FY 2011 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 2012) 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

In its second year, I^2CNER made significant advances not only in the thematic research areas, but also in staffing the institute, introducing new culture faculty programs, and broadening international activities. Some of the research highlights include: advances in how organic and inorganic semiconductors can be used and joined to produce active photoelectrochemical cells with good performance to synthesize hydrogen; elucidation of the mechanisms of hydrogen uptake in materials and discovery of fundamental deformation processes associated with hydrogen-fatigue interactions; understanding of the interactions between grain size, grain boundaries, and twins in materials for enhanced hydrogen storage performance; development of new heterogeneous and homogeneous catalysts and understanding of how catalysis and durability underscore the performance of low- and high-temperature fuel cells; determined how electrochemical processes can be used to separate CO_2 and how it can be converted to a useful product; and developed instrumentation for monitoring CO_2 in the ocean and in rock and advanced the understanding of the dynamics of CO_2 in saline aquifers.

To encourage inter-division research (fusion) within I^2CNER, the "Start-up funding for interdisciplinary research" program was started, and a total of nine projects were awarded. In addition, the Institute introduced an energy analysis thematic research area to address the roadblocks to achieving a carbon-neutral energy society due to the constraint of primary energy availability and resources on the basis of CO_2 emissions, efficiency, and cost. The goal of this division is to establish a roadmap toward a sustainable and low-carbon society over mid-and long-term scenarios by continuously assessing the relevance of the Institute's research activities. As of August 2011, the I^2CNER Satellite Institute has been in place at the University of Illinois and the kick-off symposium offered attendees an overview of current breakthroughs and identified the major science and engineering challenges to achieving a carbon-neutral energy future; Representatives of the U.S. Department of Energy, NSF, National Laboratories, and Toyota Motor Corporation presented these perspectives. Internationalization of I^2CNER is moving forward rapidly, with faculty and graduate student visits and exchanges and with the staffing of the institute. Following international searches, I^2CNER hired 11 young faculty and 3 post-docs. An associate professor was hired through the newly introduced Faculty Excellence Program. These young faculty have embarked on developing their independent research programs within I^2CNER's mission. Concurrently, I^2CNER designed and implemented a faculty evaluation process, and Kyushu University, along with the University of Illinois, continues to develop new efforts towards institutional advancement. As of April 1, 2012, the total number of I^2CNER researchers had grown to 118 (102 at Kyushu and 16 at Illinois) and the total number of I^2CNER members including both researchers and support staff had grown to 193 (161 at Kyushu and 32 at Illinois). The number of Principal Investigators (WPI PI) is 45, 10 of whom are renowned international scholars and 13 are distinguished faculty of the University of Illinois.

As a part of its outreach program, and to increase awareness of the general public about transitioning to a carbon-neutral energy society, I^2CNER organized the WPI 6 Institute Joint Symposium titled "Cutting Edge Science & Your Future." This event was attended by 573 high school students.

A new building to house the institute is under construction, and the inauguration ceremony is planned for January 29, 2013. In summary, I^2CNER, through its research, event organization, engagement of other international agencies, its transformative impact on research culture, and its outreach programs, is gaining recognition as a vital center for carbon-neutral energy and sustainability.

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 aspire to establish a “Carbon-Neutral Energy Research Institute” as a center of

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

- The International Institute for Carbon-Neutral Energy Research, (I^2CNER) officially began on December 1, 2010. The vision the Institute serves is to contribute to the creation of a sustainable and environmentally friendly society and establish an academic environment that fosters innovation through collaboration and interdisciplinary research. Within this vision framework, the Institute’s mission is to advance fundamental science to enable the technological breakthroughs that will facilitate the transition to a hydrogen-powered society with efficient CO_2 capture and storage or its conversion to a useful product. In particular, the research activities of the Institute aim to develop efficient means of hydrogen production, efficient hydrogen storage materials, hydrogen embrittlement resistant alloys, next generation fuel cells, material transformation catalysts, efficient CO_2 separation and concentration materials; and to address the science of CO_2 geo- and sub-seabed sequestration. These activities are multi/interdisciplinary in nature, as they cross-cut disciplinary boundaries for the study of phenomena occurring from atomistic to macroscopic time and length scales. The relevance of the Institute’s mission and objectives to the energy future of Japan is continuously assessed and evaluated from an energy analysis perspective in relation to other energy solution pathways, resource availability, and optimum use. The Institute’s structure has been set to attract distinguished scholars from overseas and to encourage young faculty and researchers to drive research and innovation. The Institute administration is continuously in contact with the Kyushu University administration to tackle jointly solutions to problems that arise, e.g. tenure issues, and work together on the promotion of international projects both on research and education. Lastly, the Institute is actively engaged in science dissemination and public outreach.

- On February 1 and 2, 2012, the Institute was reviewed by the External Advisory Committee (EAC) during an 1.5-day process that involved presentation of all thematic research areas and administration structure, interviews with young researchers, and exchange and discussion with Dr. Kuroki (Program Director) and Prof. Kasagi (Program Officer). According to Prof. Adrian, Committee Chair, the report from the EAC is

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 research project area as well their progress toward attaining the overall project objectives, that is, the realization of a hydrogen economy and

upcoming.

- Upon the announcement of the award and before the launching of the Institute, I^2CNER initiated an aggressive open international recruitment campaign. At the junior level, I^2CNER seeks to hire researchers who hold promise for future international recognition, and at the senior level, I^2CNER only considers candidates with international acclaim. The recruitment process is administered by the Faculty Recruiting Committee (FRC)—for more information on this committee, please see the Project Management Section. In summary, I^2CNER hired 1 researcher through the Faculty Excellence Program, and 14 researchers through 3 open international recruitment calls and FRC screenings in FY 2011. For complete details on FRC activity, please see Reference 1.

- All new hires are asked to submit a white paper describing her/his research plans, as was the case with the senior PIs. The papers were assembled into a booklet titled "Young Investigator Research Project Summaries" and reviewed by the administration of the Institute (Vice-Director, two Associate Directors, and division Lead PIs). Feedback was provided to the young investigators via the annual assessment and evaluation letter sent to the young investigators on April 1, 2012.

- To attract and recruit individuals who will contribute to transformation and positive change within their research division and across the Institute, the Director instituted the "Faculty Excellence Program." Individuals recruited through this program will have an outstanding record of accomplishment, and will clearly enhance our capacity to achieve strategic objectives and promote interdisciplinary research activities. Through this program, a female researcher was hired and appointed as a PI as of January 1, 2012.

- To promote engagement with leaders of the national and international community and enhance its visibility, the Institute launched the "I^2CNER Seminar Series" in March 2011. This seminar series features distinguished and internationally-recognized researchers from academia, national laboratories, industry, and policy makers in government agencies. In FY 2011, I^2CNER invited seventeen (17) world-class researchers for seminar presentations. Some of the notable speakers were: A. Fujishima, President of Tokyo University of

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.

Science; M. Aizawa, Executive Member of the Council for Science and Technology Policy of Japan; B. Ohtani, Professor at Hokkaido University; M. Kawaji, Professor from the University of Toronto and the City University of New York; Z. Ogumi of Kyoto University; T. Aida, Professor at the University of Tokyo; S. Iijima, Professor at Meijo University; S. Murai, Executive Director and Vice President of the Nara Institute of Science and Technology; and D. Eliezer, of the Department of Materials Engineering at Ben Gurion University in Israel.

- To foster a climate of collaboration and interdisciplinary research that cross-cuts division boundaries, the Institute launched and holds the "Institute Interest Seminar Series (IISS)." This series also serves as a forum to help our young researchers (graduate students, post-docs, assistant and associate professors) to further their abilities to present and argue for their viewpoints, scientific methods, and approach before an audience of experts. During FY 2011, sixteen (16) seminars with two presentations each were held. For complete details on the Institute Interest Seminar Presentations, please see Reference 2.

  The success of this series is demonstrated by the active participation, engagement, and debate it precipitated among the divisions for interdisciplinary research. By way of example, it was after the presentation by Prof. Nishihara (Fuel Cells), an expert on polymer science, that an interdisciplinary project titled "Theoretical and experimental design of cross-linked polymer electrolyte membranes for use in fuel cells" was initiated jointly with Prof. Staykov (Hydrogen Production), an expert on computational chemistry.

- I^2CNER instituted the "Super Research Assistants (SRA)" Program to recruit and support excellent graduate students to carry out PhD thesis work under the supervision of our WPI assistant, associate and full professors within the various divisions of the Institute. In FY 2011, two calls for recruitment were made, one in April and one in July, followed by an application process that included presentation screenings. As a result, two research assistants were hired as of July 1 and another two as of October 1, four in total. All SRAs are required to make presentations at the Institute Interest Seminar Series in English and submit progress reports, and give another presentation before the Institute's SRA Selection Committee for the renewal of their SRA status.

	As of April 1, the SRA Selection Committee decided that the progress of one of the SRAs was satisfactory. In addition, two new SRAs joined the Institute. I^2CNER aims to continue recruiting SRAs to meet its goal to train the next generation of researchers. • In order to facilitate active exchange of students between Kyushu University and University of Illinois (I^2CNER Satellite Institute) and other collaborating institutions overseas, the Institute started accepting short-term students from overseas to Kyushu University as "Visiting Students." In FY 2011, I^2CNER hosted nine (9) students. Full details are listed in Reference 3. • From FY 2012 onward, the Institute established a system to accommodate as short-term "Visiting Researchers" post-doctoral research associates who are working at Kyushu University under the supervision of foreign PIs at collaborating institutions overseas. The first associate from Tsinghua University in China is being hosted beginning April, 2012 for 3 months in the Thermophysical Properties Division.
<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> • The Institute is organized in thematic research areas (Divisions) to address individual research objectives. The divisions are o Hydrogen Production o Material Transformations (Catalysis) o Thermophysical Properties (H_2, CO_2) o Hydrogen Structural Materials o Hydrogen Storage Materials o Fuel Cells o CO_2 Separation and Concentration o CO_2 Sequestration and Storage (CCS) o Energy Analysis Each division is led by a senior WPI Principal Investigator (Lead PI) of the Institute. • The Energy Analysis division was established in response to a recommendation stated in the interim evaluation report issued by the WPI Program Committee after the 2011 WPI Site Visit ("I^2CNER should establish its own vision and roadmap toward a carbon-neutral society over time scales of short, middle and long ranges"). The idea is that

the Institute should address the roadblocks for a carbon-neutral energy society due to the constraint of primary energy availability and resources on the basis of CO_2 emissions, efficiency, and cost. The division's goals are:

- Assess the relevance of the Institute's research activities toward I^2CNER's vision for a carbon-neutral society.
- Ensure that I^2CNER research is informed of all relevant current and future energy options of Japan.
- Establish a roadmap toward a sustainable and low-carbon society over mid and long term scenarios.

The division is led by the Director and its members currently include Dr. Mark Paster (former energy analysis employee in the Energy Efficiency and Renewable Energy department of the U.S. DOE) and Dr. Kuniaki Honda (formerly with the Gas and Power Co., Ltd, Japan). Both Dr. Paster and Dr. Honda have been appointed in the Institute as WPI Visiting Professors—Dr. Honda's appointment will change to that of a WPI Professor on July 1, 2012. Prof. James Stubbins, head of the Nuclear, Plasma, and Radiological Engineering Department of the University of Illinois, is participating in the research program of the division from the Satellite Institute. An ongoing recruiting call is seeking to bring additional researchers on board.

- Upon the recommendation of the SSC, the Director reappointed the following foreign researchers who are internationally recognized scholars for their research contributions to the position of "WPI Principal Investigator" in I^2CNER for the following academic year 2012:
  - Prof. John A. Kilner, Imperial College London (UK)
  - Dr. Brian P. Somerday, Sandia National Laboratories (USA), serving as Lead PI of the Hydrogen Structural Materials Division
  - Prof. Robert O. Ritchie, University of California, Berkeley (USA)
  - Prof. Ludwig J. Gauckler, Swiss Federal Institute of Technology Zurich (ETH)
  - Prof. Harry L. Tuller, Massachusetts Institute of Technology (USA)
  - Dr. Xing Zhang, Tsinghua University (China)
  - Prof. Louis Schlapbach, Swiss Federal Institute of Technology Zurich (ETH)

	o Dr. Ping Chen, Dalian Institute of Chemical Physics (China) o Prof. Chen-Tung Arthur Chen, National Sun Yat-sen University (Taiwan) o Prof. Reiner Kirchheim, University of Göttingen (Germany) These investigators are expected to vigorously pursue collaborative research with I^2CNER researchers, offer lectures and seminar presentations, and engage with student or post-doctoral research associate supervision as well as with teaching short courses. Participating in I^2CNER, these foreign investigators are expected to continue to contribute to the excellence of our research program. In addition, the 13 Illinois Satellite faculty members are all internationally recognized researchers in their respective areas of expertise. They were specifically invited to complement the I^2CNER research activities at Kyushu as WPI PIs. • Other Principal Investigator personnel changes are: o April 1, 2011: Professor Reiner Kirchheim of the University of Göttingen (Germany) and Professor Takaki of Kyushu were appointed as PIs in the Hydrogen Structural Materials division. o January 1, 2012: Dr. Yamauchi (formerly with Hokkaido University) was appointed as a PI in the Material Transformations Division. o January 16, 2012: Professor Sakai was appointed as a PI in the Hydrogen Production Division and Dr. Shitashima was appointed as a PI in the CO_2 Sequestration and Storage Division. o March 31, 2012: Professor Kondo of the Hydrogen Structural Materials Division resigned his post as a PI due to serious health problems.
<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	<Project Management> • The Science Steering Committee (SSC) was set in place upon the launching of the Institute. The committee is chaired by the Director and its members are the Vice-Director, the two Associate Directors (see below), and the lead PIs of the thematic research areas (divisions). The SSC is the body that reviews and decides on all matters 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 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 Institute, e.g. planning and operation of research activities, budget implementation, international collaborations, and outreach. By way of example, a document that outlines the Institute's policy and terms for promotion of our assistant and associate professors is currently under discussion in the SSC. In short, an assistant professor is promoted on the basis of promise for international recognition based on interdisciplinary research carried out in I^2CNER and an associate professor is promoted when this promise has been fulfilled.

- The Director is assisted by Vice-Director, Prof. Yukitaka Murakami and the two Associate Directors Prof. Kazunari Sasaki and Prof. Tatsumi Ishihara, who was newly appointed as a second Associate Director as of February 1, 2012. The two Associate Directors are responsible for matters related to the following:
    - Prof. Sasaki (also serves as a Lead PI of Fuel Cell Division), Faculty Recruiting Committee (FRC), international collaborations and industrial collaborations such as those through the Next Generation SOFC Center.
    - Prof. Ishihara (also serves as a Lead PI of Hydrogen Production Division), Promotions Committee, I^2CNER workshop organizations, administration of our seminar series, handling of graduate student research matters and overseeing facilities and equipment.

