FY 2012 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 2013) 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 FY 2012, I²CNER, with the assistance of the Energy Analysis Division (EAD), drafted a timeline of new and advanced energy technologies aimed at achieving a ~50% CO_2 reduction for Japan by 2050. Guided by the EAD and to address specific recommendations from the review by the External Advisory Committee, research divisions formulated roadmaps to refocus the research themes to identify solutions to roadblocks for implementation of selected energy technologies.

Based on efforts over the past two years, a significant discovery on energy efficiency for organic light-emitting diodes was published in Nature by the Adachi Group and a potentially revolutionary approach to the understanding of functional [NiFe]hydrogenase in catalysis was published in Science by the Ogo group. Selected highlights of innovative ideas developed in the Institute include: how to load metal nanoparticles onto CNTs for use as electrocatalysts for fuel cells; the unveiling of the anisotropic heat conduction nature in the in- and out-of-shell thermal conductivities of multi-walled CNTs; new insights into the nature of cyclic deformation-induced microstructure evolution during hydrogen-accelerated fatigue crack growth; severely strained TiFe readily absorbs and desorbs hydrogen without activation; the influence of electrolyte composition on the electrochemical reduction of CO_2 to CO; and on the detection and monitoring of CO_2 leakage in sub-seabed storage via using seafloor-based acoustic tomography and mapping the distribution of the leakage points using novel pH/pCO_2 sensors.

To ensure fusion research within I²CNER, all projects (including those of the satellite) underwent a stringent review by the Internal Programs Review Committee (IPRC), a new ad-hoc committee formed in response to prior reviews. As a result, several "Start-up funding for interdisciplinary research" projects initiated in FY 2011 were halted, one new project was introduced, and the total budget for this program was reduced by more than 50%. Furthermore, several of the satellite programs were identified as underperforming in terms of mission/participation requirements and unless these issues are addressed immediately, these programs will end by December 2013.

To continue to advance the mission and bring in new research, resources have been set aside to launch a new initiative to reinforce programs which are advancing fusion; the Director, in consultation with the IPRC, will evaluate the submissions to this initiative. Advanced brainstorming workshops are planned in order to further consolidate the quality of the research output for this year.

I²CNER has been fully embraced and integrated within the Kyushu University structure as a unit, and will remain permanently within KU after WPI funding expires. I²CNER had the opportunity to compete for tenure track positions and has been given 4 additional tenured positions in FY 2012 by KU (all positions were for associate professors–a total of 5 have been given so far). The following is a snapshot of the staffing of I²CNER as of April 1, 2013: 9 PIs from the Faculty of Engineering transferred to I²CNER; total researchers = 150 (119 KU and 31 at Illinois); total personnel, including both researchers and support staff, = 225 (192 at KU and 33 at Illinois), of these 225, 91 are non-Japanese and 59 are female; WPI PIs total 24, of whom 6 are renowned international scholars and 2 are distinguished faculty at Illinois; postdocs numbers have grown from 6 in FY 2011 to 19 with 9 positions available; and graduate student numbers have increased from 14 to 48 graduate with 22 funded by I²CNER. The effort to bridge the Pacific continues with Illinois Faculty, postdocs, and graduate students making a total of 28 trips (144 days) to KU and KU faculty made a total of 5 trips to Illinois.

In order to advance its international visibility as a Japan-US project on energy, I²CNER hosted a symposium in Tokyo in which it brought I²CNER research to the attention of energy stakeholders of Japan and the international community.

1. Summary of center project

<Initial plan>	<Results/progress/alternations from 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 excellence in	<Center Project> • Due to changes in the Institute's structure, as well as the re-configuration and re-consideration of the thematic research areas of the Institute, the mission statement of I^2CNER was updated in FY 2012. The mission statement is now the following: At I^2CNER, our mission is to contribute to the creation of a sustainable and environmentally-friendly society by conducting fundamental research for the advancement of low carbon emission and cost effective energy systems and improvement of energy efficiency. Amongst the array of technologies that I^2CNER's research aims to enable is the innovative, safe, and reliable production, storage, and utilization of hydrogen as a fuel in a hydrogen-based economy. Our research also explores the underlying science of CO_2 capture and storage technology or the conversion of CO_2 to a useful product. Additionally, it is our mission to establish an international academic environment that fosters innovation through collaboration and interdisciplinary research (fusion). • In an effort to summarize the feedback received for each division in the FY 2012 WPI Site Visit Report, the WPI Program Committee Report, the External Advisory Committee Report, and the Internal Programs Review Committee Report, the Director created one consolidated report for each division, entitled "The Director's Assessment and Requested Action," which included all criticism and action items contained in each of the four above-mentioned reports. These consolidated reports were distributed to the Division Lead PIs on January 20, 2013. Each Division was required to respond to this report by March 31, 2013. The Internal Programs Review Committee, which is chaired by Prof. Ian Robertson, is an ad-hoc committee formed by the Director to "provide information to the Director on the entire spectrum of the Institute's research activities in anticipation of the upcoming mid-term review of I^2CNER." • In addition, each of I^2CNER's researchers was given his or her individual project review from the Internal Programs Review Committee Report.

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 the elimination of the CO_2

- Following the distribution of the Director's Assessment and Requested Action Reports, the Director required each division to host a retreat attended by all Division members by March 31, 2013 in an effort to revitalize the division and to carefully re-assess the division's research objectives, targets, and milestones. At these retreats, the division members, along with members of the Energy Analysis Division (EAD), established their relevant short-, mid-, and long-term goals vis-à-vis the Institute's research objectives, targets, and milestones, as well as the energy targets for Japan. Divisions were also asked to address the feedback provided in the Director's Assessment and Requested Action Report at these retreats. Each division was required to include a report on this retreat in the Division Lead PI's response to the Director's Assessment and Request Action report, which was due by March 31, 2013.

PI

- As of April 1, 2013, 9 I^2CNER PIs have transferred to I^2CNER from the Faculty of Engineering. This transfer was initiated and administered by the KU President in an effort to improve the mindset of the PIs and to strengthen the relationship between I^2CNER and the Faculty of Engineering. Such a relationship is advantageous within the Kyushu System since I^2CNER is now an integral unit of KU which facilitates joint proposal submissions for tenure track positions, enables the Institute's impact on the research culture, offers teaching opportunities, etc.

- Also as of April 1, 2013, the Institute reduced the number of Principal Investigators to 24. Of the 24 remaining PIs, 15 are Kyushu faculty, 2 are Satellite Faculty, and 7 are non-Kyushu/Foreign faculty.

RECRUITMENT

- It was announced on October 27, 2012 that each WPI Principal Investigator has been allocated 1 postdoctoral associate line, which he or she was encouraged to fill by April 1, 2013. The recruitment of these postdoctoral researchers followed the normal I^2CNER hiring process and screening by the Faculty Recruiting Committee (FRC). As of April 1, 2013, I^2CNER had 19 postdocs. Of these postdocs, 3 are female and 16 are non-Japanese. We plan to have 28 postdocs by the end of calendar year 2013.

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.

- Upon the announcement of the award and before the launching of the Institute, I^2CNER initiated an aggressive open international recruitment campaign, which it has continued in subsequent years. At the junior level, I^2CNER seeks to hire researchers who demonstrate 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 FRC, which is chaired by Prof. Takata as of February 1, 2013. The FRC includes key members of the Institute and any other faculty who can provide input for cases of targeted hiring. In summary, I^2CNER hired 3 faculty members and 3 postdocs as a result of 1 open international recruitment call, and 1 open call for proposals for postdoctoral lines (July 4, 2012).

EVALUATION LETTERS TO YOUNG INVESTIGATORS

- 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 are maintained in a booklet entitled “Young Investigator Research Project Summaries,” while research progress is reviewed annually by the administration of the Institute. Following the Annual Interviews and Assessments of Young Faculty conducted by the Director, the Associate Directors, and the Division Lead PIs on February 6-7, 2013, feedback was provided to the young investigators in the annual assessment and evaluation letters from the Director dated March 31, 2013.

I^2CNER SEMINAR SERIES

- In order 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, and industry, as well as policy makers in government agencies. In continuation of the successful tradition established in FY 2011, I^2CNER again managed to feature some of the most prominent figures of the international community in FY 2012. By way of example, the list of the 23 I^2CNER speakers in FY 2012 includes:
    - B. Ameduri, Research Director of the National Center of Scientific Research, France
    - T. Autrey, Scientist at Pacific Northwest National Laboratory, USA

- R. Glass, Professor at the University of Arizona, USA
- J. Kim, Professor at the University of Maryland, USA
- M. Gardiner, Technology Development Manager, U.S. Department of Energy
- K. Domen, Professor at the University of Tokyo
- S.Y. Lee, Professor at the Korea Advanced Institute of Science and Technology (KAIST)
- H. J. Sue, Professor at the Polymer Technology Center, Texas A&M University, USA
- S. Mitra, Professor at the University of Alberta, Canada
- H. Brongersma, CEO of Calipso B.V. the Netherlands and Honorary Professor at Imperial College, UK
- H. Kitagawa, Professor at Kyoto University
- M. Iwamoto, Professor at the Tokyo Institute of Technology
- S. Garimella, Professor at the Georgia Institute of Technology, USA
- P. Stephan, Professor at Technical University Darmstadt, Germany

INSTITUTE INTEREST SEMINAR SERIES (IISS)

- In order to foster a climate of collaboration and interdisciplinary research that cross-cuts division boundaries, the Institute regularly hosts the "Institute Interest Seminar Series (IISS)." This series also serves as a forum to help our young researchers (graduate students, post-docs, and assistant and associate professors) to further develop their abilities to present and argue for their viewpoints, scientific methods, and approach before an audience of experts. During FY 2012, 16 IISS were hosted, and in each seminar, two presentations were given.

