent departments, providing them with the supports for the employment of substitutes for their educational and research activities, in order to maintain the educational and research activities of the parent departments. • The university will provide flexible research infrastructures where international and national top-class researchers can perform collaborative researches which reflect the social requirements.	their engagement in the Institute's activities in coordination with the parent departments such as requests for cooperation and arrangements to the head of his/her department.
(4) Revamping host institution's internal systems to allow introducing of new management methods (e.g., English-language environment, merit-based pay, top-down decision making) unfettered by conventional modes of operation • Kyushu University is currently implementing a project for internationalization of research and education in the University, under the initiative of the president. As a part of this plan, efforts have been made, in collaboration with International Affairs Division of Kyushu University; conducting undergraduate and postgraduate degree programs in English language; increasing the number of international students and lecturers, preparing internal documents and the university webpage in English; assisting students and staff members to improve their English language skills; establishing international student and researcher support centers at every campus, in order to further accelerate the establishment of international educational and research environments. • The Institute will be established as an organization directly under the president of Kyushu University. The system will be set up for the Institute Director to be able to make decisions on research plans, research frameworks, and budget implementation, which are related to the institute management. • In regards to salary settings, there is already a system in Kyushu University to set the various range of salary based on the abilities of researchers especially for ones from external institutes. As needs arise, the system will be re-examined. • In addition, Kyushu University will work in cooperation with the	(4) Revamping host institution's internal systems to allow introducing of new management methods (e.g., English-language environment, merit-based pay, top-down decision making) unfettered by conventional modes of operation • The President of Kyushu University has initiated plans to internationalize research and education within the university. As a part of this plan, efforts have been made to prepare internal documents, and to develop an English version of the university webpage. International Student and Researcher Support Centers have been established at every campus. Additionally, the following matters will be changed by establishing new and revising current rules and regulations. • The Institute established a new salary system (Special Regulation on Employment of the International Institute for Carbon-Neutral Energy Research of Kyushu University) which deviates from the established salary ranges. The Institute also provides an "institute allowance" for existing employees. Individual faculty and researcher salaries are determined based on individual accomplishments and contributions to the interests of the Institute and also on input provided by the Program Review Meeting and External Advisory Committee.

Institute for flexible implementation, adjustment, modification of the university's internal systems, upon the requests from the Institute Director, in order to ensure smooth management of the Institute.	
(5) Accommodation of center's requirements for infrastructural support (facilities, e.g., laboratory space; equipment; land, etc.) • For the provision of the world's top-level research environment, a new research building for the WPI project with advanced equipment and facilities will be newly constructed in the new ITO campus, exclusively, under initiative of the university president. Prior to the completion of the construction of this new building, research rooms and spaces will be arranged for invited or newly employed researchers from external organizations. • In ITO campus, there are already many advanced research facilities and equipment in the research centers, for example the Central Analytical Center and High Voltage Electron Micrograph Laboratory, and the preferential usages of the equipment will be arranged for the researchers in the WPI project.	(5) Accommodation of center's requirements for infrastructural support (facilities, e.g., laboratory space; equipment; land, etc.) • New research building for the WPI project with advanced equipment and facilities will be newly constructed in the ITO campus, now working on the details of budget and designing. • Prior to the completion of the construction of this new building, a director's room, an administrative office, 5 research rooms, 5 experimental laboratories and a meeting room are arranged.
(6) Support for other types of assistance • Prof. Yukitaka Murakami, Trustee and Vice President of Kyushu University, will take on responsible roles as the chief center-project officer for this WPI research Institute, to realize the concepts and to meet the objectives of the Institute. After the establishment of the Institute, he will continue to take on responsible roles as the chief center-project officer under the direction of the president of Kyushu University, in order to effectively work in coordination with the relating departments of the university. • The promotion of the concept of this Institute as the model project for internationalization of research and education in Kyushu University, and the application of the concept of this Institute to the entire University body would contribute to reforming the university system and to training our young researchers to be internationally recognized.	(6) Support for other types of assistance • Prof. Murakami, former Trustee and Vice President of Kyushu University, serves as Vice Director of the Institute working in concert with the Director, Prof. Murakami works to realize the concepts and meet the objectives of the Institute as well as coordinating with relating departments of the university. When the Director is traveling or in Illinois, Prof. Murakami maintains daily communication with him, relaying and implementing the Director's plans.