- In the area of CO_2 Sequestration and Storage, the Director is receiving input and advice from Dr. Robert Finley, member of the External Advisory Committee and director of the Midwest Geological Sequestration Consortium at Illinois. In general, the plan is to i) streamline the research activities of the CO_2 Sequestration and Storage division in a way that the geology of Japan and time scales involved will feed back to define basic research requirements, and ii) reinforce the area of fundamental science underlying CCS as considered to be pursued by industry on an industrial scale at the Tomakomai region of Japan in Hokkaido. In this regard, the oceanographic expertise that I^2CNER possesses would be appropriate for monitoring at the seabed and in the water column as part of developing an environmental assurance program for sub-seabed sequestration.

- Prof. Ian Robertson of the University of Illinois serves as Chief Science Advisor to the Director in order to further strengthen the management

research activities of the Institute	of the Institute's diverse and growing number of activities. • Upon the official launching of the Institute, the Director and Vice-Director consulted with senior authorities in the field of renewable energy and CO_2 sequestration 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 (eight members as of March 31, 2012) o Professor Ronald J. Adrian (Chair), Arizona State University, USA o Dr. Deborah Myers (Vice-Chair), Argonne National Laboratory, USA o Dr. Robert J. Finley, Illinois State Geological Survey, USA o Professor Reiner Kirchheim, University of Göttingen, Germany o Professor Robert McMeeking, University of California, USA o Dr. Kevin Ott, Los Alamos National Laboratory, USA o Professor Tetsuo Shoji, Tohoku University, Japan o Dr. George Thomas, Retired EERE office of US DOE and Sandia National Laboratories, USA (Advisory member) • 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 (below included FRC activity details). • At the Illinois Satellite Institute, Professor Kenneth Christensen (a researcher with international acclaim on experimental turbulence) was newly appointed to serve as Associate Director. • To identify and study issues related to the cohesion of the research activities in I^2CNER across research groups and division boundaries, at the Director's request, each I^2CNER Principal Investigator (PI) submitted a white paper describing her/his research plans. In particular, the white paper addressed the grand challenge, technical barriers, goals, technical approach, near-term objectives, long-term impact, and required resources. The papers were assembled into a booklet titled "Research Project Summaries" and sent to the External Advisory Committee (EAC) for review. The reviews were communicated to the PIs and in some instances course redirection was requested. The PIs were asked to finalize and resubmit their plans by revising their papers

	along the lines suggested by the reviewers. In some cases, the Director met with individual PIs to discuss the reviews. • To promote interdisciplinary research and foster collaboration between division researchers, a) After the I^2CNER annual symposium at Kyushu University on January 31, 2012, workshops focused on individual division research thematic areas were held on February 2, 2012. In these specialized workshops, a large number of researchers from collaborating Institutes also participated. b) On March 8th, 2012, PIs from Kyushu University and the University of Illinois gathered on the Illinois campus for collaborative faculty meetings through breakout sessions in which PIs from different divisions openly discussed their research projects. Twenty-three (23) attendees from the Illinois Satellite participated in the 2012 I^2CNER Annual Symposium and thirty-five (35) attendees from Kyushu University participated in the Illinois Satellite Kick-off Symposium. Through these I^2CNER events, PIs from both universities had opportunities to directly exchange and discuss research ideas for interaction and collaboration, in addition to regular communications via email and teleconferencing.
<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	<Collaboration with Other Institutions> • Upon the signing of the agreement between Kyushu University and the University of Illinois in March 2011, the Director worked to establish the research structure of the Illinois Satellite Institute. The process involved a university-wide call for letters of intent followed by a call for proposals. The document review was carried out by Kyushu faculty and was administered by the Institute's Vice-Director. The chosen proposals were those that complemented or expanded the Kyushu research efforts. As of August 2011, the Satellite research program has been configured as follows: o Structural Materials and Hydrogen Compatibility ▪ Profs. Robertson (Mat. Sci. Eng.), Sofronis (Mech. Sci. Eng.) o Hydrogen and CO_2 Interactions with Materials Interfaces ▪ Prof. Cahill (Mat. Sci. Eng) o Conversion of CO_2 to Value-Added Products ▪ Profs. Kenis, Gewirth, Rauchfuss (Chemistry)

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.

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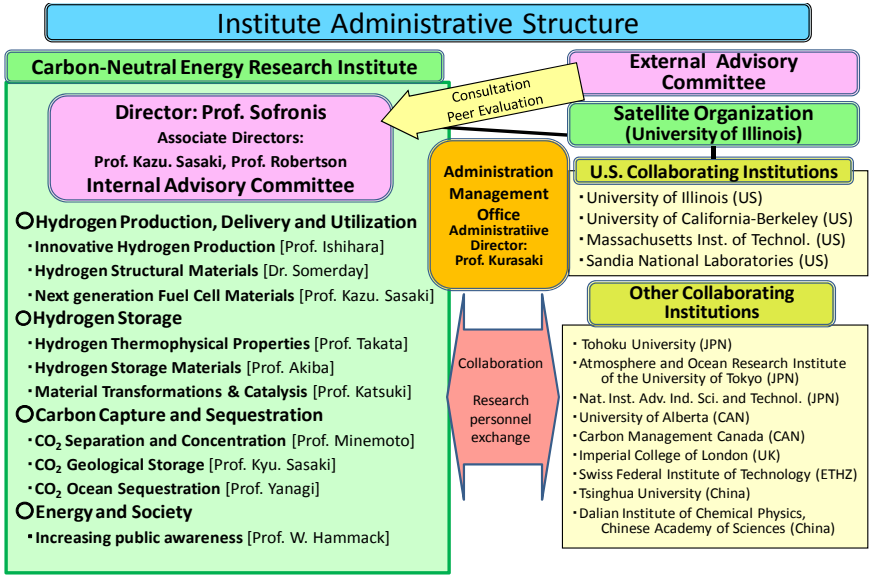

Fig. Administrative structure of the Institute

  - Energizing the Hydrogen Economy
    - Prof. Gewirth (Chemistry); Profs. Martin, Rockett (Mat. Sci. Eng.), Prof. Ertekin ((Mech. Sci. Eng.)
  - Dynamics of Multiphase Turbulent Plumes with Application to Sub-Seabed Carbon Sequestration and Buoyant Motion and Dissolution of Carbon Dioxide Drops in Water
    - Profs. Christensen, Pearlstein (Mech. Sci. Eng.)
  - Near-Critical CO_2 Flows over Active Solid Surfaces
    - Prof. Kyritsis (Mech. Sci. Eng.)
  - Energy Analysis
    - Prof. Stubbins (Nuclear. Plasma Rad. Eng.)
  - Outreach
    - Greenberg (Illinois State Geological Survey)

- I^2CNER held the Satellite kick-off Symposium March 6th through the 7th, 2012. Day One, entitled "Powering the Future," offered attendees an overview of the most current energy breakthroughs, as well as the serious barriers to a carbon-neutral energy future from the perspective of representatives of the U.S. Department of Energy, NSF, National Laboratories, and Toyota Motor Corporation. Day Two was broken into four sessions, and featured speakers from the Institute, who explained their current research projects and suggested future research directions.

- Collaborative research activities and personnel exchanges between Kyushu and the Illinois Satellite, and other collaborating institutions have also begun. Illinois graduate research assistants visited Kyushu in the summer of 2011 to carry out experiments jointly with Japanese researchers and ever since, such visits from Illinois and other institutions are contributing to the internationalization of the research activities of I^2CNER.

- I^2CNER instituted such programs as "Visiting Students" and "Visiting Researchers" to accommodate graduate research assistants and postdoctoral researchers from overseas. In this context, I^2CNER hosted a number of Visiting Students mainly from the University of Illinois during FY 2011 (full details are listed in Reference 3).

- Plans are developed for a broad I^2CNER engagement in the Livermore Valley Open Campus (LVOC) project. This project launched jointly between Sandia National Laboratories and the Lawrence Livermore

	National Laboratory aims at establishing an open campus in which foreign (non-US) researchers can participate. It is envisioned that soon the LVOC and I^2CNER will carry out joint workshops such as on the state-of-the-art for materials in a hydrogen environment. • The Director and the Vice-Director are making contacts in the US, Europe, and Japan to promote a network of interaction and exchange on research and energy policy between academia, national laboratories, industry, and government. 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 Exxon Mobil Research and Engineering Company, I^2CNER will work in concert with Mohawk Innovative Technology to coordinate material selection for future hydrogen compressor concepts, Toyota Motor Corporation on fuel cells, The Max-Planck Institute at Duesseldorf, and the Fraunhofer Institute for Mechanics of Materials IWM in Freiburg, Germany on materials under extreme hydrogen environments. The Director presented the I^2CNER project to the General Motors (Headquarters in Germany) through a webinar on February 27, 2012.

2. Research fields

<Initial plan>	<Results/progress/deviations from 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.	• The disasters caused by the Tohoku Region Pacific Coast Earthquake, tsunami and Fukushima nuclear accident, have brought to the fore serious issues related to the energy infrastructure and future of Japan. Certainly, I^2CNER will be called to participate and contribute to the national discussion on energy, and as such its mission and goals are now more relevant 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. In particular, I^2CNER through using the so-called nonlinear models for energy analysis will investigate and identify what is the best use of available energy resources of Japan is, given future energy demand vs. time

- 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 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.

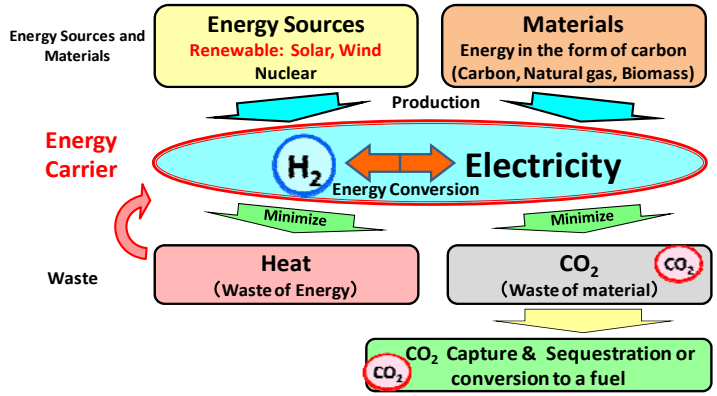

Fig. A Carbon-Neutral Energy Fueled System

b. How I^2CNER can keep its research objectives in perspective relative to other potential technologies toward a sustainable, safe, and reliable carbon-neutral energy society.

In establishing these plans, the Director is working with Dr. Mark Paster in consultation with the US Department of Energy, and the Vice-Director is consulting with corresponding agencies of Japan.

- A detailed summary of the progress made in the Institute in each individual thematic research area over the last year is presented in Section 3 of this report. The summaries reflect and integrate the research efforts at Kyushu, Illinois, and international collaborators.

- 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;
  - Development of CO_2 geological storage considering CO_2 behavior

<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 is reported in the form of executive summary that was composed from individual project reports submitted by each researcher within a specific division. In addition, the current status of our Energy Analysis Division is also reported.

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.

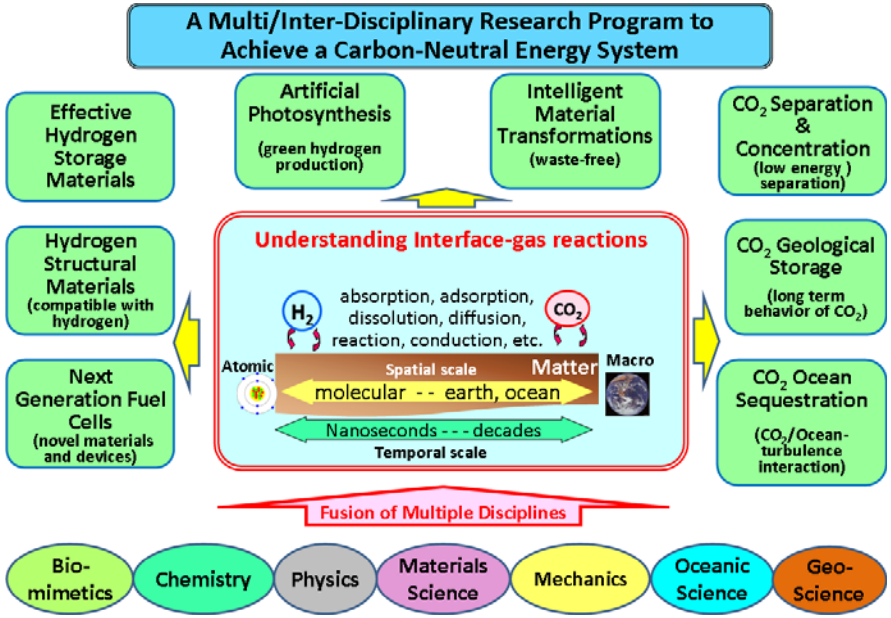

Fig. Interfaces in the multi/inter-disciplinary research program in I^{2}CNER

(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.

(Research Objectives and Methodologies)

1. **Hydrogen Production and Artificial Photosynthesis**

Goals

Activities in FY 2011 have focused on preliminary experiments and basic science directed at photovoltaic and photoelectrochemical (PEC) energy production using organic, inorganic, and hybrid devices. These materials can be used to form complete photovoltaic devices as well as electrodes in PEC devices. The latter also require catalysts to stimulate reactions and reduce required over-potentials. The project is supported

- 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.

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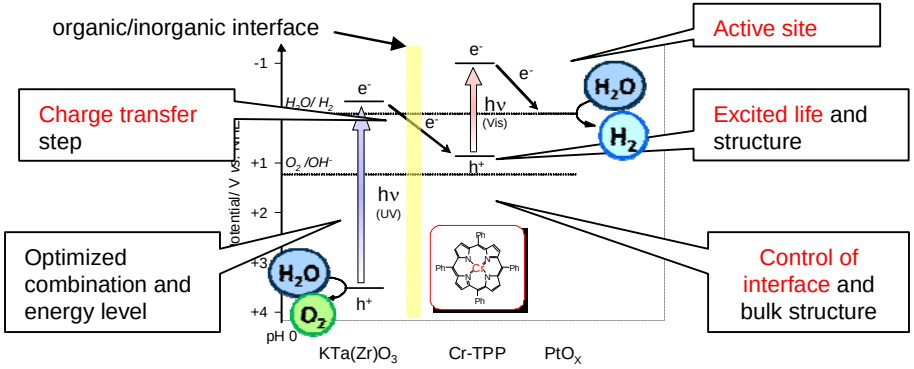

Fig. 1a. Artificial photosynthesis through complete photocatalytic water splitting

by both theoretical computations and sophisticated materials characterizations.