SRA PROGRAM

- I^2CNER instituted the "Super Research Assistants (SRA)" Program in order 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 2012, 4 recruitment calls, which were administered in December 2011, and April, July, and October 2012 resulted in 1 renewal and 6 new hires. All SRAs are required to make presentations in English at the Institute Interest Seminar Series, submit progress reports, and give an additional presentation before the Institute's SRA Selection Committee

<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.

for the renewal of their SRA status. The quality of I^2CNER SRAs is demonstrated by the fact that two former SRAs from FY 2012 have been hired as JSPS fellows (i.e. Research Fellowship for Young Scientists: doctoral course students), beginning April 1, 2013. I^2CNER aims to continue recruiting SRAs to meet its goal to train the next generation of researchers. At present, the total number of SRAs is 6 and the plan is to increase it to 10 by October 2013.

VISITING STUDENTS

- In order to facilitate active exchange of students between Kyushu University and the University of Illinois (I^2CNER Satellite Institute), and other collaborating institutions overseas, the Institute accepts short-term students from overseas as “Visiting Students” at Kyushu University. In FY 2012, I^2CNER hosted 7 students (6 from Illinois and 1 from Jamaica).

VISITING RESEARCHERS

- From FY 2012 onward, the Institute specifically established a system to accommodate post-doctoral research associates who are working at Kyushu under the supervision of foreign PIs at overseas collaborating institutions as short-term “Visiting Researchers.” In FY 2012, I^2CNER hosted:
  - 1 “Visiting Researcher” from Tsinghua University for 3 months in the Thermophysical Properties Division
  - 2 “Visiting Scholars”: 1 from Kumamoto University for 6 months in the CO_2 Separation and Concentration Division, and 1 from the VTT Technical Research Centre of Finland for 3 months in the Hydrogen Structural Materials Division.

<Research Organization>

- The Institute is organized in thematic research areas (Divisions) which address individual research objectives. Each division is led by a senior WPI Principal Investigator (Lead PI) of the Institute. The divisions are:
  - Hydrogen Production
  - Advanced Materials Transformations*
  - Thermophysical Properties (H_2, CO_2)
  - Hydrogen Structural Materials

	o Hydrogen Storage* o Fuel Cells o CO_2 Separation and Concentration o Carbon Capture and Storage* o Energy Analysis Please note that the names of those divisions marked with an asterisk (*) have been changed as of July 1, 2012. *EAD* • The Energy Analysis division was established in response to a recommendation stated in the follow-up report issued by the WPI Program Committee after the FY 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 caused by the constraint of primary energy resources and availability on the basis of CO_2 emissions, efficiency, cost, and national security. The division's goals are to: i) assess the relevance of the Institute's research activities vis-à-vis I^2CNER's vision for a carbon-neutral society, ii) ensure that I^2CNER research is informed of all relevant current and future energy options of Japan, and iii) establish a roadmap for the Institute toward a sustainable and low-carbon society over mid- and long-term scenarios. The division is led by the Director and as of April 1, 2013 its members include: o WPI Visiting Professor, Mr. Mark Paster (former energy analysis employee in the Energy Efficiency and Renewable Energy department of the U.S. DOE) o Dr. Kuniaki Honda (formerly with the Gas and Power Co., Ltd, Japan), whose title changed to WPI Professor as of July 1, 2012 o Dr. Michihisa Koyama, Professor at the Inamori Frontier Research Center of Kyushu University o Dr. Kenshi Itaoka, I^2CNER WPI Professor as of March 16, 2013 o Dr. Seiichiro Kimura, I^2CNER postdoc as of April 1, 2013 • Prof. James Stubbins, head of the Nuclear, Plasma, and Radiological Engineering Department of the University of Illinois, and Dr. Xuping Li, postdoctoral researcher at the University of Illinois, are participating in

the research program of the division from the Satellite Institute.

FOREIGN INVESTIGATORS

- 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^{2}CNER for the academic year 2013:
  - Prof. John A. Kilner, Imperial College London (UK)
  - Dr. Brian P. Somerday, Sandia National Laboratories (USA), who is serving as Lead PI of the Hydrogen Structural Materials Division
  - Prof. Harry L. Tuller, Massachusetts Institute of Technology (USA)
  - Prof. Xing Zhang, Tsinghua University (China)
  - Prof. Reiner Kirchheim, University of Göttingen (Germany)

  Appointed as WPI Professors:
  - Prof. Robert O. Ritchie, University of California, Berkeley (USA)
  - Prof. Ludwig J. Gauckler, Swiss Federal Institute of Technology Zurich (ETH)
  - Dr. Ping Chen, Dalian Institute of Chemical Physics (China)
  - Prof. Nikolaos Aravas (renewal), University of Thessaly (Greece)

  Appointed as WPI Visiting Professors:
  - Prof. Louis Schlapbach, Swiss Federal Institute of Technology Zurich (ETH)
  - Mr. Mark Paster (renewal), former energy analysis employee in the Energy Efficiency and Renewable Energy department of the U.S. DOE.
  - Prof. Kanao Fukuda (renewal), Universiti Teknologi Malaysia

  Discontinued WPI PI appointment
  - Prof. Chen-Tung Arthur Chen, National Sun Yat-sen University (Taiwan)

  These researchers are expected to vigorously pursue collaborative/fusion research with I^{2}CNER researchers, offer lectures and seminar presentations, and engage with student or post-doctoral research associate supervision, as well as with teaching short courses, depending upon their individual appointments. Through their participation in I^{2}CNER, these foreign researchers are expected to continue to contribute to the excellence of our research program.

NON-KU RESEARCHERS

Appointed as WPI PI:

- o Prof. Katsuki Kusakabe (renewal), Sojo University, Department of Nanoscience.

Appointed as WPI Visiting Professors:

- o Dr. Toyoki Kunitake (renewal), Kitakyushu Foundation for the Advancement of Industry Science and Technology.
- o Dr. Chao-Nan Xu (renewal), AIST.
- o Dr. Ziqui Xue (renewal), Research Institute of Innovative Technology for the Earth (RITE)

ILLINOIS FACULTY

- 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^{2}CNER research activities at Kyushu. In FY 2012, all Satellite faculty members were designated as WPI Principal Investigators. As of April 1, 2013, only Professors Andrew Gewirth, Kenneth Christensen, and Ian Robertson retained the title of WPI Principal Investigator. However, also as of April 1, Prof. Robertson is considered an International WPI PI (not a Satellite WPI PI), due to his new position as Dean of Engineering at the University of Wisconsin-Madison.

  The remaining 10 members of the Illinois satellite have been given the title of "Satellite Faculty." The activities of the FY 2012 members of the Illinois Satellite are:

  - o Structural Materials and Hydrogen Compatibility
    - ▪ Profs. Robertson (Mat. Sci. Eng.) and 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 (Bio. & Chem. Eng.)
  - o Catalysis
    - ▪ Prof. Rauchfuss (Chemistry)
  - o Photoelectrochemistry
    - ▪ Profs. Gewirth (Chemistry), Martin, Rockett (Mat. Sci. Eng.), Ertekin ((Mech. Sci. Eng.)
  - o CO_2 reservoir characterization and monitoring and modeling of

injected and leaked CO_2

- Profs. Christensen, Pearlstein (Mech. Sci. Eng.)

o Near-Critical CO_2 Flows over Active Solid Surfaces

- Prof. Kyritsis (Mech. Sci. Eng.)

o Energy Analysis

- Prof. Stubbins (Nuclear. Plasma Rad. Eng.)

In FY 2012, two new projects were seeded through direct funding from the University of Illinois College of Engineering. The projects were initiated to strengthen I^{2}CNER's computational capabilities in the area of modeling and simulation of CO_2 storage and devices for photoelectrochemical production of hydrogen:

o Computational Modeling of Pore-Scale Multiphase Flow and Capillary Trapping of Supercritical CO_2 in Subsurface Geological Formations

- Profs. Valocchi and Werth (Civ. Env. Eng.)

o Manufacturable Nanowire Array for Solar Hydrogen Production

- Prof. Li (Elect. Comp. Eng.)

OTHER PI PERSONNEL CHANGES

- Other Principal Investigator personnel changes as of April 1, 2013 are:
  - o Professor Shitashima's (Carbon Capture and Storage Division) appointment as WPI PI was terminated.

- The following PIs retired from KU, including their positions as WPI PIs:
  - o Prof. Murakami (former Vice Director) and Prof. Matsuoka (Hydrogen Structural Materials Division)
  - o Prof. Naruta (Advanced Materials Transformations Division)
  - o Prof. Minemoto (CO_2 Separation and Concentration Division)
  - o Prof. Yanagi (Carbon Capture and Storage Division)

<Project Management>

- One of the main goals of the Institute is the restructuring of research management at the Kyushu University. This new approach to research administration will rely heavily on the management style, academic experience, and scientific achievements of the Institute director whose duties will include the research team formation, the recruitment of the international research participants, the establishment of international collaborations and interactions with top research Institutions, the

<Project Management>

- The main feature of the new I^{2}CNER organizational structure is that the Director has direct access to all administrative, operations, and research related committees. This direct access structure was specifically adopted in order to eliminate bureaucracy and hierarchy.

- The Director is assisted by two Associate Directors, Prof. Tatsumi Ishihara and Prof. Yasuyuki Takata. Prof. Takata was newly 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 research activities of the Institute

appointed as of February 1, 2013, after Prof. Kazunari Sasaki stepped down from his post as Associate Director on November 30, 2012. The two current Associate Directors are responsible for matters related to the following:

  - Prof. Ishihara (also serves as a Lead PI of Hydrogen Production Division): Promotions Committee, I[2]CNER workshop organization, administration of our seminar series, and oversees facilities and equipment.

  - Prof. Takata (also serves as a Lead PI of the Thermophysical Properties Division): Faculty Recruiting Committee (FRC), international collaborations and industrial collaborations, and graduate student research matters.

IAN ROBERTSON

- Prof. Ian Robertson, Dean of Engineering at the University of Wisconsin-Madison serves as Chief Science Advisor to the Director in order to further strengthen the management of the Institute in relation to its research activities.