11. FY 2010 funding

(Exchange Rate: JPY/USD=100)

Cost Items	Details	Costs (ten thousand dollars)
Personnel	Center director and Administrative director	3
	Principal investigators (17 persons)	36
	Other researchers (28 persons)	18
	Research support staffs (0 persons)	0
	Administrative staff (15 persons)	24
	Total	81
Project activities	Gratuities and honoraria paid to invited Principal investigators (17 persons)	3
	Cost of dispatching scientists (0 persons)	0
	Research startup cost (3 persons)	32
	Cost of satellite organizations (1 satellite Organization)	58
	Cost of international symposiums (1 Symposium)	4
	Rental fees for facilities	0
	Cost of consumables	43
	Cost of utilities	1
	Other costs	8
	Total	149
	Domestic travel costs	2
	Overseas travel costs	1

Ten thousand dollars
(Exchange Rate: JPY/USD=100)

WPI grant for FY 2010 346
(WPI grant includes 357,252 dollars for the balance carried forward)

Cost of establishing and maintaining facilities in FY 2010: 0

Costs of equipment procured in FY 2010: 611

- 3 TV Conference Systems 15
- 3 Microscope Stages 15
- 1 3-D Measuring Laser Microscope 13
- 1 Multipurpose X-ray Diffraction System 8
- 1 High-Frequency Induction Heating Device 8
- Others 552

Travel	Travel and accommodations cost for invited scientists (4 domestic scientists) (26 overseas scientists)	15
	Travel cost for scientists on secondment (0 domestic scientists) (0 overseas scientists)	0
	Total	18
Equipment	Depreciation of buildings	0
	Depreciation of equipment	163
	Total	163
Other research projects	Projects supported by other government subsidies, etc.	54
	Comissioned research projects, etc.	144
	Grants-in-Aid for Scientific Research, etc.	32
	Total	230
Total		641

12. Efforts to improve points indicated as requiring improvement in application review and results of such efforts	
-Points specified as needing improvement • The committee has concerns about the director not being based in Kyushu. His presence at Kyushu University should be significantly enhanced and be clearly committed for at least next 5 years. The relationship between the University of Kyushu and the University of Illinois, including scope, obligations, methods of collaboration, and responsibility/role of the center director, needs to be defined in more depth and formalized in written agreement. The commitment of the host organization, addressed in the hearing, is requested to be more concrete including continuous financial support to the center. Finally, there were concerns about the apparent focus on a single research area, hydrogen, and other research area including CCS needs to be explored more in detail to match the title of the center.	-Efforts to improve them and results 1) The Memorandum of Understanding and the agreement establishing the I^2CNER satellite institute between Kyushu University and University of Illinois were concluded and entered into on December 1, 2010. The satellite location designates the framework for mutually beneficial collaborations in academic and research endeavors. The latter stipulates the Director's role and duties. Director Sofronis communicates with Vice Director Murakami, Administrative Director Mr. Kurasaki, Director's assistant, Ms. Utamaru every day, including weekends, via e-mail and videoconferencing. Following the Director's instruction, the institute is being operated and managed during his absence from Kyushu University with the support of the Administrative Office. 2) Policies have been established to reform hiring practices within Kyushu University, including: a. Processes to provide the Director with the authority to make decisions on matters concerning the Institute in consultation with the Science Steering Committee (consisting of Director, Vice Director, Associate Director, and Lead PI of each research division). b. Processes to authorize the Director to make the final decisions on new faculty and post-doctoral research associate recruitment. New faculty hires will be internationally sought based upon the recommendations of the Faculty Recruiting Committee. Applicants that do not meet or international standards as required by first-tier US and Japanese universities are not considered. In addition, the Faculty Excellence Program is in place to recruit faculty capable of bringing transformational change across the Institute. c. Authorization of the director to make the final decisions on the posting, title, research activities, and compensation of the newly-hired researchers based upon recommendations from the Faculty Recruiting Committee.

3) After an international open recruitment call for researchers in all areas of carbon-neutral energy, one associate professor has been hired in the area of CO_2 sub-sea bed storage and one assistant professor for CO_2 geological storage will join the Institute on June 1, 2011.

    a. I^2CNER is aggressively working toward building partnerships major domestic research institutes in the field of geological CO_2 storage, e.g. RITE.

4) Adhering to its commitments, Kyushu University provided the funds for the hiring of one professor in the Hydrogen Storage Materials Division and four associate professors in the fuel cell division.

5) Each PI completed a white paper which detailed her/his concrete research plans and included sections describing the grand challenge, technical barriers, goals, technical approach, near-term objectives, and long-term impact. The Director reviewed the papers and conducted hearings with each PI to make revisions. The papers are currently being reviewed by the External Advisory Committee.
    a. Currently, the CO_2 Geological Storage plan and objectives are being formulated with input from Dr. Robert Finely, director of the Midwest Geological Sequestration Consortium at Illinois and a member of the External Advisory Committee.

6) In view of the recent disasters in the northeastern part of the country and the emerging discussion for the creation of a new energy policy for Japan, I^2CNER is planning to:
    a. Strengthen research on carbon capture and storage since fossil fuels are now expected to play a significant role in the country's energy portfolio as a short term solution.

    b. Continue fundamental research that will enable the technology for a hydrogen-powered society.

    c. Provide a thorough assessment of the new energy carrier—hydrogen—as a long term energy solution relative to other renewable energy sources.

To this end, the Director is consulting with the US Department of

	Energy and the Vice Director is consulting with corresponding agencies of Japan.