Research Team

Division Leader — Tatsumi Ishihara (Applied Chemistry), Chihaya Adachi (Applied Chemistry), Elif Ertekin (Mechanical Science and Engineering, UIUC), Kenichi Goushi (Applied Chemistry), Hidehisa Hagiwara (Applied Chemistry), Shintaro Ida (Applied Chemistry), John Kilner (Imperial College, London), Lane Martin (Materials Science and Engineering, UIUC), Hiroshige Matsumoto (Inamori Frontier Research Center), Angus Rockett (Materials Science and Engineering, UIUC), Aleksandar Staykov (I^2CNER), Atsushi Takahara (Materials Chemistry and Engineering), Keiji Tanaka (Applied Chemistry), Takuma Yasuda (Applied Chemistry), Kazunari Yoshizawa (Fundamental Organic Chemistry), Ken Sakai (Chemistry).

Research Highlights and Accomplishments

In the past year our results have demonstrated fundamental differences in the electronic structure of chalcopyrite semiconductors as a function of group I cation and the corresponding d-orbitals. They have shown how growth kinetics may be modified by energetic particle bombardment, how organic layers can provide enhanced exciton blocking layers in OPV devices with improved device performance, how organic and inorganic semiconductors can be used and joined to produce active photoelectrochemical cells with good performance, and ultimately how hydrogen can be synthesized by the approaches studied. We have produced a wide range of organic and inorganic materials and demonstrated preliminary experimental results highlighting their potential in devices and fundamental science.

In the area of inorganic materials, we are looking at a range of materials spanning fluorides, oxides and chalcogenides. Ln_2NiF_4 and $(Pr,La)_2NiO_4$ are being studied as electrodes of electrochemical cells, and their surface properties. In the oxides Cu_2O and TiO_2 have been grown as epitaxial single crystals on $SrTiO_3$. This work has been enhanced by theoretical modeling of the interface between Cu_2O and TiO_2, and how this can result in photovoltaic activity has been further evaluated. We have demonstrated a connection between the adatom energy and flux rate to both the epitaxial relationships and shape of the resulting nanostructures. Rh-doped $CaNbO_3$ nanosheets were synthesized and shown to exhibit high photocatalytic activity. Bridging the oxide/chalcogenide materials, we have examined Bi_2O_2S and

demonstrated novel synthesis methods. Heterojunctions with In_2O_3 have been shown to exhibit excellent photochemical activity.

I^2CNER research confirmed the performance of a number of photocatalysts under study. $AgInSe_2$ has been deposited as a single crystal epitaxial layer and studied by scanning tunneling spectroscopy. This showed the basic nature of band edge fluctuations in the material and how it differs from other chalcogenides. We have deposited $CuInSe_2$ and studied it as a component of an organic/inorganic hybrid electrode material and tested the catalytic activity of the structure.

Hybrid electrodes studied have included GaN:ZnO combinations with Cr-TPP and other organic molecules. The energy of the LUMO in the organic material was found to be critical to the formation rate of H_2 in the resulting photoelectrochemical cells. In purely organic materials, the nature of interfaces between candidate materials has been examined by ultrasmall angle x-ray scattering, and organic photovoltaics have been synthesized and characterized for current-voltage characteristics and fundamental optoelectronic properties.

Future Directions

The team will expand interactions among the participants through visits and increased collaboration. Materials studies will provide guidance on the best choices among the anions in the inorganic materials and will ultimately lead to downselection of the candidate materials.

Impact on Science and Engineering

Energy generation is fundamental to the project and to the future world economy. In addition the science of these materials will provide general understanding of photovoltaic and photoelectrochemical materials.

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

2. Hydrogen Structural Materials

Goals

The technical barriers identified in this division include the limited understanding of hydrogen-surface interactions, hydrogen uptake, and material degradation mechanisms; the need to develop next-generation materials having improved resistance to hydrogen embrittlement at higher strength levels; and the need to improve

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 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.

fatigue and fracture property measurements in hydrogen gas.

Research Team

Division Leader — Brian Somerday (Sandia National Laboratories), , Yoshihiro Fukushima (Mechanical Engineering), Shigeru Hamada (Mechanical Engineering), Yoshiyuki Kondo (Mechanical Engineering), Masanobu Kubota (Mechanical Engineering), Saburo Matsuoka (Mechanical Engineering), Takehiro Morita (Mechanical Engineering), Yukitaka Murakami (I^2CNER), Nobuo Nakada (Materials Science and Engineering), Robert Ritchie (University of California, Berkeley), Ian Robertson (Materials Science and Engineering, UIUC), Yoshinori Sawae (Mechanical Engineering), Petros Sofronis (I^2CNER, and Mechanical Science and Engineering, UIUC), Joichi Sugimura (Mechanical Engineering), Setsuo Takaki (Materials Science and Engineering), Hiroyoshi Tanaka (Mechanical Engineering), Toshihiro Tsuchiyama (Materials Science and Engineering), Chao Nan Xu (AIST), Junichiro Yamabe (International Research Center for Hydrogen Energy).

Research Highlights and accomplishments

A combined experimental-modeling effort amplified understanding of the effects of oxygen impurities on hydrogen-gas accelerated fatigue crack growth in low-strength steels, and hydrogen uptake was numerically modeled at the crack tip for a low-strength steel in hydrogen gas. An analytical model based on oxygen diffusion in the crack channel was developed that predicts the effects of variables such as oxygen concentration and load ratio on hydrogen-accelerated fatigue crack growth. In addition, density functional theory (DFT) modeling provided new insights on the mechanisms of competitive co-adsorption for oxygen and hydrogen on iron surfaces. These activities involved international collaboration among multiple institutions (Sandia National Laboratories, UIUC, University of Göttingen) and collaboration across I^2CNER division boundaries (Hydrogen Structural Materials-Hydrogen Production).

Experiments of cyclic contact between steel surfaces revealed that hydrogen uptake was enhanced by cyclic normal contact but suppressed by cyclic contact with sliding. Surface analysis suggested that the permeation of hydrogen was affected by the formation and removal of oxide films on the steels. This activity on characterizing hydrogen uptake to understand basic processes in hydrogen-affected friction and wear complements work on characterizing hydrogen uptake at crack tips to define basic mechanisms of hydrogen-affected

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.

- 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

fatigue and fracture.

Using Transmission Electron Microscopy of samples extracted from beneath fatigue fracture surfaces by Focused Ion Beam machining, we investigated microstructural differences caused by the presence of hydrogen. For the first time, the microstructure beneath fatigue striations has been elucidated, and it appears that fatigue causes a refinement of the grain structure immediately below the fracture surface. Hydrogen causes a further refinement of microstructural features.

A new inclusion rating method by the positive use of hydrogen embrittlement phenomenon was proposed. This new method is the most reliable and efficient method among the existing inclusion rating methods in the world.

As a result of joint studies conducted with manufacturers of materials and hydrogen-supply components, a high-strength austenitic stainless steel was identified that is resistant to hydrogen embrittlement. The steel has minute amounts of N, Nb and Mo added to the chemical composition of Type 304, the tensile strength is at least 800 MPa, and the reduction of area and fatigue crack growth properties in 100 MPa hydrogen gas are almost the same as in atmospheric air.

Impact on Science and Engineering

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

Future Directions

Among our future plans are to simulate hydrogen adsorption with hydrogen transport and elastoplastic deformation to develop a fracture criterion that is predicated on the underlying fracture mechanism(s) acting at the microscale. In this framework, the extent by which surface oxidation affects the uptake process and how the competition between hydrogen and oxygen for surface adsorption sites controls the amounts of hydrogen that reaches the fracture initiation sites will be explored. We expect to continue studies on hydrogen-affected friction and wear, and explore the role of nonmetallic inclusions on hydrogen embrittlement of high strength steels. In particular, we hope to clarify the roles of trace elements in promoting embrittlement resistance in a

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.

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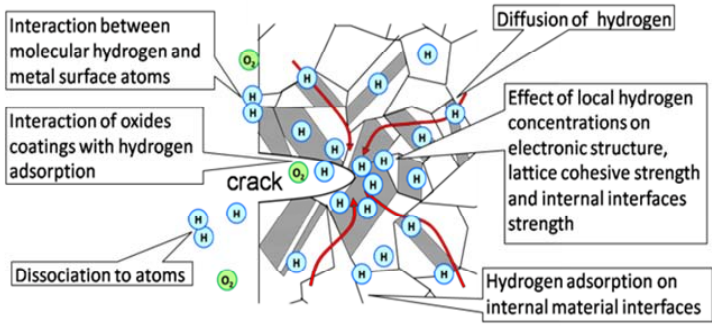

Fig. 2a. Fundamental processes around a crack in the presence of hydrogen

high-strength stainless steel. Finally, we will quantify effects of hydrogen on tensile deformation and fracture behavior, as well as deformation-induced martensite transformation in stainless steels.

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

Goals

The goal of this program is to develop efficient, cost-effective, and stable methods to convert hydrogen and other fuels into electricity using a fuel cell. Both high temperature solid oxide fuel cells (SOFC) and low temperature polymer electrolyte membrane (PEM) fuel cells are examined. For the former, efforts are directed at developing lower temperature conductors, higher durability materials, and more effective catalysts. In the latter, efforts are directed at developing more durable and effective catalyst supports, carbons which facilitate water management, and more effective and cheaper catalysts, especially for the oxygen reduction reaction. A parallel effort seeks to use CO_2 as a feedstock to produce value added chemicals. While a practical focus on new systems remains at the forefront of this effort, more fundamental studies provide insight to inform future directions.

Research Team

Division Leader — Kazunari Sasaki (Mechanical Engineering), Sean Bishop (I^2CNER), Tsuyohiko Fujigaya (Applied Chemistry), Andrew Gewirth (Chemistry, UIUC), Ludwig Gauckler (Swiss Federal Institute of Technology), Akari Hayashi (International Research Center for Hydrogen Energy), Kohei Ito (Mechanical Engineering), Tatsumi Kitahara (Mechanical Engineering), Michihisa Koyama (Inamori Frontier Research Center), Stephen Lyth (I^2CNER), Hironori Nakajima (Mechanical Engineering), Naotoshi Nakashima (Applied Chemistry), Yasuro Niidome (Applied Chemistry), Masamichi Nishihara (I^2CNER), Yusuke Shiratori (Mechanical Engineering), Harry Tuller (Massachusetts Institute of Technology).

Research Highlights and Accomplishments

Over the past year there have been a number of accomplishments. In the SOFC area, developments include new cathode materials exhibiting improved oxygen reduction kinetics, synthesis and characterization of thin ('nanoscopic') platinum films and dealloyed Pt-Al films exhibiting strain dependent changes in activation energies for oxygen reduction. Important chemical degradation mechanisms for SOFCs where characterized, including such causes as impurity poisoning, interdiffusion, and thermal cycling. Measurement of the surface temperature distribution in a microtubular SOFC is part of this characterization effort. Fundamental efforts directed at understanding the important rate limiting steps for the oxygen exchange reactions

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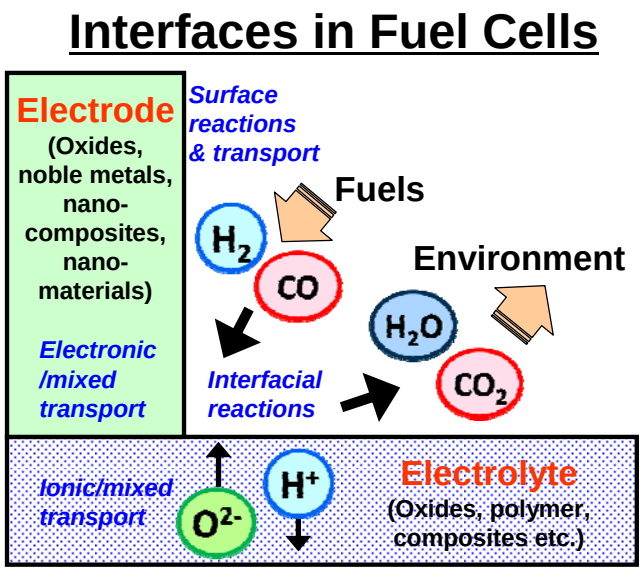

Fig. 3a. Transport and reaction processes around the electrode/electrolyte interfaces

operative at electrode interfaces were developed.

In the PEM area, I^{2}CNER Principal Investigators have continued characterization of a SnO_2 support for Pt electrocatalyts. These electrocatalyst supports exhibit substantially increased durability relative to the more commonly used carbon materials. Nano-channel mesoporous carbons have been developed as catalyst supports for PEM fuel cells. The nano channels can isolate and promote electrochemical reactions. Hybrid PEM membranes incorporating sulfonated polyimides exhibit enhanced durability and improved oxygen reduction kinetics. A new microporous layer-coated gas diffusion layer enhances PEM fuel cell performance under conditions of zero humidification. New methods to support catalyst structures were investigated, involving the interplay of mesoporous materials and ionic liquids.

Finally, new molecular-based catalysts for CO_2 conversion were developed which exhibit higher selectivity for CO production relative to hydrogen; this new catalyst may allow more practical conversion of CO_2 to fuels.

Future Directions

Research into both high- and low temperature fuel cells will continue. Promising directions in hybrid materials, both as electrolytes in the high temperature process and as membranes and catalyst supports in the low temperature area. Characterization of fundamental processess, particularly in the SOFC area, has the promise of leading to development of new electrolyte materials having both conductivity and activity at reduced temperatures. Micro SOFCs continue to provide convenient testbeds for concepts in catalysis and fuel cell durability. Studies of alternative combinations of materials to form more effective, durable, and active fuel cell structures will be a further emphasis. Durability, supports, and catalysis also form the focus of future directions for PEM fuel cells. The SnO_2 materials are highly durable, but less active relative to carbon. Increasing activity is clearly a necessity. The polyimide materials provide considerable new opportunities both as membranes and as supports. New catalysts for CO_2 conversion will require investigation into the interplay between ligand structure, metals, and supports.