SSC

- The Science Steering Committee (SSC) was established upon the launching of the Institute. The committee is chaired by the Director, and its members are the two Associate Directors and the lead PIs of the thematic research areas (divisions). The SSC is the body that reviews and decides on all matters of the Institute, e.g. planning and operation of research activities, budget implementation, international collaborations, and outreach. In FY 2012, the SSC voted to invite Professor Honda of the EAD to join the SSC meetings as a non-voting member in order to keep the EAD informed of the course of the Institute. In addition, as of April 1, 2013, Professors Fujikawa and Tsuji have been invited to represent their divisions (CO_2 Separation & Concentration and Carbon Capture & Storage, respectively) in the SSC due to the retirement of the former division lead PIs.

EAC

- As of March 31, 2013, the External Advisory Committee (EAC) had eight members:
  - Professor Ronald J. Adrian (Chair), Arizona State University, USA

- Dr. Deborah Myers (Vice-Chair), Argonne National Laboratory, USA
- Dr. Robert J. Finley, Illinois State Geological Survey, USA
- Professor Reiner Kirchheim, University of Göttingen, Germany
- Professor Robert McMeeking, University of California, USA
- Dr. Kevin Ott, Los Alamos National Laboratory, USA
- Professor Tetsuo Shoji, Tohoku University, Japan
- Dr. George Thomas, Retired EERE office of US DOE and Sandia National Laboratories, USA (Advisory member)

On July 19, 2012, the EAC submitted to the Director the report from their review of the Institute, which was held February 1-2, 2012 at Kyushu University. An I^2CNER Retreat with the EAC at the University of Illinois at Urbana-Champaign will be held May 30-31, 2013.

KU-IL COLLABORATION AND EVENTS

- Collaborative research activities and personnel exchanges between Kyushu and the Illinois Satellite, and other collaborating institutions are ongoing. Illinois graduate research assistants continually visit Kyushu to carry out experiments jointly with Japanese researchers. In FY 2012, 5 graduate students and 2 postdocs from the University of Illinois visited Kyushu. In addition, 2 young faculty members from Kyushu University were hosted by Prof. Cahill at the Illinois Satellite for a longer term (more than 2 months). One of them, Prof. M. Kohno, visited UIUC for 6 months from the end of October 2012 to April 2013.

- In order to promote interdisciplinary research and foster collaboration between I^2CNER's researchers, workshops focused on the individual divisions' thematic research areas were hosted on January 31, 2013, following the I^2CNER Annual Symposium and New Building Completion Ceremony at Kyushu University on January 29, 2013. 17 attendees from the Illinois Satellite participated in the 2013 I^2CNER Annual Symposium. A large number of researchers from collaborating foreign institutions participated in these specialized workshops, as well. The Illinois Satellite is planning an international workshop on "Catalytic Concepts for Fuel Cells" in September 2013 which involves speakers from both KU and Illinois. Through such I^2CNER events, and mutual visits of faculty and students between the two universities, researchers from both universities have opportunities to directly exchange and discuss research ideas for interaction and collaboration, in addition to their regular communications via email and teleconferencing.

- The Director began publishing a newsletter entitled "I^2CNER P.I.peline" in FY 2012. This publication was started in the spirit of keeping the researchers of the Institute informed of important events and changes that are happening within I^2CNER. The first issue of I^2CNER P.I.peline was published in December 2012.

DIRECTOR'S PHYSICAL PRESENCE AT KU

- The Director's physical presence in I^2CNER for FY 2012 increased to 46%. In FY 2012, the Director made ten (10) trips and spent a total of 103 days of his time in Japan By comparison, in FY 2011, he made 5 trips and spent 54 days in Japan.

FACULTY COUNCIL

- As part of the ongoing transition of I^2CNER into the permanent unit of the Kyushu University system, a Faculty Council was established. The establishment of the Faculty Council helped to facilitate the transfer of 9 PIs from the Faculty of Engineering, which was mentioned under *PI* in this Section (1. Summary of center project).

BUDGET

- The fraction of WPI fund spent in FY 2012 is listed below.

･Personnel	3.1 million USD (314 million JPY)
･Project activities	7.1 million USD (714 million JPY)
･Travel	0.8 million USD (76 million JPY)
･Equipment	2.2 million USD (220 million JPY)
Total	**13.2 million USD (1.32 billion JPY)**

- In FY 2012, KU researchers of the center have acquired a total amount of 31.56 million US dollars (3.16 billion yen), which amounts to a 93% increase compared to FY 2011. Please refer to Section 8 for more details.

- 6 of the Illinois Satellite Researchers have won a total of 15 external funding projects by leveraging their I^2CNER research, which resulted in the total amount of 4,643,514 US dollars of extra award grants at Illinois (only projects whose period/duration included FY 2012 were counted).

<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.

  - Satellite Institute, University of Illinois at Urbana-Champaign, USA
    - The Director of the WPI Institute, Professor Petros Sofronis, is a faculty member at the University of Illinois at Urbana-Champaign, Illinois, and is an internationally recognized expert on the effects of hydrogen on the mechanical properties of materials. Other research activities at Illinois mirror parts of the proposed program. Therefore a satellite office will be established at Illinois to facilitate cooperative research activities as well as personnel exchanges. In addition to conducting Institute related research, the satellite office will serve as the base for identifying and engaging key research programs and faculty at Universities and Institutions nationally and internationally. As Director of the WPI Institute, Professor Sofronis will serve as the Director of the satellite institute. In this latter capacity he will report directly to the Dean of the College of Engineering at the University of Illinois. Appropriate agreements between Kyushu University and the University of Illinois, other than an exchange of students which is already in place, will be negotiated if the Institute is funded. Both parties have expressed interest and support for establishing this satellite institute at the University of Illinois.

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

<Collaboration with Other Institutions>

- Plans have been 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. Dr. Brian Somerday, Lead PI of the Hydrogen Structural Materials Division, is a distinguished member of the technical staff of Sandia National Laboratories.

- The Director made 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, a joint workshop between I^2CNER and NTNU/SINTEF took place in Trondheim, Norway in Nov. 15-16, 2012 to explore potential collaborations between the three Institutions. Legal issues for an MOU for collaboration on CO_2 Capture and Storage (CCS), Energy Analysis, and Structural Materials are currently being resolved. On January 16, the Director presented the I^2CNER project at the Sandia National Laboratories at Albuquerque, NM and a potential collaboration is now being explored in the area of CCS, given that Sandia is running an Energy Frontiers Research Center (EFRC) on CCS funded by the U.S. DOE. Similar collaborations to strengthen I^2CNER's computational capabilities in the areas of captured CO_2 and catalysis are currently being explored with Dr. Bruce Garrett, the Director of the Chemical and Materials Sciences Division of the Pacific Northwest National Laboratory (PNNL).

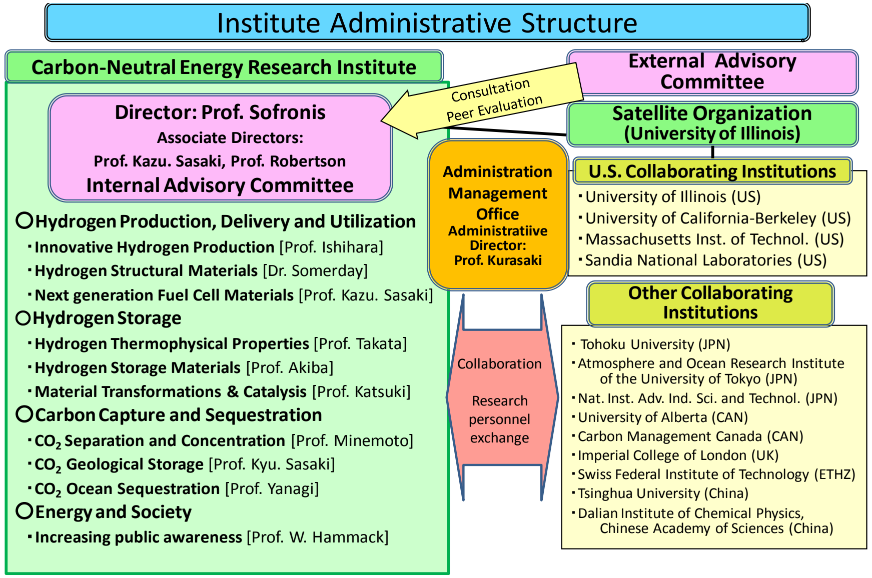


Fig. Administrative structure of the Institute

2. Research fields

<Initial plan>

Research Field

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

Significance of the Proposed Project

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

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

<Results/progress/ alternations from initial plan>

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. The fundamental science I^{2}CNER is conducting for the realization of a carbon-neutral energy society remains unaltered from the initial plan. The establishment of targets/milestones, along with a roadmap toward removing the roadblocks for enabling the energy technologies for a carbon-neutral energy future, has been and is being worked out by the EAD in collaboration with the individual research Divisions.

- 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.

- 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.

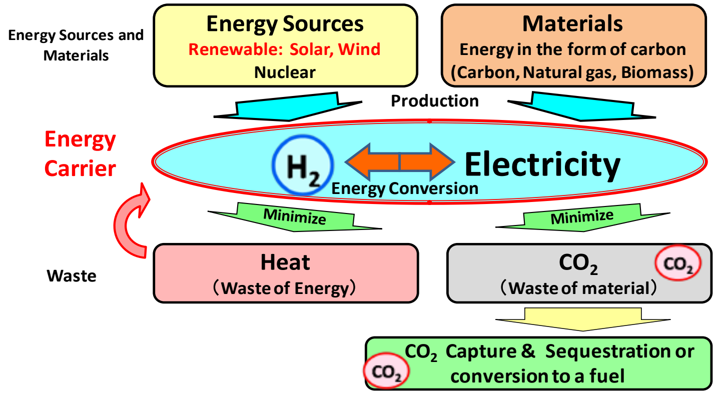


Fig. A Carbon-Neutral Energy Fueled System

• 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>	<Results/progress/alternations from 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: o Development of high efficiency material conversion processes without any by-products such as waste and CO_2. o Development of innovative and sustainable hydrogen production processes, such as photocatalytic water splitting; o Development of novel hydrogen storage materials with storage capacity of over 6wt% H_2; o Design of hydrogen-embrittlement resistant materials for the development of a safe and reliable material infrastructure; o Development of the next generation of fuel cells by the research on novel materials and devices; o Development of low-energy carbon separation and concentration processes; o Development of CO_2 geological storage considering CO_2 behavior and chemical interactions;	• 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 an 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.

- o Development of ocean sequestration by understanding CO_2 behavior in ocean;
- o Increase public awareness for hydrogen technologies and long-term CO_2 behavior in each earth and ocean.

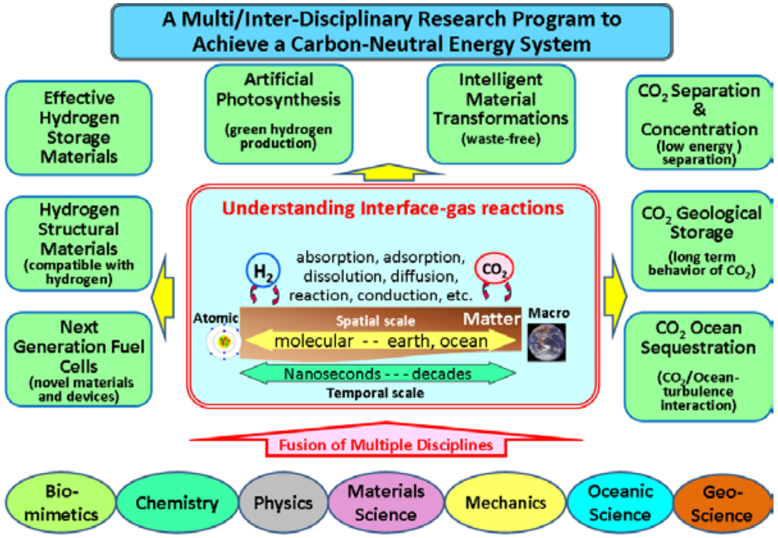


Fig. Interfaces in the multi/inter-disciplinary research program in I^{2}CNER

(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.
- 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

(Research Objectives and Methodologies)

1. Hydrogen Production and Artificial Photosynthesis

Goals

The efforts of this Division focus on the science and engineering of technologies to produce and conserve energy and to use that energy to reduce hydrogen to a storable fuel. The Division is developing photoelectrochemical cells for direct conversion of sunlight to hydrogen and photovoltaics combined with steam electrolysis as a two-step hydrogen reduction process. As a complement to photovoltaics, organic light emitting devices are being developed both for high efficiency lighting to contribute to energy consumption and because the underlying science is very valuable to organic photovoltaics, an energy production method being studied. Research also includes use of microstructural characterization techniques for analysis of the interface structure of organic dye and inorganic semiconductors in photocatalysts.

The research in the division falls under the themes of energy production, development, and ii) conversion of CO_2 to functional compounds in combination with electrolytic techniques mimicking dark reactions.

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

Reference

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

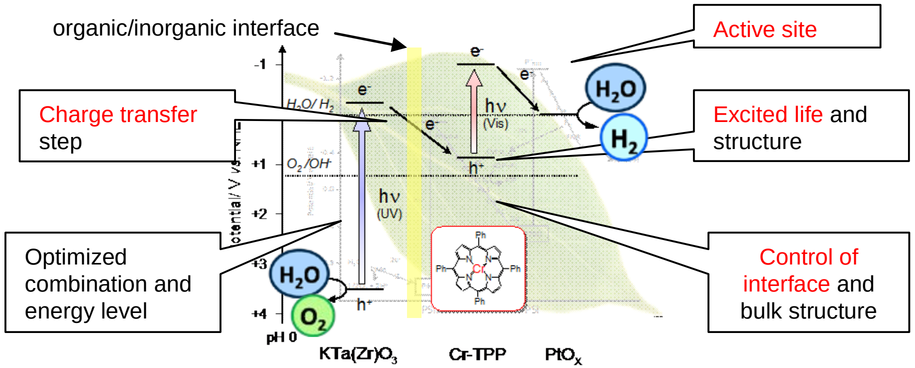


Fig. 1a. Artificial photosynthesis through complete photocatalytic water splitting

conservation, and storage. Energy production is based on conversion of solar to electric energy. Conservation is through enhanced lighting efficiency based on high efficiency solid state lighting. Finally fuel production is through hydrogen reduction. The work includes experimental materials synthesis, device fabrication and testing, and theory-based materials development. Projects encompass novel inorganic and organic photocatalysts and electrodes, synthesis of novel molecules for organic light emitters and photoelectrochemical and photovoltaic cells, and materials for electrochemical and electrolytic water reduction. The research targets and objectives are shown in the roadmap of the Division (Fig. 1) that has been formulated in consultation with the Energy Analysis Division.

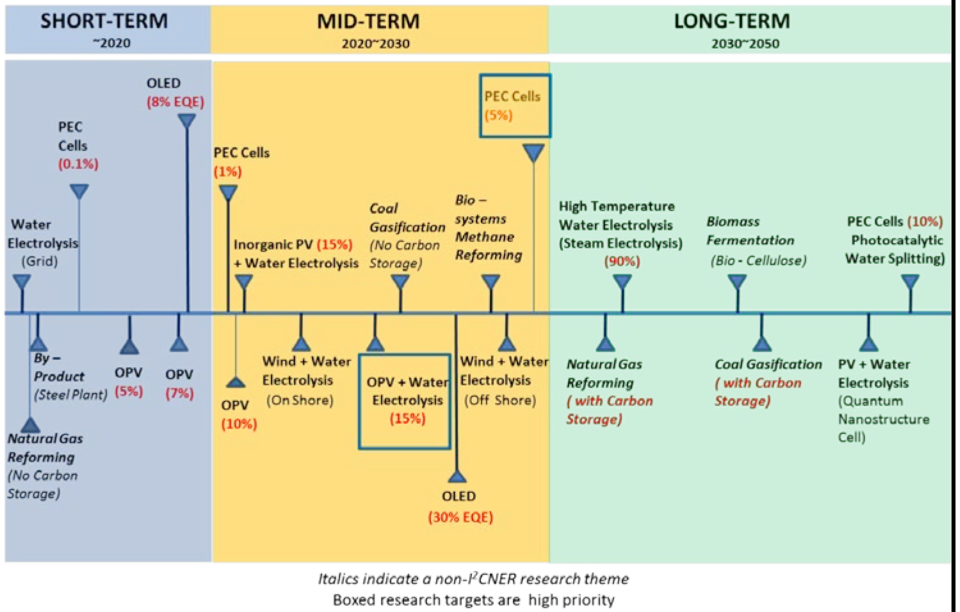


Fig. 1. Hydrogen Production Division Roadmap

Research Highlights

Ishihara and his group (Kyushu University) have designed, synthesized, and demonstrated novel organic dye molecules for improved photocatalysis devices. Octaphirine was shown to exhibit much higher activity than Cr-TPPCl with extended wavelength sensitivity. In inorganic materials, they showed that Ga(Zn)N(O) produced with proper composition and processing shows extended photon absorption with photoelectrochemical decomposition of water demonstrated from 350 and 650 nm photons.

Kilner and his group (Imperial College) have examined the stability of some $Pr_{2-x}La_xNiO_{4+\delta}$perovskite oxides with promise for application as anode materials in steam electrolyzers. The "A site" cation was shown to segregate on the surface of the material. Much of this work was performed by John Druce, Post-doc, using the low energy ion scattering facilities at Kyushu. The polarization resistance at open circuit was found to be comparable to those reported for some of the currently best performing $Pr_2NiO_{4+\delta}$and $La_2NiO_{4+\delta}$ end members.

Adachi and his group (Kyushu University) have demonstrated a 7% efficient organic photovoltaic device based on ITO/MoO_3/DBP/C_{70}/BCP/Ag device structure. In addition the group has achieved very high internal quantum efficiency and materials exhibiting a very low energy gap between singlet and triplet states, promoting highly efficient conversion of the triplet to the singlet state. This contributes to high intrinsic fluorescence efficiency and an overall external electroluminescence efficiency of more than 19%, comparable to that achieved in high-efficiency phosphorescence based OLEDs.

Ken Sakai and his group have designed, synthesized, and demonstrated novel organic molecules for water oxidation based on various new pigment-multiacceptor systems. For example, multi-viologen frameworks tethered to a single $Ru(bpy)_3^{2+}$-derived chromophore, have been developed and their detailed photophysical properties together with their multi-electron storage behaviors have been successfully characterized. The exceptionally long-lived charge separated states realized in these new systems have been interpreted in terms of electron migration among the multi-viologen residues, since it substantially suppresses the probability of the backward electron transfer events. Other results include a relatively simple Pt(II) complex that was developed to serve as a 'photo-hydrogen-evolving molecular device' which photocatalyzes H_2 evolution from water based on a very unique simulated 'artificial Z-scheme photosynthesis' concept, the mechanisms of which have been developed in collaboration with investigators at Osaka University.

Angus Rockett and his group (University of Illinois) in collaboration with T. Yasuda of Kyushu University have developed simulations of organic photovoltaic devices produced at Kyushu. These simulations give a direct interpretation of the recombination charge transport across the device heterojunction, which controls the dark current and specific recombination mechanisms. This is then compared with the light current/voltage characteristics to demonstrate the balance between charge collection in the heterojunction and charge recombination across the junction. The Rockett group has also conducted scanning tunneling spectroscopy measurements on $AgInSe_2$, a promising photovoltaic material and has shown how the band edge fluctuations in this material compare with $CuInSe_2$. The resulting understanding can improve inorganic photovoltaic device performances. This work is now being extended through ion surface scattering in collaboration with Druce at Kyushu using the I^2CNER ISS facility.