Impact on Science and Engineering

The work on both high and low temperature fuel cells speaks to important issues surrounding the interplay between catalysis, the

support, and the electrolyte. The development of a relatively low temperature SOFC (550 °C) in the micro fuel cell configuration and the related materials development and characterization is an important step toward practical realization of these devices. Integration of PEM and SOFC ideas (such as might occur with the polyimide materials) provides new opportunities for both systems. New catalyst development for fundamental processes is significant in all areas.

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.

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4. Thermophysical Properties

Goals

The goals of this effort are to (i) advance fundamental understanding of the interactions of H_2 and CO_2 with material interfaces; (ii) develop real-time, in-situ experimental methods with greater sensitivity to interfacial phenomena in high pressure environments than are currently available; and iii) establish a comprehensive understanding and a database for the thermophysical properties of hydrogen, CO_2 and other working substances for carbon-neutral solutions.

Research Team

Division Leader — Yasuyuki Takata (Mechanical Engineering), David Cahill (Materials Science and Engineering, UIUC), Masamichi Kohno (Mechanical Engineering), Shigeru Koyama (Energy and Material Science), Xing Zhang (Tsinghua University, China).

Research Highlights and Accomplishments

We developed a transient short-hot-wire method and applied this new method to determine the thermal conductivity of hydrogen up to 100 MPa and 500°C. We proposed a new correlation equation for hydrogen thermal conductivity accurate to within ±2%. We initiated in-situ studies of charging and discharging of an oxide cathode used in Li ion batteries. The elastic constants of the $Li_{1-x}CoO_2$ soften as Li is removed from the planes between the CoO_2 layers and the thermal conductivity decreases with cycling.

Future Directions

Our main research direction in the near-term is to establish experimental capabilities at Kyushu University for pump-probe measurements of thermophysical properties and develop the high pressure optical cells needed for these experiments at both Kyushu University and University of Illinois. We will continue our *in-situ*

measurements of thermophysical properties of oxide cathodes and will continue to develop high-throughput and high-precision measurements of GHz surface acoustic wave velocity acoustic damping. We will provide new high accuracy data for the viscosity and equation of state of hydrogen up to 100 MPa and 500°C.

Impact on Science and Engineering

An enhanced ability to characterize high pressure reactions at material interfaces will have broad and long-term impacts on our ability to engineer materials with greater reliability and higher performance in high pressure H_2 environments. The unique data acquired in our studies will provide critical test of theory and computational models. Thermophysical properties measurements and the development of predictive correlations and databases for high pressure hydrogen will contribute to the hydrogen economy by supplying accurate data for the design of production, delivery, and storage systems.

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.

5. Hydrogen Storage Materials

Goals

The Hydrogen Storage Division brings together leading researchers with expertise in the fundamental design, analysis, and engineering aspects of systems for hydrogen storage. With an emphasis on reducing system weight, volume, and cost, and increasing efficiency, durability, and charge/discharge rates, researchers in this division focus on the design and demonstration of hydrogen systems to enable a sustainable, safe, and affordable method for the storage and transport of hydrogen fuel. Specific goals include elucidating and exploiting the role of defects such as grain boundaries, dislocations, and twins in metallic and intermetallic hydrogen storage materials, and using state-of-the-art characterization tools to describe the microstructural changes that take place in hydrogen storage materials as hydrogen gas is absorbed and released.

Research Team

Division Leader — Etsuo Akiba (Mechanical Engineering), Ping Chen (Dalian Institute of Chemical Physics, China), Zenji Horita (Materials Science and Engineering), Hai-Wen Li (International Research Center for Hydrogen Energy), Junko Matsuda (I^2CNER), Louis Schlapbach (Federal Institute of Technology, Zurich), Huaiyu Shao (I^2CNER).

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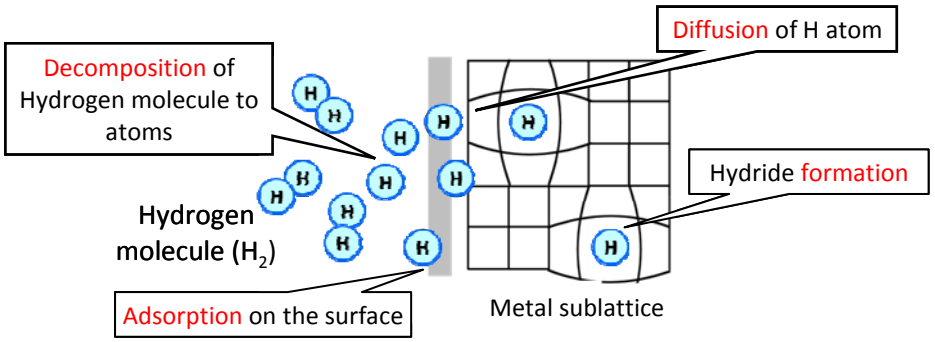

Fig. 5a. Fundamental processes at the surface of hydrogen storage materials

Research Highlights and Accomplishments

A number of technical accomplishments were achieved by the team over the course of the last year. To explore in detail the atomic scale microstructural changes that take place in storage materials during hydrogen absorption and release, the team has developed ex situ transmission electron microscopy tools that are now being applied to hydrogen storage alloys such as Ti,V. Through joint investigations between the Hydrogen Storage and Hydrogen Structural Materials Division, these tools are offering new insights into the microstructural changes that accompany hydrogen absorption and release, which point to the formation of twin boundaries and stacking faults during hydrogenation.

The effects of lattice geometry (lattice size, atomic radii) on hydrogen diffusion kinetics have been explored in Mg-Co alloys, the results of which have initiated new collaborations combining experiment with atomic-scale modeling and simulation at Illinois. Further study has demonstrated the role of nanostructuring and catalysts on the performance of Mg-based materials. In collaboration with the Hydrogen Production Division, the Hydrogen Storage Division demonstrated that grain boundary refinement achieved via high-pressure torsion (HPT) in metallic compounds improves their hydrogen storage capability. Experiments revealed that the grain refinement achieved through HPT is most important for improving the hydrogen absorption rate, pointing to grain boundaries as active storage centers that can be exploited for enhanced performance. HPT was also applied to the nanoscale grain refinement in (typically hard to refine) intermetallic compounds. The team has also demonstrated that HPT-processing of metals such as Pd can minimize structural deformation such as volume expansion during hydrogen uptake.

Future Directions

Using the newly-developed TEM characterization tools, the team will establish the formation mechanism of lattice defects in Ti,V BCC alloys and other hydrogen storage materials during hydrogenation/ dehydrogenation towards the guided design of high performance materials. In collaboration with nanoscale synthesis and computational modeling capabilities at UIUC, the team will explore geometrical effects on performance. Building on the accomplishments of the team, future efforts will target a number of avenues related to elucidating and exploiting microstructural effects on hydrogen storage. These include

continued efforts to exploit HPT for microstructure refinement and enhanced performance. The team will explore the reduction of hydrogen absorption temperature in metallic compounds via the introduction of catalysts, the application of HPT to the hydrogen storage intermetallic FeTi, and the quantitative evaluation of the effect of grain structure on volume expansion and microstructural changes in Pd and other metals of interest during hydrogen cycling.

Impact on Science and Engineering

By establishing the role of microstructural defects such as grain size, grain boundaries, and twins in hydrogen storage materials, the Hydrogen Storage Team is unlocking insights to exploiting properties for enhanced hydrogen storage performance. To date there have been few reports on defects and microstructure change due to hydrogenation in metals/intermetallics, although it has an important role in hydrogen pressures, reaction rates, effective absorbing capacity and cyclic stability. The impact of the work conducted by the hydrogen team has been demonstrated through a number of recognitions, including a Japanese Society of Applied Physics Excellent Paper Award for 2011 for Prof. Akiba's research; and Prof. Horita's work on HPT processing for nanostructure control of metallics was recognized as a top cited paper of 2011.

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

6. Materials Transformations—Catalysis

Goals

Activities in FY 2011 focused on investigations of catalysis-related, waste-free and low-carbon technologies combining the individual strengths to form a strong team with excellent coverage of relevant topics. The program is unified with a focus on transformations of "small molecules" (H_2, O_2, H_2O, CO_2), all of which impact green technologies. This interdisciplinary knowledge is also required for training the next generation of scientists.

Research Team

Division Leader — organic chemist Tsutomu Katsuki (I^2CNER), Kazuhiro Matsumoto (Chemistry), Takahiro Matsumoto (Applied Chemistry), Annada Maity (Institute for Materials Chemistry and Engineering), Hidetaka Nakai (Applied Chemistry), bioinorganic chemist Yoshinori Naruta (Institute for Materials Chemistry and Engineering), inorganic chemist Seiji Ogo (Applied Chemistry), Takehiro Ohta (Institute for

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 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.

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Materials Chemistry and Engineering), organometallic chemist Thomas Rauchfuss (Chemistry, UIUC), Tatsuya Uchida (Chemistry), and physical Chemist Miho Yamauchi (I^2CNER).

Research Highlights and Accomplishments

A central theme in catalysis — both green and "real-world" — is the oxygen reduction reaction (ORR), which is a major barrier to the further development of fuel cells (FCs). Several aspects of the problem have been attacked — new catalyst designs, use of earth-abundant metals, and new ways of supporting catalysts for low overpotentials and easier implementation. New catalysts have been developed in the form of carbon nanostructure-controlled electrocatalysts that exploit polymer-wrapped carbon nanotubes. The work puts an emphasis on materials processing with attention to both traditional fuel cells using polymer-wrapped, multi-walled carbon nanotubes, and next generation catalysts that either avoid or more effectively utilize precious metals for ORR.

Inspirations for our work on FCs are the enzymes that support life in air-breathing organisms. Progress has been made on biomimetic Fe-Cu catalysts that reduce dioxygen to water at low overpotentials. The work has also led to the detection of O_2-bound intermediates in homogeneous systems. These developments underpin a powerful new concept of membrane-less FCs that contain catalysts selective for both cathode and anode reactions.

Overlapping with work on ORR, another theme deals with oxidative processes, exploiting our skills in materials science and organic synthesis. New heterogeneous catalysts have been developed consisting of alloys of iron-group metals, Fe-Co-Ni and applied to the oxidation of the commodity chemical ethylene glycol. Correspondingly, we have developed homogeneous catalysts composed of Fe-imino-naphthoxide complexes, which catalyze the corresponding aerobic conversions of secondary alcohols. The work has been extended to broadened substrate range, exploiting the role of hydrogen-bonding between substrate and catalyst, a theme of continuing interest across the entire team. Advances have also been made in catalysts for water oxidation and proton reduction. These two reactions comprise the ultimate devices that will produce solar fuels.

Future Directions

The team will expand cross-training of students leading to

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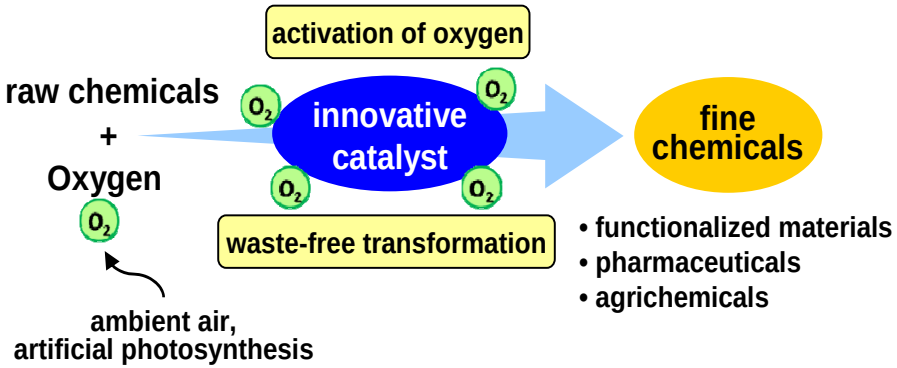

Fig. 6a. Concept of a catalyst process for a "zero-waste/no-carbon" reaction

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

cross-fertilization of projects. Emphasis on small molecules and fuels cells and solar energy will continue.

Impact on Science and Engineering

Catalysis is central to all technologies related to energy management from capture of solar photons to the consumption of fuels.

7. CO_2 Separation and Concentration

Goals

The objective of this work is to determine and exploit the unique physical and chemical characteristics of CO_2 that will diminish the cost of its capture and/or sequestration, and hence impel carbon-neutral power generation. This is a highly interdisciplinary line of work that brings to bear expertise in electrochemistry, interfacial science, and experimental fluid mechanics to advance three major technologies: (i) advanced absorbent materials; (ii) electrochemical methods for CO_2 separation; and (iii) near-critical CO_2 flows over solid active surfaces.

Research Team

Division Leader — Masaki Minemoto (Chemical Engineering), Shigenori Fujikawa (I^2CNER), Katsuki Kusakabe (Nanoscience, Sojo University), Dimitrios Kyritsis (Mechanical Science and Engineering, UIUC), Yosuke Matsukuma (Chemical Engineering), Paul Kenis (Chemical and Biomolecular Engineering, UIUC).

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.

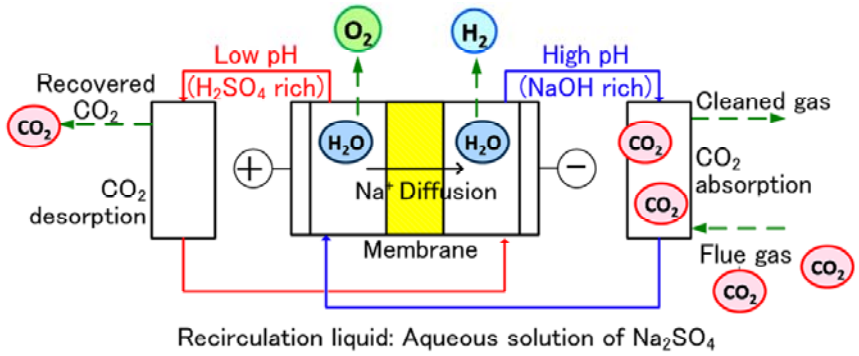

Fig. 6a. An advanced CO_2 separation and concentration system

Research Highlights and Accomplishments

In the area of advanced adsorbent materials, substantial progress was made towards overcoming the caveat of zeolites for CO_2 adsorption that relates to competing adsorption of water vapor. Prof. Kusakabe's group developed a Metal Organic Framework based on Zn (MOF-5, $Zn_4O(1,4\text{-benzenedicarboxylate})_3$) that can be produced from relatively cheap raw materials and achieve specific surface area in excess of 1000 m^2/g. MOF-5 crystals with a crystal size on the order of 20 μm were formed on α-alumina substrates through immersion into dimethylformamide solutions of $Zn(NO_3)_2$. The crystalization reaction commences approximately six hours after reactant preparation and is completed within 21 hours.