Elif Ertekin and her group (University of Illinois) have conducted density functional theory simulations of organic and inorganic materials in collaboration with A. Staykov (Kyushu University). She has calculated electronic states of polar interfaces for photo-catalytic water-splitting. These were applied to Cuprous Oxide/TiO_2 and $BaTiO_3$/TiO_2 heterojunctions in collaboration with Martin and the observed behaviors were successfully simulated. The group is also working on elucidating and optimizing the charge transfer mechanism in the porphyrin-GaN:ZnO photocatalyst synthesized by the Ishihara group at Kyushu. Her electronic structure modeling efforts are being used to suggest a suitable combination of organic dyes for optimal photocatalytic performance. Additionally, with Profs. Staykov, Hagiwara, and Ishihara, we are simulating the mixed organic – inorganic junction composed of the inorganic perovskite semiconductor $KTaO_3$ and the organic molecule Cr-Tetraphenylporphirin-Cl (Cr-TPPCl), in which charge carrier separation is enabled by a unique molecular switching mechanism.

Lane Martin (University of Illinois) and his group have demonstrated TiO_2/$SrRuO_3$ heterostructures exhibiting hot carrier injection from $SrRuO_3$ into TiO_2 and it was found that this gives rise to interactions with sub-band gap radiation, and enhanced activity under visible light irradiation. This can potentially enhance the performance of photoelectrochemical cells being developed by Ishihara and coworkers. Strong photovoltaic responses were observed under AM1.5G light and even when the vast majority of light absorption in the TiO_2 was removed. Andrew Gewirth (University of Illinois) and his group showed that by using nitrogen-containing ligands to control CO and H_2 production on supported silver nanoparticle catalysts and decorating Ag particles with the N-containing molecules that increased selectivity toward CO production relative to H_2 could be accomplished. This is important to designing a high performance electrochemical method for reduction of both hydrogen in various forms and carbon dioxide. In collaboration with Prof. Hagiwara (Kyushu University) oxysulfide electrodes were modified by adsorbing an organometallic light absorber on the surfaces. In combination with a cocatalyst, the collaboration was able to achieve substantial O_2 and H_2 evolution activity following visible light exposure. In particular, the dye modification – achieved following protocols developed at Kyushu University – led to enhanced activity. The exact efficiency of gas production in this system is currently being determined.

Takahara and team have employed tomographic imaging in the transmission electron microscope to investigate the aging processes of fuel cell electrodes (FCEs) in terms of morphology, e.g., size and distribution of Pt catalysts, from which a new insight of degradation process of the FCEs are proposed. Planned research also includes the use of small angle x-ray scatterning for analysis of the interface structure of organic dye and inorganic semiconductors in photocatalysts. Preliminary work using this technique has established some aspects of the nanostructure in polymer blends. Materials synthesis efforts in the group include plans to develop novel polyelectrolyte films for fuel cells.

Significant Accomplishments

Uoyama, Hiroki; Goushi, Kenichi; Shizu, Katsuyuki; Nomura, Hiroko; and Adachi, Chihaya. "Highly efficient organic light-emitting diodes from delayed fluorescence." Nature, 492, 234-238, 2012.

Description of Scientific Achievement:

The Adachi group has developed, synthesized, and demonstrated excellent luminescence from an all-organic light emitting device with no expensive and rare transition metal atoms incorporated in the molecules. Light emission in OLEDs requires quantum mechanical selection rules to be obeyed, which imposes a restriction on spin and phase of the carbocation and carbanion in the excitons responsible for light emission. Typically the allowed fluorescent transition of the "singlet" state has a much higher energy than the triplet state that does not permit light emission. Therefore light emission is normally weak without specific molecules that mediate conversion from the triplet to the singlet state. These molecules normally incorporate a heavy rare element such as iridium. The Adachi group has used time-dependent density functional theory coupled to advanced organic chemical synthesis to produce organic molecules with exceptionally low transition energies from the triplet to the singlet, promoting efficient fluorescence without the use of expensive metal atoms. A class of new molecules, carbazolyl dicyanobenzene (CDCB), were synthesized from commonly available materials in a single synthesis step reaction. No rare elements were required as catalysts. The single synthesis step without rare element catalysts makes the molecules cost effective to produce. The light emission wavelength of the molecules could be tailored by modification of the molecular structure, guided by DFT calculations. Peak emission wavelengths were obtained from ~450 to ~590 nm spanning blue to orange colors. Total external electroluminescence quantum efficiencies of 8-20% were obtained for devices emitting in the red, green, and blue portions of the spectrum, which is higher than is obtained from conventional OLEDs with conventional singlet-to-triplet converter molecules.

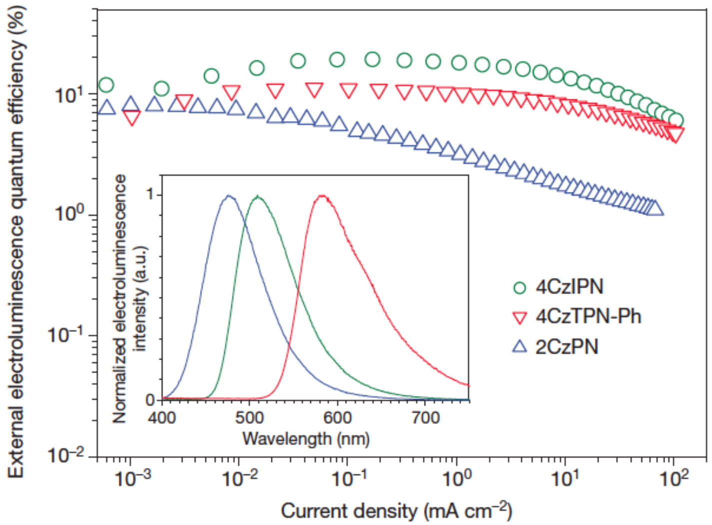
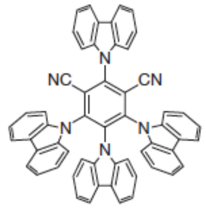


Fig. 2



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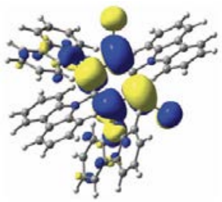

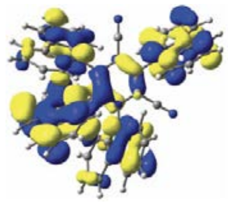

Fig. 3 Fig. 4 Fig. 5

Figures show Fig. 2 the external electroluminescence efficiency of OLEDS obtained with three different related carbazolyl dicyanobenzene molecules, Fig. 3 the structure of one of the new molecules created, Fig. 4 the lowest unoccupied molecular orbital and Fig. 5 the highest occupied molecular orbital of the molecule shown in Fig. 3.

Kobayashi, Masayuki; Masaoka, Shigeyuki; and Sakai, Ken. "Photoinduced Hydrogen Evolution from Water by a Simple Platinum(II) Terpyridine Derivative: A Z-Scheme Photosynthesis." Angewandte Chemie International Edition, 51, 7431-7434, 2012.

Description of Scientific Achievement:

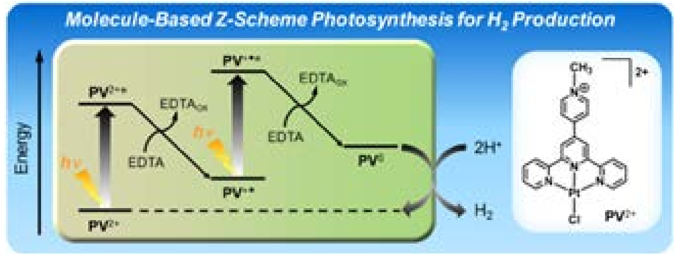

Fig. 6

Extensive studies have been carried out on the Pt(II)-based molecular catalysis for H_2 production from water using $Ru(bpy)_3^{2+}$-sensitized photosystems. As part of those studies, we previously reported that a Pt(II) complex having 2,2':6',2''-terpyridine as a ligand ($[Pt(terpy)Cl)^+$) serves as a bifunctional photocatalyst promoting both photosensitization and hydrogenic activation (Okazaki et al., Dalton Trans. 2009). In the present work, a new $[Pt(terpy)Cl]^+$ analog having a viologen-like acceptor unit (PV^{2+}) was designed and synthesized, and the mechanism of photochemical H_2 production catalyzed by PV^{2+} has been clarified in detail. Under visible light irradiation, PV^{2+} was shown to promote H_2

production from water in the presence of EDTA as a sacrificial electron donor. Interestingly, the photo-hydrogen-evolving activity was found to be dramatically enhanced by the presence of a Pt(II)-based molecular co-catalyst such as *cis*-$PtCl_2(NH_3)_2$. Next, the photochemical behaviours of PV^{2+} were elucidated by monitoring the time-course of UV-vis spectra under light illumination. In the first step, a reductive quenching of the photoexcited state of PV^{2+} (PV^{2+}*) proceeds to give a one-electron-reduced species of PV^{2+} ($PV^{+\bullet}$). Interestingly, $PV^{+\bullet}$ was found to be quite stable in the dark. It was clarified that effective H_2 formation proceeds only through the formation of PV^0, which is given by further reductive quenching of the photoexcited state of $PV^{+\bullet}$. This is the first example of study in which two-step photo-excitation of a molecular system drives hydrogen evolution from water, as nature does in the photosynthesis. Thus, we called it "Z-scheme".

Future Directions

Specific shorter term future directions involve collaborative development of novel inorganic group I and III oxides and their optimization for photoelectrochemical and photovoltaic cells by the Martin and Ishihara teams. These will be coupled to novel organic ligands that will produce hybrid organic/inorganic electrodes for photoelectrochemical cells and will be applied directly in next-generation inorganic photovoltaics. Additional materials science in support of inorganic photovoltaics enhancing current leading technologies manufactured in Japan will be developed by Rockett, Ishihara, and Kilner teams. Organic materials for OPV and OLEDS will be developed by the Adachi team. Both of these efforts will be supported by Ertekin, Staykov, and Rockett conducting simulations using density functional theory approaches and photovoltaic and photoelectrochemical device simulations. Steam electrolyzers will be optimized through inorganic materials development by Kilner supported by Ertekin and Staykov.