The adsorption work is closely interwoven with the absorption-desorption electrochemical method that has been developed and utilizes an aqueous K_2CO_3 solution in order to capture CO_2 in the form of $KHCO_3$, and then desorb it using cation and anion exchange membranes. Desorption happens in vacuo (0.05-0.10 atm), but the power needed to preserve the vacuum clearly outweighs the heat necessary for a classical desorption process. The energy consumption for separation with the newly established technology is on the order of 1000 kJ/kg of CO_2, which is roughly equal to one quarter of the corresponding consumption for current technologies. Moreover, the innovative process that has been devised can proceed at room temperature. We note that the work in electrochemistry for CO_2 separation couples with fusion work on electrochemistry for CO_2 conversion to high-value chemicals.

The separated CO_2 will have to be compressed in high-pressure, low-temperature reservoirs, which will bring CO_2 to the near-critical regime. A near-critical flow facility was established in the University of Illinois and laser-induced fluorescence measurements were performed to establish the anomalous entrainment of compressor oils by near-critical CO_2. In particular, it was shown that mass flow rate of entrained fluid was closely proportional to the fourth root of the pressure differential, a result that is clearly distinct from the square-root scaling predicted in classical fluid mechanics. It was established that complex flows can be utilized to reject the oil from the CO_2 stream. The application of laser-based diagnostics was pursued with the establishment of the fundamentals of a Raman-based measurement of greenhouse potential.

Future Directions

In the next year, the work on advanced adsorbent materials will be integrated with the electrochemical separation efforts. The determination of thermophysical properties for near-critical flow will benefit from the KU/Illinois collaboration, where Brillouin-scattering measurements will be performed in the optically accessible apparatus in Illinois. The ultimate goal is to couple the separation and sequestration activities in order to provide efficient capture technologies based on the unique physical chemistry of CO_2.

Impact on Science and Engineering

Pioneering work on adsorption and electrochemistry has advanced interfacial science through the establishment of materials with exceptionally high specific surface. Adsorption engineering has been promoted with the demostration of micro-porous organic/inorganic composites as absorbents. The unique electrochemical properties of aquaeous carbonic solutions have been shown to be able to provide CO_2 -separation methods that require roughly one quarter of the energy needed for currently used technologies. Moreover, the near-critical flow research highlighted the anomalous behavior of the thermal and transport properties in the vicinity of the critical point, as well as the elimination of the distinction between the two phases in supercritical conditions. As a result, a novel flow regime has been established that sits at the border of the classical disciplines of single-phase and two-phase flow.

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

8. CO_2 Storage

Goals

The goal of the CO_2 Sequestration and Storage Division is to develop scientific understanding, tools, and technology to enable design, analysis, and risk assessment of approaches to geologic storage of CO_2, both in onshore and sub-seabed locations. The work includes experimental, computational, observational, and analytical components, as well as educational and public outreach. We develop techniques and instrumentation to monitor CO_2 storage in onshore and sub-seabed reservoirs, to understand fundamental mechanisms of CO_2 behavior in porous geological formations, and to assess safety.

Research Team

Division Leader — Tetsuo Yanagi (Research Institute for Applied

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.

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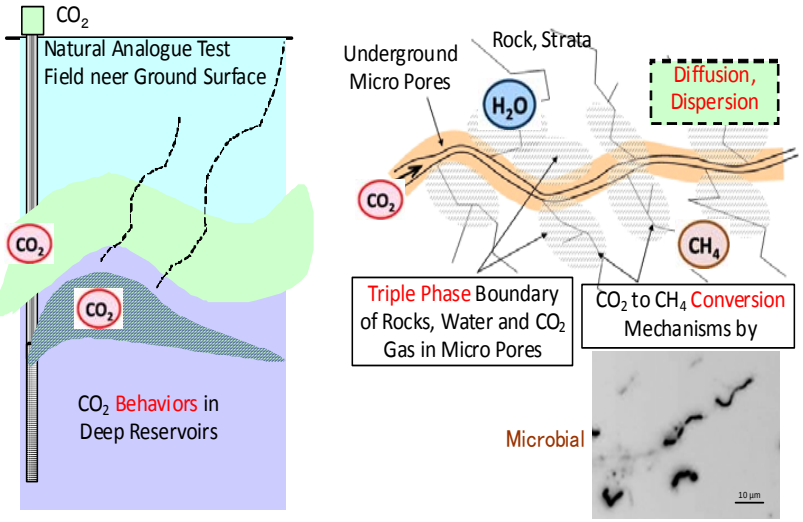

Fig. 8a. CO_2 geological storage

Mechanics), Chen-Tung Arthur Chen (National Sun Yat-Sen University, Taiwan), Kenneth Christensen (Mechanical Science and Engineering, UIUC), Robert Finley (Illinois Geological Survey), Sallie Greenberg (Illinois Geological Survey), Changhond Hu (Research Institute for Applied Mechanics), Hiroyuki Kajiwara (Marine Systems Engineering), Keigo Kitamura (I^2CNER), Masahiko Nakamura (Research Institute for Applied Mechanics), Kiminori Shitashima (I^2CNER), Arne Pearlstein (Mechanical Science and Engineering, UIUC), Makoto Sueyoshi (Research Institute for Applied Mechanics), Jong Hwan Yoon (Research Institute for Applied Mechanics).

Research Highlights and Accomplishments

At Kyushu University (KU), a high-pressure system for measurement of relevant properties under conditions of supercritical CO_2 storage has been built. Numerical studies of CO_2 behavior in porous heterogeneous Tako sandstone show that behavior is strongly influenced by small-scale porosity. Instrumentation continues to be developed for monitoring liquid, gaseous, and dissolved CO_2 in the ocean and in rock under high pressure. Collaboration has been initiated with the Illinois State Geological Survey, the Midwest Geological Sequestration Consortium (MSGC), and other foreign and Japanese partners in the area of rock physics, as well as fusion research to develop instrumentation to quantify relevant metal ions in brine. Planning has been completed for additional observational campaigns to study CO_2 drops and bubbles rising from natural vents in the Western Pacific, Kagoshima Bay, and near the Italian island of Panarea. The dynamics of CO_2 in saline aquifers is being studied in a Refractive Index Matched (RIM) facility by flowing surrogate fluids through a permeable bed, allowing high-resolution optical measurements in geometrically complex domains. In addition, an optically-accessible flow facility was built to probe the fundamental physics and three-dimensional interactions of a bubble plume with surrounding liquid, with application to CO_2 leakage into the ocean from sub-seabed storage. Computational work has developed an initial model for the case of axisymmetric flow driven by a density difference between the CO_2 drop and the aqueous phase, with a "clean" interface.

A significant element involves field studies of CO_2 drops and bubbles rising from natural vents in the Western Pacific and Japanese coastal waters. Work at Illinois uses experimental and computational approaches to understand multiphase flow relevant to risk assessment

of CO_2 storage. Experiments focus on dynamics of supercritical CO_2 in porous media, fault formation due to over-pressurization, and behavior of gaseous and liquid CO_2 inadvertently released into the ocean from sub-seabed storage. Computations focus on predicting motion and dissolution of escaped liquid drops in the ocean. Collaborative efforts include use of KU field data to validate and refine computational models developed at Illinois, joint development of hydrate film models, and the use of Illinois experimental data and computational results in risk-assessment modeling at KU.

Future Directions

Future work will use high-pressure facilities to measure elastic wave velocities, relative permeability, and resistivity of various rock types from MGSC and other cores, and will provide estimates of CO_2 saturation. We will also study the geochemical evolution of rocks, develop a reservoir model using geophysical and geological data, and perform reservoir-scale simulations of long-term CO_2 storage. We will continue field observation of naturally-vented CO_2 bubbles and drops, develop a 3,000 m class virtual mooring system and towed vehicle system, and participate in UK-based experimental and field work directed to monitor and assess marine impacts of geological storage of CO_2. Future Illinois experimental work on CO_2 migration through porous media will introduce an immiscible fluid to simulate CO_2, allowing study of fluid-fluid interactions. We will also develop microscale pore-space models to study interactions between infiltrating and pore-saturating fluids. Two-phase plume measurements will consider dispersion of drops rising into the surrounding liquid. On the computational side, we will complete axisymmetric computations for rising CO_2 drops, absent dissolution, pressure dependencies and the presence of a hydrate film, and accounting for variation of density and viscosity with pressure/depth. We will formulate detailed models for the hydrate film, with emphasis on its mechanics and mechanisms by which CO_2 diffuses through it.

Impact on Science and Engineering

The I^2CNER effort will have major impact on risk assessment for potential CO_2 injection sites. It will contribute to protocols to monitor, verify, and account for injected CO_2 using seismic, gravity, resistivity, surface deformation, and fluid sampling measurements. Understanding the dependence of elastic wave speeds on CO_2 saturation will be key to seismic estimation of the latter. CO_2 -monitoring instrumentation will

find use in other marine applications. Observational data will provide insight into natural venting processes, and help refine drop dynamics computations and develop interfacial hydrate film models. Our experimental work addresses issues of risk assessment and mitigation with respect to geological storage of CO_2, including in the sub-seabed. As reservoir-scale prediction of CO_2 fate depends on pore-scale mechanisms, our experiments seek to provide detailed data at these scales, from which accurate microscale models can be developed and validated for use in larger-scale simulations. Our computational work will produce a code capable of predicting the fate of liquid CO_2 drops in the ocean and as they rise through faults. Ultimately, results can be incorporated (e.g., as a subgrid-scale model) into reservoir-scale simulations of long-term viability of sub-seafloor CO_2 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

The CO_2 ocean sequestration division was consolidated with the Geological Storage Division into one division titled "CO_2 Storage" as presented above.

9. Energy Analysis

Goals

The goals of the Energy Analysis Division (EAD) are to ensure that the I^2CNER research is relevant to the future carbon-neutral energy infrastructure for Japan, ensure that I^2CNER research is informed of all relevant current and future energy options, and to help enable an I^2CNER Vision and Roadmap for a low carbon energy infrastructure for Japan.

All analyses will include cost, energy use, and greenhouse gas (GHG) emissions. Analyses will be done on a Well to Wheel (WTW)/Cradle to Grave (CTG) basis where all activities, costs, and energy flows will be tracked throughout the energy pathway from the source of the primary energy (e.g. a natural gas well) through the final use of that energy (e.g. as electricity from a gas turbine for use in the residential market or hydrogen from natural used in a fuel cell vehicle).

Research Team

Kuniaki Honda (Gas and Power Co.), Mark Paster (US Department of Energy, Retired), James Stubbins (Nuclear, Plasma, and Radiological Engineering, UIUC).

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.

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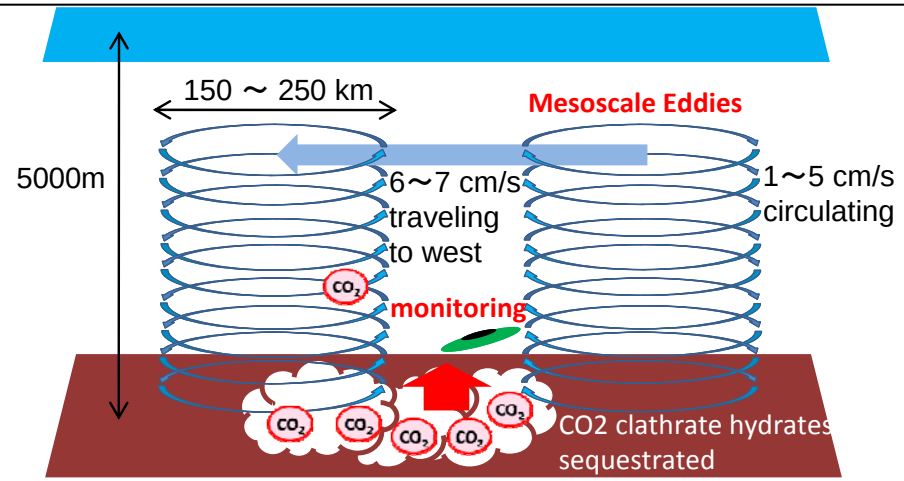

Fig. 9a. CO_2 ocean sequestration

Research Highlights and Accomplishments

The EAD will begin its efforts by understanding the current energy picture in Japan and its future needs. It will analyze the current energy pathways used and the future potential energy pathways that reduce carbon emissions including those that could utilize the I^{2}CNER research efforts. It will compare the I^{2}CNER technology linear WTW/CTG energy pathways to both current and other future potential energy pathways to ensure that the I^{2}CNER research is relevant from a cost, energy use, and low GHG gas emissions basis. In time the EAD will employ the use of energy macro-system models to analyze how I^{2}CNER technologies can penetrate the Japan energy infrastructure. Through the use of both linear WTW/CTG energy pathway and energy macro-system modeling, The EAD will help enable I^{2}CNER to develop a Vision and Roadmap for a low carbon energy infrastructure for Japan.

The Energy Analysis Division has only recently been initiated. So far its efforts have been focused on establishing a plan and scope as well as beginning to hire resources for the effort. The accomplishments achieved so far include: a Draft Plan for the I^{2}CNER Energy Analysis Division , several sources of data on the current energy situation in Japan have been identified and are starting to be compiled, the list of all energy pathways that will be examined is being defined, and U.S. analyses of several important hydrogen production and hydrogen delivery pathways have been identified. The latter includes an initial analysis of the potential cost for the production of hydrogen utilizing sunlight to split water which is a key pathway being researched by I^{2}CNER.

Future Directions

The near term tasks for the I^{2}CNER EAD effort include: complete the staffing for the EAD, gather the data required to quantify the cost, energy use, and GHG emissions for the current energy pathways in use in Japan, and begin to analyze and model the potential energy pathways that could utilize the I^{2}CNER research efforts.

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 new Administrative Director was assigned to the Administrative Office as of August 1, 2011. 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 19 staff members (as of April 1, 2012) have established support systems under the supervision of the Administrative Director and the Associate Administrative Directors.

- 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. Two members in the research support and international affairs group hold PhDs, which enables them to better communicate with I^2CNER researchers.

- Administrative staff members have a good command of English, which allows for smooth English communication between the Institute Director and other 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, and offers full-time support to international researchers in the area of invitation procedures including visa application processing and accommodations on campus. Additionally, the I^2CNER Administrative Office provides extensive living support and assistance with medical checkups, private accommodations, family support, travel arrangements, and introduction to the Japanese social insurance system including medical, just to name a few.

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. • The Institute will be established as an organization under the direct	2) Decision-making system • The Director's decision-making authority has been established by preparing applicable governing documents to apply a top-down approach, in consultation with the Science Steering Committee that consists of the Institute Director, Vice-Director, Associate Directors and division leaders on the following topics: o Research policy o Personnel affairs o Important matters on Institute research o Establishment, revision, or abolition of rules

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.	Compensation considerations based upon a special agreement between I^{2}CNER and Kyushu University entitled "Regulations on Special Measures on the Hiring of National University Corporation Kyushu University International Institute for Carbon-Neutral Energy Research Employees" • The Institute has established the following "Governing Documents:" o Rule of Members o Science Steering Committee o External Advisory Committee o Program Evaluation Process o Faculty Recruiting Process o Faculty Excellence Program o Research Assistant (RA) Program o Postdoctoral Research Associates for Foreign Principal Investigators o Roles and Responsibilities of Administrative Office o Organization and Sponsoring of Conference or Workshop o Start-up Funding for Interdisciplinary Research o Guidelines for Visiting Student Acceptance o Guidelines for WPI Visiting Researchers o Guidelines for International Institute for Carbon-Neutral Energy Research Project Funds, Kyushu University o Rules on Indirect Cost of Competitive Funds o Faculty Promotion • The Director is assisted by Vice-Director Yukitaka Murakami, Associate Directors Kazunari Sasaki, and Tatsumi Ishihara, who was newly appointed as the second Associate Director as of February 1, 2012. At the Illinois Satellite Institute, Professor Kenneth Christensen serves as Associate Director. An External Advisory Committee comprised of national and international distinguished 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 2011	Results at end of April 2012
Researchers from within host institution	16	16	16 (March, 2011)	21	20
Foreign researchers invited from abroad	11	11	11 (March, 2011)	11	24
Researchers invited from other Japanese institutions	3	3	3 (March, 2011)	1	1
Total principal investigators	30	30	30 (March, 2011)	33	45

All members

- In the “Researchers” column, put the number and percentage of overseas researchers in the < > brackets and the number and percentage of female researchers in the [ ] brackets.
- In the “Administrative staffs” column, put the number and percentage of bilingual staffs in the ( ) brackets.

	At beginning	Planned for end of FY 2010	Final goal (Date: month, year)	Results at end of FY 2011	Results at end of April 2012
Researchers	71 <21, 30%>	92 <36, 39%>	130 <54, 42%> (March, 2014)	84 <26, 31%>[4, 5%]	117 <41, 35%> [7, 6%]
Principal investigators	30 <11, 37%>	30 < 11, 37%>	30 <11.37%> (March, 2011)	33 <11, 33%>[2, 6%]	45 <24, 53%> [3, 7%]
Other researchers	41 <10, 24%>	62 < 25, 40%>	100 <43, 43%> (March, 2014)	51 <15, 29%>[2, 4%]	72 <17, 24%> [4, 6%]
Research support staffs	32	37	51 (March, 2013)	39	58
Administrative staffs	23	23	23 (March, 2011)	18 (16, 89%)	21 (19, 90%)
Total	126	152	204	141	196

-“Results at end of April 2012” are calculated by including the total of 31 Illinois Satellite members (15 researchers, 14 research support and 2 admin. staff members)

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	ii) Satellites <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. (please also see <Collaboration with Other Institutions> under section 1.)
iii) Partner institutions <Initial plan> <u>Institution (1)</u> 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)	iii) Partner institutions <Results/progress/alternations from initial plan> The Participating Institutions, Personnel, and collaborating divisions are: • Atmosphere & Ocean Research Institute at the University of Tokyo, Dr. Mitsuo Uematsu, CO_2 Sequestration and Storage Division • National Institute of Advanced Industrial Science & Technology (AIST), Visiting Researchers to HYDROGENIUS, AIST: Professors Matsuoka, Sugimura from Hydrogen Structural Materials Division, and Takata from Thermophysical Properties Division • University of California, Berkeley, Professor Robert Ritchie, Hydrogen Structural Materials Division • Massachusetts Institute of Technology, Professor Harry Tuller, Fuel Cells Division

• Massachusetts Institute of Technology (USA) • Sandia National Laboratories (USA) • 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)	• Sandia National Laboratories, Dr. Brian Somerday, Hydrogen Structural Materials Division • Imperial College of London, Professor John Kilner, Hydrogen Production Division • Swiss Federal Institute of Technology Zurich (ETH), Professor Ludwig Gauckler, Fuel Cells Division • Tsinghua University, Professor Xing Zhang, Thermophysical Properties Division • Dalian Institute of Chemical Physics, Chinese Academy of Sciences, Professor Ping Chen, Hydrogen Storage Materials Division • University of Göttingen, Professor Reiner Kirchheim, Hydrogen Structural Materials Division • Swiss Federal Institute of Technology Zurich, Professor Louis Schlapbach, Hydrogen Storage Materials Division • National Sun Yat-sen University, Professor Chen-Tung Arther Chen, CO_2 Sequestration and Storage Division • Sojo University, Professor Katsuki Kusakabe, CO_2 Separation and Concentration Division • Central Research Institute of Electric Power Industry, Dr. Kimio Miyakawa and Dr. Hideshi Kaieda, CO_2 Sequestration and Storage Division • Research Institute of Innovative Technology for the Earth, Dr. Jun Kita, CO_2 Sequestration and Storage Division • Kyoto University, Professor Toshifumi Matsuoka, CO_2 Sequestration and Storage Division • National Oceanography Center, Professor Ian Wright, CO_2 Sequestration and Storage Division • University of Nottingham, Dr. G. Caramanna, CO_2 Sequestration and Storage Division • The Scottish Association for Marine Science, Dr. Henrik Stahl, CO_2 Sequestration and Storage Division • University of Tokyo, Professor Toru Sato, CO_2 Sequestration and Storage Division • Royal Norwegian Embassy, Dr. Per Christer Lund, CO_2 Sequestration and Storage Division • Japan Agency for Marine-Earth Science and Technology, Dr. Toshiro Saino, CO_2 Sequestration and Storage Division

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, advertisements for the positions will be placed on the web site of the Kyushu University, the Kyushu University Offices overseas in Great

<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 Directors. As of April 1, 2012, the General Affairs and Human Resources group had 6 members; the Research Support and International Affairs group had 3 members, two of which possess a doctoral degree and the technical background necessary to successfully administer this office; the Public Relations had 4, and Accounting and Contracting group had 4 members.

- A rule was established that one technical staff member should be hired for every PI of Kyushu University that is hired and 7 technical staff members were newly hired during FY 2011.

2) Startup research funding

- To encourage inter-division research within I^2CNER, we have set up "Start-up funding for interdisciplinary research." In FY2011, nine (9) projects have been approved and started (Please see details in Reference 14 "Fusion of Research Areas")

- Start-up research funding has been allocated to newly hired I^2CNER full-time researchers to develop their research environment.

3) Postdoctoral positions resulting from open international solicitations

- From October to December 2010, the first open international recruiting call was conducted. Advertisements were published in international academic magazines such as Nature and Science and yielded 61 faculty

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.	applicants and 75 postdoctoral applicants. The Faculty Recruiting Committee reviewed the applications and identified candidates for an on-site interview. As a result, 8 faculty members (1 associate professor, 7 assistant professors) and 1 post-doctoral research associate joined the Institute on or after April 1, 2011.
• 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."	• From March to June 2011, the second open international recruiting call was conducted. Out of 32 faculty applicants, 4 were invited for on-site interviews and presentations and 1 was hired as an associate professor. Out of 50 postdoctoral applicants, 6 were invited for on-site interviews and presentations, and 1 was hired.
• 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.	• From August to November 2011, the third open international recruiting call was conducted. Out of 13 faculty applicants, 6 were invited for on-site interviews and presentations and 2 were hired (1 associate professor and 1 assistant professor). Out of 12 postdoctoral applicants, 2 were invited for on-site interviews and presentations, and 1 was hired.
• We also plan to recruit an international research assistant or a research administrator (RA) for the Institute's administration management department.	• 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.
	• I^2CNER's fourth international open recruiting call began in March 2012.
	• 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. Through this program, a female researcher was hired and appointed as a PI as of January 1, 2012.
	• In total, 15 researchers (12 faculty members and 3 post-doctoral research associates) joined the Institute in FY 2011.
4) Administrative personnel who can facilitate the use of English in the work 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.	• Administrative staff members have an excellent command of English. Drawing on this experience, the Administrative Office has been organized in such a way that enables the development of a research

• 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 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.	environment where researchers will be able to concentrate on research activities. • In cooperation with the International Affairs Division at Kyushu University, English versions of various applications and other forms have been introduced. Additional training and workshop opportunities are offered to assist in the transition for international researchers while they are 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 (a special agreement between I^2CNER and Kyushu University entitled "Regulations on Special Measures on the Hiring of National University Corporation Kyushu University International Institute for Carbon-Neutral Energy Research Employees") which deviates from the established salary ranges. Individual faculty and researcher salaries are determined based on individual accomplishments and contributions to the interests of the Institute. • The Institute provides a "site allowance" for jointly-appointed KU faculty members based on performance evaluation. A salary increase for the following fiscal year has been given to I^2CNER full-time faculty members who were highly evaluated.
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	6) Equipment and facilities, including laboratory space, appropriate to a top world-level research center • In order to continue developing a research environment befitting a top world-level research institute, a new building has been under construction, will be completed in autumn 2012, and will open in

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 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.

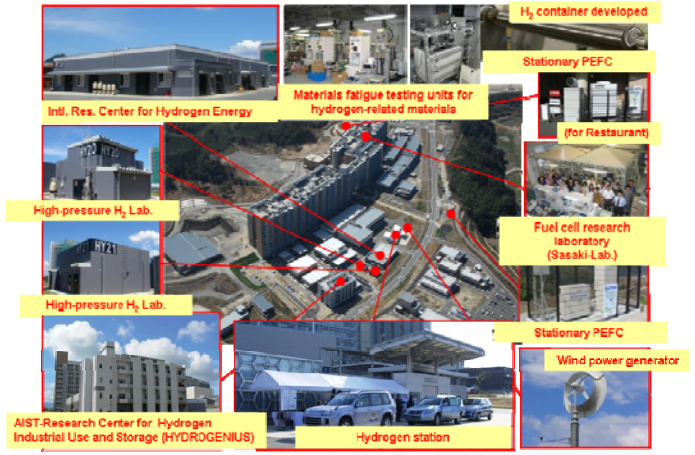

Fig. Overview of the Hydrogen Energy Research Facility in the ITO-Campus of Kyushu University, with ca. 100 research staffs and 100 students in >5000m^2 laboratory area.

January, 2013. The Institute is planning to complete the move in winter 2012/2013.

- Six (6) common-use laboratories have been secured and shared by researchers from various fields.

- Three (3) laboratories have been secured for I^{2}CNER full-time researchers, where new equipment has been installed, and where some researchers brought equipment from their previous work place, as well.

- The following pieces of equipment have been purchased:

  -Horiba EMGA-930 (O_2, H_2, and N_2 analyzer)
  -High speed Laser Raman Spectroscopy
  -SmartLabTM Automatic X-Ray Diffractometer
  -Mode-locked Femto-second Ti: Sapphire Laser System
  -Fatigue Testing Machine combined with Scanning Electron Microscope
  -Pulsed Laser Deposition (PLD) Apparatus (Thin Film Deposition Methods)
  -NanoTR: Thermal Analysis System for Thin Films (Nanosecond thermoreflectance method)
  -PicoTR: Thermal Analysis System for Thin Films (Picosecond thermoreflectance method)

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 Annual Symposium 2012
  - Date: Jan. 31, 2012
  - Attendance: 170 national/international attendees
  - Description: I^2CNER's international symposium with 18 presentations from the following nine divisions were held at Kyushu University, Ito Campus:
    - Energy Analysis
    - Hydrogen Production
    - Hydrogen Storage Materials
    - Fuel Cells
    - Thermophysical Properties
    - Material Transformations
    - Hydrogen Structural materials
    - CO_2 Separation and Concentration
    - CO_2 Capture and Storage

- I^2CNER International Workshop 2012
  - Date: Feb. 2, 2012
  - Attendance: 109 national/international attendees
  - Description: Held in conjunction with the I^2CNER Annual Symposium 2012 on January 31, 2012 in Fukuoka Japan. Four workshops with a focus on individual research fields were held at Kyushu University, Ito Campus:
    - CO_2 Capture and Storage
    - Hydrogen Storage Materials
    - CO_2 Separation & Concentration
    - Material Transformations

- HYDROGENIUS & I^2CNER Joint Research Symposium
  - Date: Feb. 2, 2012
  - Attendance: 266 national/international attendees
  - Description: Held in conjunction with the 2012 International Hydrogen Energy Development Forum held on February 1, 2012 in Fukuoka, Japan. Five research symposia with a focus on individual research fields were held at Kyushu University, Ito

Campus:

- Hydrogen Fatigue and Fracture
- Hydrogen Polymers
- Hydrogen Tribology
- Hydrogen Thermophysical Properties
- Fuel Cells and Hydrogen Production

- I^2CNER Satellite Kick-off Symposium
  - Date: Mar. 6-7, 2012
  - Attendance: Around 100 national/international attendees
  - Description: Entitled "Powering the Future," the symposium offered attendees an overview of the most current energy breakthroughs, as well as the serious barriers to a carbon-neutral energy future. PIs from Kyushu and Illinois University explained their current research projects and suggested future research directions.

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 way 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. For a complete list of seminars hosted in FY2011, please see Reference 4.

C) Sponsoring of International Conferences

I^2CNER encourages its PIs to organize international conferences which are related to and promote the institute's specific goals and objectives:

- The 3rd ERATO Soft Interfaces Seminar (co-sponsored)
  - Date: Jul. 14, 2011

- The 4th International Conference on Heat Transfer and Fluid Flow in Microscale (co-sponsored)
  - Date: Sep. 4-9, 2011

- The 3rd Asian Symposium on Advanced Materials (co-sponsored)
  - Date: Sep. 19-22, 2011

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.	• The 3rd Dalton Transactions International Symposium (co-hosted) o Date: Nov. 16, 2011 • Nobel Prize Forum (co-hosted) o Speaker: Prof. Ei-ichi Negishi o Date: Feb. 16, 2012 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. • "Ito Guest House," an on-campus housing accommodation facility for short-stay researchers from overseas, was newly built on Ito campus, where I^2CNER is located. • International initiatives such as bilingual display (Japanese and English) of bus time tables at campus bus stops and destination signs of buses running between the nearest train station and campus, in addition to cafeteria menus that are available for the convenience of foreign researchers.