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

2. Hydrogen Structural Materials

Goals

Deployment of hydrogen fuel-based technologies requires that high-pressure hydrogen storage and distribution systems are safe, reliable, structurally efficient, and cost-effective. One safety and reliability consideration for hydrogen containment systems is the effect of degradation of metals is well documented and significant progress has been made in the discovery of the fundamental mechanisms for particular loading conditions (cf. work of Murakami, Kondo, Matsuoka, Robertson, and Sofronis), there remains a paucity of information about the wide spectrum of pathways through which hydrogen degrades the material properties and how these depend on the in-service conditions. A few examples should suffice to demonstrate the magnitude of the challenge: In hydrogen-accelerated fatigue failure, we do not understand how relatively low pressures of hydrogen degrade the material resistance by orders of magnitude. At a more fundamental level, we do not understand how relatively low pressures of hydrogen degrade the material resistance by orders of magnitude. At a more fundamental level, we do not know if vacancy stabilization by hydrogen is a potential fracture mechanism, let alone the operation and loading conditions under which vacancy formation can potentially bring about failure. Further, we do not know whether gaseous hydrogen serves as a lubricant in dry sliding seals or whether it couples with wear mechanisms to hasten failure. The systems that will be used in production, delivery, storage, and dispensing will contain non-metallic components. For example, polyethylene may be used as the liner in the pressurized tanks envisioned for use in automotive applications, and elastomers will be used in seals. In comparison to metallic systems, our knowledge base for hydrogen effects on the structural properties of non-metallic systems is, at best, rudimentary.

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

hydrogen on material degradation (e.g., hydrogen embrittlement). Hydrogen-material interactions can accelerate fatigue crack propagation, reduce fracture toughness, and enhance wear of structural components, which can lead to unexpected and catastrophic failures unless the related material degradation phenomena are understood and accommodated. The objective of the research in this division is to establish the fundamental knowledge that enables the development of new tools and technology: reliable and efficient test methods for measuring the effects of hydrogen on the fatigue, fracture, and wear properties of materials; models of hydrogen-assisted fatigue, fracture, and wear that include the detailed physics of hydrogen uptake, hydrogen-defect interactions, and material degradation; and next-generation materials having lower cost and improved performance (e.g., higher strength) without compromising resistance to hydrogen-induced degradation. This fundamental knowledge is attained by conducting complex mechanical property measurements on materials in challenging environments that include both high-pressure hydrogen and low temperature. In addition, physical models of hydrogen-induced material degradation derived from the mechanistic studies serve as the foundation for developing predictive model frameworks. The research activities in this division will ultimately lead to hydrogen containment systems that are optimized in terms of cost, performance, and safety.

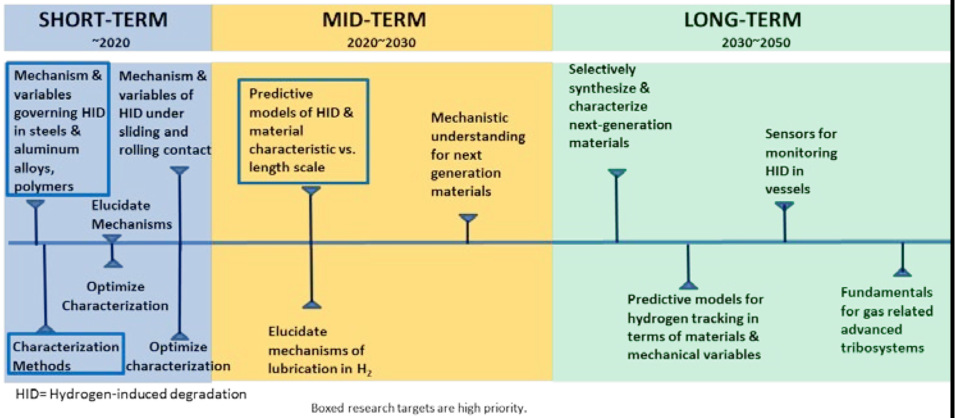

Fig. 7. Hydrogen Structural Materials Division Roadmap

Research Highlights

The research accomplishments from the Hydrogen Structural Materials division are in accord with the short-, mid-, and long-term technology experimental methods and such a team has been assembled. In particular, we plan to:

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

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

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

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

- 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.

and research objectives. An overview of progress toward objectives in the first two time horizons is provided in this section, and two corresponding significant accomplishments are detailed in the following section.

The short-term technology objective addressed by this division is deploying safe and reliable components (valves, piping, seals, etc.), vessels, and compressors for hydrogen gas storage and distribution. The work described here was motivated by several basic research objectives derived from the technology objectives, including elucidating the salient variables and mechanisms governing hydrogen-induced degradation in structural metals and optimizing methods for characterizing hydrogen-induced degradation in materials. The former research objective related to elucidating mechanisms of hydrogen-induced degradation pertains to fatigue and fracture as well as friction and wear.

One of the significant accomplishments described in the following sections relates to research objectives in the short-term horizon. These results from Prof. Robertson's team provide new insights into the nature of cyclic deformation-induced microstructure evolution during fatigue crack growth. In addition, the results show that such deformation-induced microstructure evolution is notably influenced by hydrogen. These elusive observations were only possible because of the development of advanced material characterization methods. These accomplishments recently documented in the *International Journal of Fatigue* demonstrate that the activity reported last year has progressed toward a clear story. Complementary results were produced by other research teams on different material systems. For example, Prof. Kubota's team demonstrated that hydrogen affected cyclic deformation in copper as well. In this new activity, it was observed that hydrogen significantly enhanced the development of slip bands. Although copper is not a high-priority structural metal for hydrogen technology, it is a model material for gaining fundamental insights about hydrogen-deformation interactions. In addition, Prof. Yamabe proposed that the mechanism of intergranular hydrogen embrittlement in high-strength steels includes the interaction of deformation twins with grain boundaries. This mechanistic interpretation was published in the *International Journal of Fracture* during 2012.

Two other activities represent an extension of work reported last year. In

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

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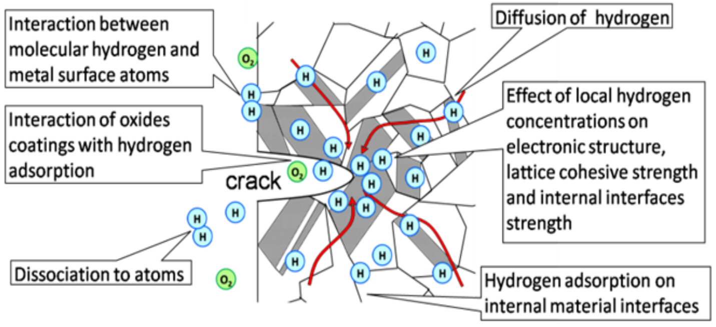

Fig. 2a. Fundamental processes around a crack in the presence of hydrogen

the 2012 report, Dr. Somerday indicated that the mechanism of hydrogen-assisted fatigue crack growth in low-strength steels involves intergranular fracture. Since then, Dr. Somerday has been collaborating with Prof. Takaki's team to design experiments that can test proposed mechanisms. These experiments require model Fe-C alloys, which Prof. Takaki's team have procured and characterized. In the friction and wear activities supervised by Prof. Sugimura, the notable result in last year's report was that hydrogen uptake into steel is blocked by oxide films formed under sliding at low contact pressure. The progression of this work has revealed that other variables contribute to surface oxide formation and its effect on hydrogen uptake, including contact pressure and temperature. These efforts to characterize the basic processes and variables affecting hydrogen uptake during sliding and normal contact between surfaces complements work on characterizing hydrogen uptake at crack tips to define basic mechanisms of hydrogen-affected fatigue and fracture.

Significant Accomplishments

Tsuboi, Koichi; Macadre, Arnaud; Tsuchiyama, Toshihiro; and Takaki, Setsuo. "Surface-layer microstructure control for metastable austenitic stainless steel plate to improve hydrogen embrittlement resistance." CAMP-ISIJ, 25, 1185, 2012.

Description of Scientific Achievement:

The ultimate goal is to develop lower-cost and higher-strength steels with excellent hydrogen embrittlement resistance by a variety of microstructural control techniques, such as ultrafine grain refinement, solid solution strengthening by high content of interstitial alloys, and so on. This emphasis on lower-cost and higher-strength steels is consistent with mid-term and long-term technology objectives identified for the division. Metastable austenitic steels are relatively cost-effective due to their low nickel content. In this class of steels, the formation of deformation-induced martensite markedly contributes to high strengthening. However, when martensite grains are connected to each other, a preferred path for hydrogen diffusion is created. As a result, hydrogen embrittlement is enhanced. In order to control the distribution of stable austenite and deformation-induced martensite phases, we applied a solution nitriding to metastable type 304 austenitic stainless steel sheet. Almost 80% of austenite transformed to martensite at each position below the surface in non-nitrided material, while deformation-induced martensitic transformation was suppressed and austenite was fully stabilized in the complete-nitrided material (86.4 ks). On the other hand, it is found that a stable austenite layer exists only at the surface in the incomplete-nitrided materials, and this austenite surface layer grows with increasing nitriding period (0.18 and 3.6 ks). The effectiveness of such an austenite surface layer against hydrogen embrittlement is measured in terms of tensile testing with and without electrolytic hydrogen-charging (Fig. 8). It should be noted that the embrittlement sensitivity is drastically reduced by stable austenite surface layer of only 10 μm in thickness. A patent has already been obtained on this technology.

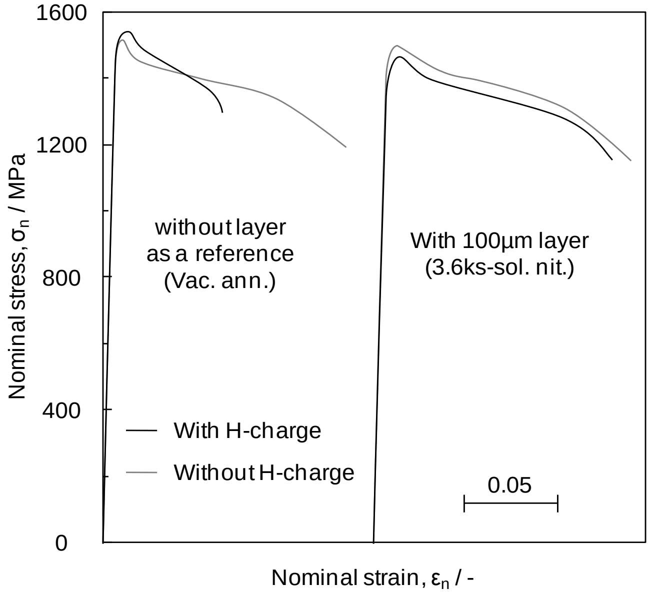

Fig. 8. Comparison of nominal stress-strain curves for hydrogen-charged and non-charged solution-nitrided (3.6ks) and 60% cold-rolled SUS304 steel sheets (100μm austenite phase layer).