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;	<Current assessment> • There has been no deviation from the initial criteria and methods for self-evaluation. Using the indicators on the left, we assessed our activities from April 2011 to March 2012 as noted below: **1. WPI-Affiliated Publications** In FY 2011, there were 51 publications indicating WPI affiliation. Institute researchers published 27 joint papers with WPI acknowledgment in journals with an impact factor greater than 2. For a complete list of publications, please see Reference 5.

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 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.

2. Keynote and Plenary Lectures

The Institute's researchers were invited to give a total of 20 invited keynote and/or plenary lectures in FY 2011. For a complete list of Keynote and Plenary lectures, please see Reference 6.

3. Invited Lectures

The Institute's researchers were invited to give a total of 79 invited lectures in FY 2011. For a complete list of invited lectures, please see Reference 7.

4. Symposia organization in international conferences by Institute Researchers

The Institute's researchers contributed to the organization of a total of 21 symposia in FY 2011. For a complete listing of Symposia Organization, please see Reference 8.

5. Trend-setting workshops that attract participation of national agencies such as MEXT, JSPS, US NSF, US DOE, European Commission, etc.

The Institute's researchers conducted a total of 5 trend-setting workshops in FY 2011. For a complete list of Trend-setting Workshops, please see Reference 9.

6. Organization of International Conferences

The Institute's researchers participated in the organization of a total of 21 International Conferences. For a complete listing of Organization of International Conferences, please see Reference 10.

7. Participation of the Institute's researchers in international conferences (e.g. Gordon Research Conferences)

The Institute's researchers participated in a total of 88 international conferences. For a complete listing of Participation in International Conferences, please see Reference 11.

8. Invitations to the Institute's researchers for participation in government panels and national laboratory efforts

	The Institute's researchers served on a total of 14 government panels in FY 2011. For a complete listing of Participation in Government Panels, please see Reference 12. **9. Patents and technology accomplishments** The Institute's researchers contributed to a total of 22 patents. For a complete list of Patents, please see Reference 13. **10. Visitors to I^2CNER and Researchers Exchange between I^2CNER and collaborating institutions** Over the past year, as I^2CNER has become increasingly international, the number of visitors to I^2CNER has increased steadily. At the same time, many I^2CNER researchers are invited to and visiting foreign institutions such as the Illinois satellite institute. In particular, there were 32 visits made to I^2CNER by international WPI PIs. Among them, 15 visits were made by Illinois Satellite PIs.

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 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.	• The research funding shown on the left column also includes the funding for the Institute for Hydrogen Industrial Use and Storage at Kyushu University (HYDROGENIUS). If the HYDROGENIUS funding is excluded, the annual research funding average of KU PIs who work for I^2CNER was 9.5 million dollars for the period FY2006-FY2009. The corresponding total amount for FY 2011 is 16.36 million US dollars (Exchange rate: JPY/USD = 100), which amounts to a 30% increase.

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

<Initial plan>	<Results/progress/alternations from 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.	• 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. • KU has introduced a robust system in which the KU president reviews and examines all the structural reform plans submitted by each department every fiscal year, and provides a relevant number of faculty positions for the selected superior initiatives. Tenured faculty lines are extremely important for the recruitment and retention of young faculty. I^2CNER is in a continuous communication with the KU President regarding the introduction of tenured faculty lines in the Institute. So far, I^2CNER was allocated and filled one tenured position with an associated professor hired through its Faculty Excellence Program. • I^2CNER worked to advance interactions between the KU and Illinois Libraries. M. Schlembach and W. Mischo of the Grainger Engineering Library Information Center at Illinois visited KU Library on January 30, 2012. President Arikawa, Dr. T. Kuroki of WPI, Prof. Y. Fujiki (Executive Vice President) visited the Grainger Library on March 7. Areas of collaboration to be pursued are: the development of special tools and services for I^2CNER researchers; the implementation of a custom database of researcher publications and associated project data; A just-in-case document delivery for I^2CNER researchers; a joint data curation and data stewardship support structure; and coordination and assistance with depositing reports in the two library Institutional Repositories.

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 University will proactively support researchers, such as on information gathering and strategic advice on grant applications. In addition,

<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 information regarding research grants, providing strategic advice on grant applications, etc. In addition, two of the administrative staff

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.	members with a doctoral degree have taken charge of research support and international affairs. These staff members provide 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 December 2012. The Institute is planning to complete the move in winter 2012/2013. • Until the completion of the new facility, the Institute has secured temporary arrangements for the Director's office, the Administrative Office, 8 rooms for researchers, 9 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. • A salary increase for the following fiscal year has been given to I^2CNER full-time faculty members who were highly evaluated.
(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 project, the university will work in coordination with the parent	(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 their engagement in the Institute's activities in coordination with the

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. (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 Institute for flexible implementation, adjustment, modification of the university's internal systems, upon the requests from the Institute Director, in order	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 • 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 (a special agreement between I^2CNER and Kyushu University entitled "Regulations on Special Measures on the Hiring of National University Corporation Kyushu University International Institute for Carbon-Neutral Energy Research Employees") which deviates from the established salary ranges. The Institute also provides a "site allowance," as listed on p. 49, 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 External Advisory Committee. • A salary increase for the following fiscal year has been given to I^2CNER full-time faculty members who were highly evaluated.

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. (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.	(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 is currently under construction and is due to be completed around December 2012. • Prior to the completion of the construction of this new building, a Director's room, an administrative office, 8 research rooms, 9 experimental laboratories and a meeting room are arranged. (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. Efforts to improve points indicated as requiring improvement by Program Committee and results of such efforts	
-Points specified as needing improvement (as noted in Item 3 "Actions Required and Recommendations" in the FY2010 follow-up results)	-Efforts to improve them and results *If you have already described these in other parts of this report, please indicate where for reference.
1) The physical presence of Director Sofronis in KU should be at least more than 50% of his time, which should be reached earlier.	1) Director Sofronis intends to increase his physical presence at KU up to 50% and effort rate to 75% in 3 years. So far, his effort rate is certainly 75%. In the meantime, he will continue to utilize modern communication tools in order to effectively manage research and programmatic issues in addition to weekly videoconference meetings between Kyushu and Illinois division leaders. In FY 2011, the total number of days the Director was away from Illinois, working at Kyushu, promoting I^2CNER activities, looking for new talent, and building U.S. and international partnerships was 92. This number corresponds to 41.25% of his time. Out of the 92 days, 54 were spent at Kyushu University, which corresponds to a physical presence of 24.21%. So far, in FY 2012 (months of April, May and June), the Director spent 34 days traveling for I^2CNER business, including 31 days in residence at Kyushu University, time that was spread over the three months. These 31 days correspond to a physical presence at Kyushu of 55.6%. His plan is to continue in the future with such monthly visits to Kyushu.
2) The number of researchers is not yet at the required level. At this early stage it is critical that the Institute's recruitment of additional researchers proceeds expeditiously but at the same time attracts the very best candidates.	2) The agreement between KU and Illinois was concluded on March 25, 2011. Immediately upon the signing of the agreement the process of setting up the Satellite Institute got underway through a campus-wide call for proposals (see in <Collaboration with Other Institution> under 1. Summary of center project). The Satellite institute was fully established by August 2011. Thus, as of April 1, 2012, the total number of I^2CNER researchers is 118 (102 at Kyushu and 16 at Illinois) and the total number of I^2CNER members including both researchers and support staff is 193 (161 at Kyushu and 32 at Illinois). The number of Principal Investigators (WPI PI) is 45, 10 of whom are renowned international scholars and 13 are distinguished faculty of the University of Illinois. The Institute conducts recruitment campaigns semi-annually, looking for

	top-notch researchers whose research interests are in line with those of the Institute. The interview process which is carried out by the Faculty Recruiting Committee involves seminar presentations and interviews with the candidates. In addition, when a researcher is identified by any individual PI and is deemed a potential asset to the Institute by the SSC, the Faculty Recruiting Process is initiated. In particular, the latter approach is used for the Energy Analysis Division that was established recently given that it is generally difficult to find candidates through the standard advertisement process.
3) The effort rates of PIs should be raised to a reasonable level, at least more than 50%, as a WPI center. More active participation from Illinois is necessary. At least 10-20% of center-residing foreign PIs should be achieved.	3) In the I^2CNER report submitted for the 2011 WPI Site Visit, the reported PI effort rates were low because of a misunderstanding on behalf of the PIs in evaluating their participation effort in I^2CNER. This time, the PIs were asked to recalculate their efforts and also count as I^2CNER effort their engagement with other projects that are I^2CNER related. Since I^2CNER does not support the PIs' research budget, the PIs are seeking funding from other sources, thus establishing other I^2CNER related research projects. Further, the PIs were asked to count the training of their graduate students as I^2CNER related activity. Thus, after the recalculation of the effort rates by the PIs, the participation effort of half of the Kyushu PIs is larger than 80% (6=over 90%, 6= 80~90% , 5=70~80%, 3=60~70%). Though the Institute has yet to achieve the target rate of 10-20% of center-residing foreign PIs, the overall effort rates among the foreign PIs is on the rise (e.g. Professor Harry Tuller of MIT stayed at KU for collaborative research activities for about 1 month). While I^2CNER still maintains 0% center-residing foreign PIs, the foreign PIs who participate in I^2CNER have become fully engrained in the I^2CNER research culture. In fact, I^2CNER's research objectives are ideally pursued through this integral interaction and engagement of its foreign PIs. Additionally, I^2CNER is making a constant effort to recruit permanent-staying PIs by running semi-annual recruitment calls.
4) I^2CNER should establish its own vision and roadmap toward a carbon-neutral society over time scales of short, middle and long ranges.	4) A new Energy Analysis division has been established to address the issue of a roadmap. Please see details in <Research Organization> under 1. Summary of center project.

5) The mission of the WPI program does not seem to be exactly understood among scientific and administrative staff members.	5) PI meetings and orientation for new-hires have been conducted to ensure that I^2CNER research and administrative personnel understand the nature of the WPI program and its mission. In particular, the Director has met with individual PIs and clearly explained the four tenets of the WPI program, namely cutting edge research, interdisciplinary research approach (fusion), international collaborations, and system reformation. By way of example, in his annual evaluation letters to I^2CNER WPI faculty, the Director emphasized that publications addressing interdisciplinary research jointly with researchers across division boundaries and possibly with our international collaborators (e.g. Illinois) will weigh heavily on their promotion to the next level. More specifically, if the comment "The mission of the WPI program does not seem to be exactly understood among scientific and administrative staff members." is meant to imply that I^2CNER does not as of yet have at least 10-20% of center-residing foreign PIs, we would like to state the following: While I^2CNER still maintains 0% center-residing foreign PIs, the foreign PIs who participate in I^2CNER have become fully engrained in the I^2CNER research culture. Indeed, I^2CNER's research objectives are ideally pursued through the ongoing integral interaction and engagement of its foreign PIs who are actively involved in interdisciplinary research with their Kyushu counterparts. Additionally, I^2CNER is making a constant effort to recruit permanent-staying PIs by running semi-annual recruitment calls. We have received many applications from senior researchers from all over the world, but we have been very thorough in our screening process. Our approach is not to hire any senior faculty who would not be hired at a first-tier, world-renowned college of engineering in the United States, such as the University of Illinois, MIT, Stanford, or Caltech.

12. Efforts to improve points indicated as requiring improvement by the Working Group

-Points specified as needing improvement (extracted from the FY 2010 WPI Site Visit Report)	-Efforts to improve them and results *If you have already described these in other parts of this report, please indicate where for reference.
1. Quality of Science 1) WPI program generally requires core-mass of 10-20 world top class PIs. I^2CNER still does not meet this criterion. Another concern is the age of some of the top-level researchers that are close to the end of their career (retirement). It is strongly recommended to recruit first-class scientists, and also replacements must be sought in the near future to maintain and even increase the level of science with new perspectives.	1. Quality of Science 1) Please see response in 11. -2) and 11.-3) In addition, as of April 1, 2012, the list of WPI PIs includes 32 researchers linked with KU and Illinois. This brings the total number of researchers to 45, given that the Illinois Satellite has 13 participating faculty PIs. The future of our faculty who approach retirement has already been discussed in the SSC. We carry out biannual recruiting campaigns and we aggressively look to hire young and talented researchers.
2) There is no PI from Illinois participating at the time of the site visit. Although 9 foreign PIs are listed, their effort rates are low ranging from 3 to 35%. They should more proactively participate in the activities of I^2CNER. As for the fund committed, it is necessary to define a clear structure for the finances, money allocation etc. for both center partners, and to define rules of accountability. Illinois partners must use the given resources as leverage to secure additional block funding from the US, which is critical to the success of the partnership.	2) Please see response in 11. -2) and 11.-3). In addition, as of April 1, 2012, thirteen (13) faculty of the University of Illinois participate in the Satellite Institute. After the establishment of the Satellite, the Illinois researchers do participate in I^2CNER activities. By way of example, the Satellite faculty and a large number of foreign PIs participated en masse in the Annual Symposium at KU on January 31, 2012. As for the fund committed, the Institute handles the finances based on the agreement between Kyushu University and the University of Illinois. In order to share the same understanding of WPI fund allocation and its handling, efforts have been made such that personnel visits (persons responsible for the finances) between the two universities are properly implemented with regard to accounting at both ends. The Illinois faculty have already leveraged their I^2CNER funding to obtain block funding by submitting proposals to NSF for the following programs: a) PIRE (Partnerships for International Research and Education) jointly with KU; b) Interdisciplinary Graduate Education and Research Training (IGERT); c) The G8 Research Councils Initiative on Multilateral Research Funding: Material Efficiency. The Illinois efforts shall continue.