Martin, M.L.; Sofronis, P.; Robertson, I.M.; Awane, T.; and Murakami, Y. "A microstructural based understanding of hydrogen-enhanced fatigue of stainless steel." International Journal of Fatigue, DOI: 10.1016/j.ijfatigue.2012.08.009, 2012.

Description of Scientific Achievement:

This project is motivated by the short-term technology objective of deploying safe and reliable components for hydrogen gas storage and distribution. Consistent with the related basic research objective, the methods and results described here elucidate the salient variables and mechanisms governing hydrogen-induced degradation in steels and optimize methods for characterizing hydrogen-induced degradation in materials. We have developed the capability to extract using the focused-ion beam (FIB) lift-out technique, transmission electron microscopy (TEM) samples from site-specific locations on fracture surfaces with irregular topography. This new technique has led to a significant advance in our understanding of microstructure evolution under fatigue loading as it makes it possible for the first time to observe the microstructure immediately beneath the fracture surface. Most notably, we have discovered that the microstructure developed beneath striations consists of a layered structure with the complexity decreasing with distance from the fracture surface. Furthermore, the presence of hydrogen modifies and refines the microstructure to an extent greater than achievable in its absence. This refinement in the absence and presence of hydrogen in 316 stainless steel is compared and contrasted in the micrographs presented in Fig. 9.

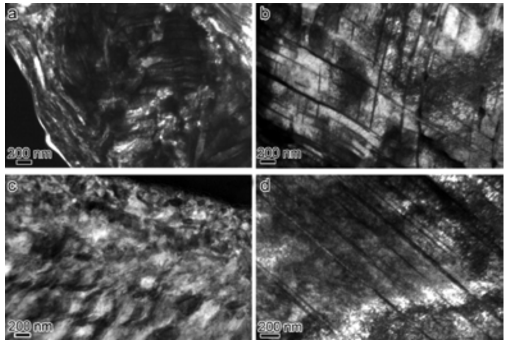

Fig. 9. Microstructures immediately beneath the fatigue fracture surfaces of 316 stainless steel fractured in both the absence (a-b) and the presence (c-d) of hydrogen. a) Microstructure immediately beneath the fracture surface (left side) produced in air consisting of a banded structure indicative of high levels of strain. b) Microstructure 5 μm from the fracture surface produced in air consisting of an array of planar structures (twins). c) Microstructure immediately beneath the fracture (top side) produced after hydrogen charging consisting of fine grains. d)

Microstructure 5 µm from the fracture surface produced after hydrogen charging consisting of planar structures (twins).

The uniqueness of these results is they demonstrate the microstructure beneath striations has evolved to an unanticipated state and the presence of hydrogen induces refinement but of a different nature. These results emphasize the need to understand the degree of microstructure development during fatigue loading but prior to crack propagation as this microstructure determines and dictates crack propagation and growth. Furthermore, the microstructural complexity suggests that a fundamental understanding of the fatigue processes is still lacking and that further studies using advanced experimental, modeling and simulation techniques are needed.

Future Directions

The future directions for Hydrogen Structural Materials are oriented toward the short-, mid-, and long-term technology and basic research objectives identified for the division. The common thread for these future activities is an emphasis on collaboration. These collaborative relationships will be fostered within the division as well as across division and institutional boundaries. Examples of collaborative activities that impact the short- and mid-term objectives are highlighted below.

(i) Short term

Future directions that impact the short-term horizon focus on the basic research objective of elucidating salient variables and mechanisms governing hydrogen-induced degradation in steels under mechanical loading conditions that induce fatigue, fracture, friction, or wear. By way of example, a new collaboration that fuses expertise from the fatigue/fracture (Prof. Robertson team) and friction/wear (Prof. Sugimura team) technical areas will determine how the microstructure evolution under wear conditions is influenced by the presence of hydrogen. The collaboration has already been established and characterization of samples with known wear properties has started. Another collaborative activity that addresses the short-term research objective of elucidating salient variables and mechanisms governing hydrogen-induced degradation in steels involves Dr. Somerday and Prof. Takaki's team. This collaboration represents an extension of work previously reported by Dr. Somerday, in which evidence from fatigue crack growth tests conducted on low-strength steels in hydrogen gas indicated that hydrogen embrittlement involved intergranular fracture. Dr. Somerday proposed several mechanistic scenarios for the hydrogen-induced intergranular fracture, and these will be tested by performing experiments on model Fe-C alloys. The first experiments will be conducted on two Fe-C alloys with varying grain size, which the Prof. Takaki team has already procured and characterized. The initial fatigue crack growth tests on these alloys will be a joint effort between Dr. Somerday and a member of Prof. Takaki's team (Dr. Arnaud Macadre) at Sandia National Laboratories in late summer/early fall.

(ii) Mid term

Future directions that impact the mid-term horizon focus on the basic research objective of developing models that predict the relationship between hydrogen-induced degradation and material characteristics at different length scales. In pursuit of this objective, Prof. Sofronis' team will facilitate a collaboration to finalize the new hydrogen-mediated crystal plasticity constitutive model. While the model framework now exists due to efforts by WPI Prof. Aravas, further progress depends on insights that must be derived from experiments. These experiments are extremely complex, involving compression tests on hydrogen-exposed single-crystal metals. Both the mechanical loading and hydrogen concentration boundary conditions must be accurately controlled. Design and execution of the experiments will be led by Dr. Somerday and WPI Prof. Kubota.

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.

3. Fuel Cells

Goals

The goal of the Fuel Cell Division is to develop efficient, cost-effective, and stable methods to convert hydrogen and other fuels into electricity using a fuel cell. Both high temperature (HT) and low temperature (LT) solid oxide fuel cells (SOFC) and low temperature polymer electrolyte membrane fuel cells (PEFC) are examined as shown in the roadmap figure. For the former, efforts are directed at developing lower temperature conductors, higher durability materials, and more effective electrode materials (catalysts). In the latter, efforts are directed at developing more durable and effective catalyst supports, more efficient and cheaper catalysts, and ionic membranes which can function at high temperature. While a practical focus on new systems remains at the forefront of this effort, more fundamental studies provide insight to

- 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.

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

inform future directions. All these efforts and the related research targets are shown in the Division's roadmap in Fig. 10.

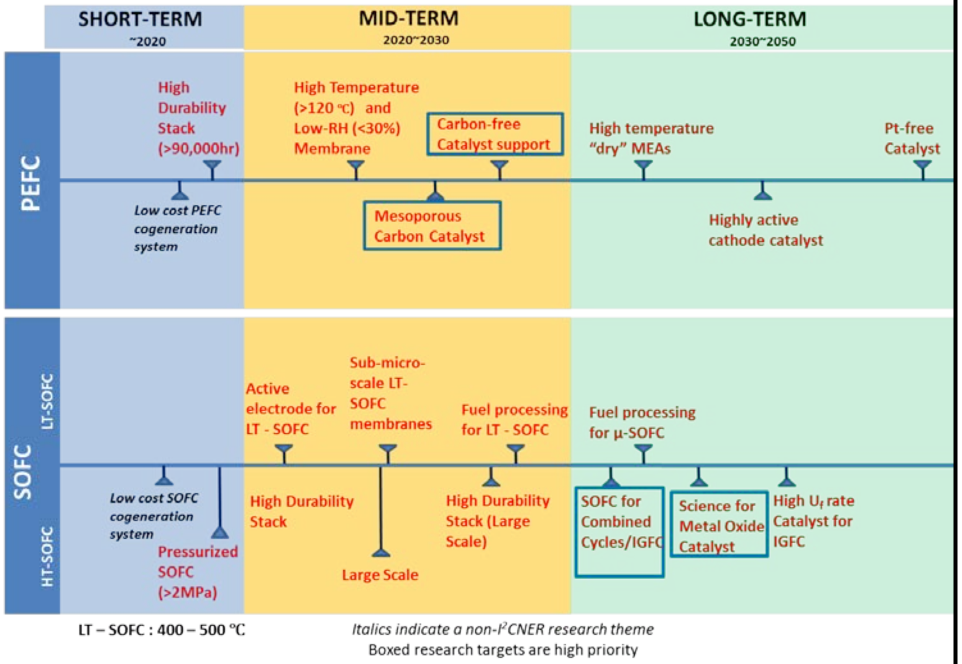


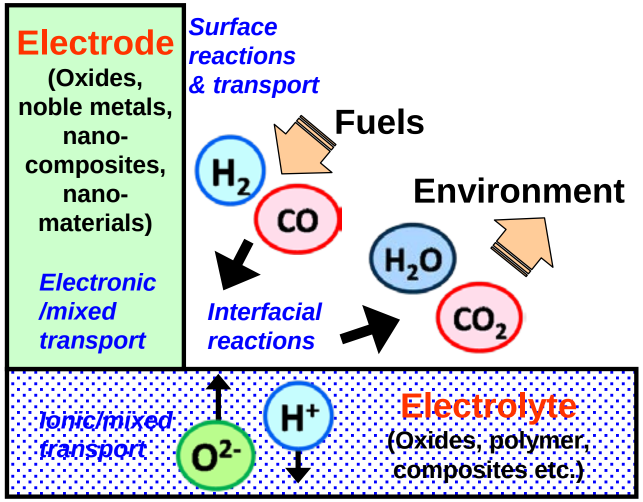
Fig. 10. Fuel Cells Division Roadmap

Research Highlights

In **PEFCs** efforts are directed at exploring durable materials to enhance device lifetime and to achieving higher temperature operation (>100°C), in order to improve efficiency. Specific objectives include: a) increasing system level durability and efficiency with a focus on new gas diffusion layers to improve water management, b) finding and evaluating durable supports including carbon-based nanomaterials and SnO_2, c) finding and evaluating a high temperature electrolyte. An emphasis has been on a polybenzimidazole (PBI)-based ionomer in combination with carbon nanotubes, but other materials such as graphene and charge-transfer complexes are also examined and d) finding Pt-free catalysts, such as nanostructured nitrogen-doped carbons, especially for the oxygen reduction reaction (ORR). Higher temperature operation is expected to improve the reaction kinetics of these materials, increasing their viability for use in commercial fuel cells

In **LT-SOFCs** efforts are directed at increasing the oxygen exchange

Interfaces in Fuel Cells



yte interfaces

activity of electrodes, developing high conductivity, stable, thin films, and developing more active electrodes to enable internal to SOFC reforming of fuels. A general goal is robust low temperature fuel cell operation. Specific activities include: a) developing thin film electrodes to enable both faster oxygen exchange kinetics b) developing low temperature (ca. 400 °C) thin film electrodes to act as proton conducting materials with an emphasis on interfaces between electrode and electrolyte and c) exploring mechanisms and materials (particularly ceramics) for low temperature hydrocarbon or alcohol reforming at SOFC anodes.