3) To obtain information from industries or other related projects of NEDO and RITE would be beneficial to update the vision. It is also recommended to obtain the advice of organizations in hydrogen (DOE in the US, for example) and of experts that have accomplished significant work on hydrogen production and utilization.	3) The Director and the Vice-Director are making contacts in the US, Europe, and Japan to promote a network of interaction and exchange on research and energy policy between academia, national laboratories, industry, and government. The Director is consulting frequently with members of the Energy Efficiency and Renewable Energy Office of the U.S. DOE to make sure that the I^2CNER research program is always informed on the latest technology and economic developments. By way of example, I^2CNER researchers already collaborate with researchers from the Exxon Mobil Research and Engineering Company, I^2CNER will work in concert with Mohawk Innovative Technology to coordinate material selection for future hydrogen compressor concepts, and Toyota Motor Corporation on fuel cells.
2. Fusion of research areas 1) It is again too early to comment on fusion research, but any fusion between different research teams was not much evident during the site visit.	2. Fusion of research areas 1) Certainly, by June 2011, it was too early to showcase any fusion research in the Institute. The Director and Vice Director were still studying the capabilities of the I^2CNER researchers before they could initiate any fusion projects.
2) I^2CNER should initiate proper action toward creation of fusion studies. New interdisciplinary projects should be created to cover the gap between existing team projects by the top-down suggestions from I^2CNER leader and senior PIs. To do this, the issue-driven research would be a promising pathway. As the bottom-up approach, frank discussion should be most important for the development of fusion. A major effort will be required to create the atmosphere and opportunities for fusion to well up at the initiative of the PIs, graduate students, and post-doctoral scholars. The regularly scheduled seminars are a good example in general, with the directed seminars of issues in common research areas ("Institute Interest Seminar Series") being especially effective. The Director must work with Kyushu University to assure that faculty performance review credits (rather than faults) for participating in, and contributing to interdisciplinary research.	2) To promote interdisciplinary research across division boundaries, the SSC introduced a new program titled "Start-up Funding for Interdisciplinary Research" to solicit research proposals for start-up funding. Only joint proposals by faculty from at least two divisions are considered for review. So far, nine (9) proposals have been selected after rigorous screening and the full listing of the ongoing interdisciplinary research projects can be found in Reference 14. In addition, to promote the "Fusion" mode of operation at all levels of the Institute, I^2CNER instituted division seminars (weekly or bi-weekly) and plans to organize retreats and open planning meetings, to further cultivate interdisciplinary activities. The "Institute Interest Seminar Series," where PIs and young researchers from different divisions interact with one another has been found to be especially effective in advancing fusion research (e.g. seed project titled "Theoretical and Experimental Design of Cross-linked Polymer Electrolyte Membranes for Use in Fuel Cells"). Further, as the culture of the institute advances with time, this fusion mode of operation is becoming the norm. Some of the newly hired faculty have already

	embarked on interdisciplinary/collaborative research on their own (e.g. Profs. Yamauchi and Sadakiyo)
3. Establishment of globally visible research center 1) More publicity effort may be necessary, particularly in terms of public relations and mass media. New research findings should be press-released without time lag. A team for publicity may be effective.	3. Establishment of globally visible research center 1) The Institute's Public Relations (PR) group currently has four (4) members working on outreach activities such as the publication of the "Hello! I^2CNER," the Institute's tri-annual newsletter that targets the general public and in particular, high school students. The PR Group is also responsible for the organization of public events to promote the Institute's research activities on a steady basis. Such a successful event was the WPI 6 Institutes Joint Symposium for high school students in November 2011. The PR group also administers the internal newsletter publication called "Fuse News" in collaboration with the Illinois Satellite office for the purpose of publicizing and sharing the I^2CNER's scientific activities, researchers (both senior and junior scientists), event calendar, etc. among all the I^2CNER members at both Kyushu and Illinois. I^2CNER organized (co-hosted/sponsored) and participated in the following events in FY 2011. For a complete listing of these events, please see Reference 15. Regarding the immediate press release of research findings, the PR group is working with the Public Relations Office of Kyushu University in creating a manual for researchers so their research outcomes are publicized without delay. By way of example, on September 9, 2011 there was a press release for the article on "Molecular catalysis in fuel cell" by Prof. Ogo that appeared in "Angewandte Chemie - International Edition" on November 18, 2011. The Administrative Office, especially the PR group is working aggressively on organizing public outreach events for FY 2012. For a complete listing of these events, please see Reference 16. The PR group arranges I^2CNER facility/laboratory tours for various guests/visitors to Kyushu University. During FY2011, the following numbers are indicative of the large scale of activities by the PR group: • I^2CNER visitors: 111

	• I^2CNER Seminar Series Speakers: 9 • Ad hoc visitors (from overseas, governments and universities): 84 • Facility-tour participants during 2012 annual symposium: 18 I^2CNER researchers present the Institute's activities worldwide by participating/attending international/national conferences, meetings, symposia, and workshops. By way of example, in the Gordon Research Conference Series, which is universally recognized for its importance and visibility, I^2CNER was represented by four (4) invited speakers in the 2011 Hydrogen Metal Systems Gordon Conference in Boston in July 2011. This is indeed a tremendous international recognition of the Institute and its stature in the international community.
2) I^2CNER still needs some time and continuous efforts to achieve high quality research work and to publish quality papers in major journals. It would also be most important to invite very active world-top level researchers as PIs and/or short-term visiting collaborators so that I^2CNER looks like a Mecca of the research on carbon-neutral society. Recruitment of top young scientists is mandatory; there was unfortunately no proof of competitiveness in this respect at the global level or even nationally during the site visit.	2) I^2CNER has adopted an aggressive semi-annual international recruiting program. This campaign through advertisements placed in high impact international journals (e.g. Science, Nature) has so far resulted in the hiring of 3 associate professors, 8 assistant professors, and 3 post-doctoral research associates. These researchers come from top tier universities from around the world: Leipzig University, Imperial College, Kyushu University, M.I.T., Tokyo Institute of Technology, A.I.S.T., Max Planck Institute, Kyoto University, Tokyo University, The Institute of Physical and Chemical Research (RIKEN), Central Research Institute for Electric Power Industry (CRIEPI), and Research Institute of Innovative Technology for the Earth (RITE). In addition, these faculty and post-docs were chosen from a strong pool of applicants that included researchers from universities and institutions from around the world such as Stanford University, Brookhaven National Laboratory, Lawrence Berkeley National Laboratory, Colorado School of Mines, Hitachi Zosen Corporation, Korea Advanced Institute of Science and Technology, National University of Singapore, Shanghai Institute of Microsystem and Information Technology, School of Mines Nantes, Chinese Academy of Sciences, Korea Institute of Science and technology, NIMS, Royal Institute of Technology, Stockholm, IIT, Dehli, Politechnico di Milano, Tokyo Institute of technology, and The Atomic and Alternative Energy Center (CEA) in Grenoble. In particular, Prof. Yamauchi from Hokkaido University, one of the nationally recognized young faculty in Japan, was hired through the Faculty Excellence Program. This is a

	program I^2CNER introduced to facilitate the recruitment of top tier researchers. Another indication of the high quality of our young faculty is their exceptional ability to acquire external funding—of the 12 young faculty that were hired in FY 2011, 5 were awarded the prestigious KAKENHI award. The young professors who received this award are: Prof. Junko Matsuda (Scientific Research (C)/ 4.2 million yen), Prof. Masamichi Nishihara (Young Scientists (B)/ 3.4 million yen), Prof. Kiminori Shitashima (Challenging Exploratory Research/ 3.1 million yen), Prof. Miho Yamauchi (Challenging Exploratory Research/ 3.2 million yen), and Prof. Huaiyu Shao (Research Activity Start-up/ 1.2 million yen/ continued). The list of our PIs currently includes a large number (10) of very active foreign world-top researchers (see in <Research Organization> under 1. Summary of center project) in addition to the 13 Illinois Satellite PIs.
3) I^2CNER, in addition to hosting conferences, may consider joining academic based annual international conferences in the areas germane to the I^2CNER's Goals (e.g., the International Colloquium on Environmentally Preferred Advanced Generation, ICEPAG), sponsored annually by the U.S. Department of Energy (among others).	3) I^2CNER is part of the Fukuoka Strategy Conference for Hydrogen Energy (FSCH), and its researchers participate in the Annual Merit Review (AMR) Meetings of the Hydrogen Program of the U.S. DOE. The FSCH is a key organization of Japan in which 480 companies participate, including the three major automotive companies, Toyota, Honda, and Nissan. The AMR is the key meeting in the U.S. in which the entire hydrogen program from production to utilization is outlined. Also, I^2CNER researchers participate in the HYDROGENIUS Institute funded by METI. HYDROGENIUS' mission is to provide solutions to technology problems related to applications for the hydrogen economy. I^2CNER is scheduled to carry out the 2012 International Conference on Hydrogen in Materials in September 2012—the main worldwide event in the area of fundamental research on hydrogen/materials compatibility. Lastly, I^2CNER will strive to increase its visibility and engagement with the international community by joining important conferences and interacting with world-class Institutes and Corporations in the area of hydrogen related technology (please also see <Collaboration with Other Institutions> under section 1.)

4. Break of administration limitation 1) The Vice-Director and Associate Director seem to be collaborating well with the Director to cover his absence. However, the administrative structure of I^2CNER is a bit complicated to produce understandable decisions and actions. So, definitions and/or clarifications are necessary for the role of the US partner in this administrative structure, the responsibilities of the external advisory committee, and the responsibilities of the science steering committee. It is needed to define and formalize the specifics of the collaboration with Illinois.	4. Break of administration limitation 1) The Science Steering Committee (SSC) is the faculty body that discusses and advises the Director on all matters of the Institute. The final decisions are made by the Director in consultation with the Vice Director and the two Associate Directors. The decision making process is fully described in the relevant governing document (please see Section 4, <Management>, under <Decision-Making System>). The External Advisory Committee (EAC) advises the Director and the Institute on all matters, including research and administration, again as described in the relevant governing document. The role of the satellite Institute is described in the agreement between Kyushu University and the University of Illinois. In short, the Satellite Institute is administered by the Director in consultation with an Associate Director. The research program of the Satellite Institute is complementary to that of Kyushu.
2) Various ambitious trials such as the appointment procedure, the independent working style of all faculty members including young, and the research proposal assessment based on a white paper should be pursued further.	2) All these trials now constitute the norm at the Institute.
3) Young researchers seem to have some freedom of research work and be satisfied with the working environment, but it is hoped that they should have a mindset of creating a research theme independently, selecting own research approach and developing collaboration beyond the control and influence of PIs.	3) The development of independent research programs by our young faculty and researchers is one of the most important goals of I^2CNER. The director himself oversees the progress and development of all young researchers by meeting with them regularly. The interaction between the director and young researchers is summarized in the annual evaluation letters that are given to the researchers at the end of each FY. Lastly, the seed projects on fusion research mentioned in 2. -2) are essentially run by assistant and associate professors. In particular, 6 out of those 9 projects are run exclusively by assistant and associate professors.
5. Actions to the comments previously raised by the program committee 1) The regularly scheduled seminars, the teleconferencing, the regular engagement of the Director in the seminars, the ability of Director to respond to emails from PIs and researchers quickly, and the supportive role of the I^2CNER administration are all attributes that need to be acknowledged and encouraged to continue. Something more should be done to overcome the current difficulty caused by the two separated research locations and even make it advantageous.	5. Actions to the comments previously raised by the program committee 1) Graduate student exchange and visits between Kyushu and Illinois have been found to be a very effective means of communication between the Institute at Kyushu and the Satellite. We plan to increase the number of students travelling across the Pacific.

6. Actions required and recommendations 1) I^2CNER should establish its own vision and roadmap toward a carbon-neutral society over time scales of short, middle and long ranges. It is necessary to develop a quantifiable strategy to reach the goals, and define technology needs/gaps and time frames to close them. The ongoing research themes must be assessed within the framework of I^2CNER's vision so that their merits and relationship are made clear.	6. Actions required and recommendations 1) A new Energy Analysis division has been established to address the issue of a roadmap. Please see details in <Research Organization> under 1. Summary of center project.
The following are recommended: 1) Kyushu University's commitment for a pool of positions must be made formally and all young professors must be accordingly informed. This is a must for sustainability after 10-15 years.	1) Please see Section 9. third bullet paragraph.
2) Young researchers should be provided with interdisciplinary research subjects in order to enhance collaboration and fusion of research areas between PIs. The driving force for the fusion must be young researchers.	2) All young researchers have been prompted to take advantage of our "Start-up funding for interdisciplinary research" program. This program requires proposal submission by faculty from two or more separate divisions. In fact, all assistant and associate professors hired through the first and second recruitment calls do work on such interdisciplinary programs. Young faculty hired through the third recruitment call started working at the Institute on April 1, 2012. They, too, will be encouraged to apply for fusion seed projects.

13. FY 2011 funding

(the exchange rate used: JPY/USD=100)

i) Overall project funding

Ten thousand dollars

Cost Items	Details	Costs (10,000 dollars)
Personnel	Center director and Administrative director	15
	Principal investigators (no. of persons): 21	218
	Other researchers (no. of persons): 48	199
	Research support staffs (no. of persons): 12	23
	Administrative staffs (no. of persons): 22	92
	Total	547
Project activities	Gratuities and honoraria paid to invited principal investigators (no. of persons): 62	11
	Cost of dispatching scientists (no. of persons): 0	0
	Research startup cost (no. of persons): 25	297
	Cost of satellite organizations (no. of satellite organizations): 1	175
	Cost of international symposiums (no. of symposiums): 2	7
	Rental fees for facilities	4
	Cost of consumables	30
	Cost of utilities	4
	Other costs	31
	Total	559
Travel	Domestic travel costs	12
	Overseas travel costs	45
	Travel and accommodations cost for invited scientists (no. of domestic scientists): 64 (no. of overseas scientists): 47	23
	Travel cost for scientists on secondment (no. of domestic scientists): 6 (no. of overseas scientists): 4	4
	Total	84
Equipment	Depreciation of buildings	0
	Depreciation of equipment	458
	Total	458
Other research projects	Projects supported by other government subsidies, etc.	115
	Commissioned research projects, etc.	449
	Grants-in-Aid for Scientific Research, etc.	620
	Total	1,184
Total		2,832

WPI grant for FY 2011			1,334
Costs of establishing and maintaining facilities in FY 2011			0
Establishing new facilities			
(Number of facilities: , m²)		Costs paid:	0
Repairing facilities			
(Number of facilities: , m²)		Costs paid:	0
Others			0
Cost of equipment procured in FY 2011			892
Name of equipment: Fatigue testing machine combined with scanning electro microscope			
Number of units: 1		Costs paid:	49
Name of equipment: Mode-locked femto-second ti: sapphire laser system			
Number of units: 1		Costs paid:	49
Name of equipment: SmartLabTM automatic X-ray diffractometer			
Number of units: 1		Costs paid:	42
Name of equipment: High speed laser raman spectroscopy			
Number of units: 1		Costs paid:	40
Name of equipment: Pico TR: thermal analysis system for thin films			
Number of units: 1		Costs paid:	28
Name of equipment: O2, H2, N2 analyzer			
Number of units: 1		Costs paid:	16
Others			668

ii) Costs of Satellites and Partner institutions

Cost Items	Details	Costs (10,000 dollars)
Personnel	Researchers (no. of persons): 9	
	Managing director (no. of persons): 1	
	Research support staff (no. of persons): 17	
	Others (no. of persons): 3	
	Total	83
Project activities		33
Travel		19
Equipment		40
Other research projects		0
Total		175