In **HT-SOFCs** efforts are directed at exploring durable, high temperature/high pressure/integrated gasification SOFCs for large-scale power generation. Specific activities include a) determining mechanisms and rate-determining steps for SOFC electrodes, b) developing impurity tolerant electrode materials for practical fuels, such as coal gas, c) combining SOFC technology with other processes, including electrolyzers, and d) developing an understanding of degradation mechanisms with a particular focus on the atomistic origins of chemical expansion.

Common goals for the division relate to electrode stability and durability, increasing the operating range to lower or higher temperatures, developing enhanced understanding of both anode and cathode catalysis, and developing electrolyte materials with enhanced conductivities.

Significant Accomplishments

The division boasts a number of important accomplishments over the previous period. These range from work using PBI modified CNTs for PEMs to Zr modified Ce for SOFCs.

Fujigaya, T. and Nakashima, N. “Fuel cell electrocatalyst using polybenzimidazole-modified carbon nanotubes as support materials.” Advanced Materials, 25, 1666-1681, 2013.

Description of Scientific Achievement:

In the first highlight, PBI-modifed CNTs are used as a support for fuel cell electrocatalysts. The use of carbon nanotubes (CNT) as a supporting material for PEFC electrocatalysts is ideal due to the high durability coming from the highly graphitized structure of CNTs. However, the homogeneous loading of metal nanoparticles onto the CNT surface is difficult due to the highly graphitized structure. Typically, the graphitized surface is treated by severe oxidation in order to introduce binding sites for metal nanoparticles. However, such oxidation treatments damage the graphitic structure, resulting in poor durability. Therefore, a novel idea of how to load metal nanoparticles onto undamaged CNTs was required. In this research we used PBI wrapped onto untreated CNTs to act as a biding site for Pt nanoparticles. By this approach, CNT-based electrocatalysts were obtained without introducing any damage into the CNT structure. In addition, PBI served as a proton conductor so that the composite of CNT, PBI and Pt possesses electron conductivity, proton conductivity and a reaction site, all of which are required for PEFC electrocatalysts. Since PBI shows proton conductivity at higher temperature ~200 °C compared to conventional polyelectrolytes such as Nafion, our PBI-containing electrocatalysts are utilized in a PBI-based PEFC. PEFC operation at temperatures over 100 °C afford many benefits including i) enhancement of reaction rates, ii) high CO tolerance and iii) replacement of Pt to the other cheaper metal, all of which contribute to the reduction of the cost of PEFC systems. Furthermore, the PEFC operation at higher temperatures results in high power generation efficiency.

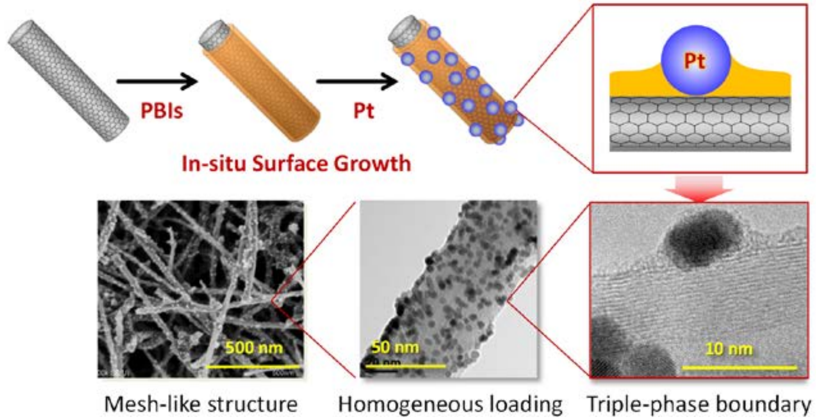
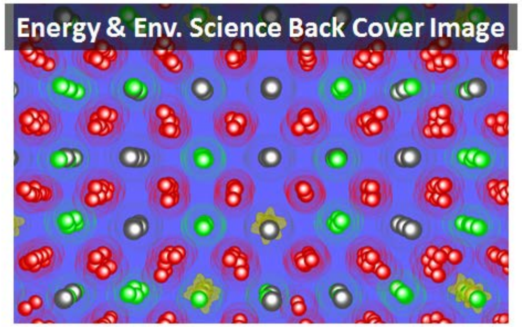


Fig 11. (TOP) Schematic diagram of platinum nanoparticles decorated on PBI-coated carbon nanotubes. (BELOW) Electron microscopy of this same CNT-PBI-Pt electrocatalyst system.

Bishop, S.R.; Marrocchelli, D.; Fang, W.; Amezawa, K.; Yashiro, K.; and Watson, G.W. "Reducing the chemical expansion coefficient in ceria by addition of zirconia." Energy and Environmental Science, 6, 1142-1146, 2013.

Description of Scientific Achievement:

The second highlight addresses SOFCs. In many advanced electrodes for SOFCs, non-stoichiometry induced dilation, known as chemical expansion, can lead to large strains with consequent stresses during operation, ultimately resulting in mechanical failure. Previous work by Kyushu University researchers showed that lattice relaxation around oxygen vacancies was a potential key method to manipulate, by cation substitution, the chemical expansion coefficient. For the first time, the role of isovalent Zr substitution in cerium oxide on the non-stoichiometry induced dilation (chemical expansion) was investigated. Chemical expansion was derived experimentally using HTXRD, dilatometry, and TGA measurements on $Pr_{0.1}Zr_{0.4}Ce_{0.5}O_{1.95-\delta}$ and computationally with DFT calculations on $Zr_{0.5}Ce_{0.5}O_{2-\delta}$. Though Zr was found to increase the reducibility and the corresponding chemical expansion of ceria (in the studied range), the relationship between chemical expansion and non-stoichiometry (the chemical expansion coefficient) was significantly smaller (54% less) than that observed in ceria, and consistent with predictions from our previous work. The origin of the reduced chemical expansion coefficient, associated with a larger contraction of the lattice around oxygen vacancies, was explained using DFT calculations and corroborated with prior investigations of enhanced reducibility of ceria-zirconia. This discovery has strong implications for reducing chemical expansion in SOFCs, thus increasing their durability, and that the studied material has potential for use in SOFC electrode functional layers.



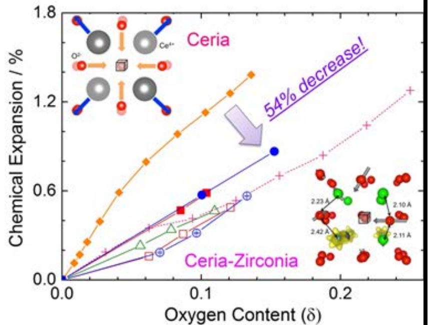


Fig. 12. By tailoring the lattice relaxation around oxygen vacancies by adding Zr to CeO_2, the chemical expansion was significantly reduced as computationally predicted by our group.

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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[2] P.L. Woodfield, S. Moroe, J. Fukai, M. Fujii, K. Shinzato, M. Kohno, and

Future Directions

Future directions will be focused on the themes shown in the roadmap and more specifically on carbon-free catalyst, mesoporous carbon catalyst, and high active cathode catalyst. In the case of high temperature SOFCs, according again to the roadmap, research will be done on durability and performance of the metal oxide catalysts for the anode of the SOFCs that will be part of the "novel SOFC combined cycle." This is a new cycle contemplated in Japan for power production—it combines an SOFC from which the exhaust gas is fed into a steam turbine to produce electricity. The anode needs to be resistant, durable, and performing, as it receives the impurity gas from all gasification. This cycle is viewed as an advancement in relation to the cycle to the left that is the so called Triple Combined Cycle.

4. Thermophysical Properties

Goals

In consultation with the Energy Analysis Division, the Division's research objectives are now covering the broader area of thermal science and engineering. The Division's roadmap and research targets are shown in Fig. 13. As can be seen, the overarching objective is the reduction of CO_2 emissions through efficient use of thermal energy. Moreover, almost all energy conversion processes suffer from losses associated with the transfer of thermal energy (heat) from higher to lower temperatures. Fundamental progress towards more intelligent and efficient energy utilization could be made if heat is transferred with the smallest possible temperature difference. For instance, Thermoelectrics, the direct thermal-to-electrical energy conversion systems, which could operate at lower temperatures (100–700ºC), will significantly expand the possibilities for waste heat recovery applications.

Further advancement and optimization of new energy technologies will be inhibited without an expansion of our knowledge base of the thermophysical properties of key substances projected for widespread use in the future low-carbon emission society. To lay the foundation for a wide range of low-emission technologies, in this regard, we need to expand the thermal properties database of relevant substances to a wider range of conditions and we need to generate data to understand

Y. Takata, "Techniques for Accurate Resistance Measurement in the Transient Short-Hot-Wire Method Applied to High Thermal-Diffusivity Gas," *Int. J. Thermophysics*, **30** (6), 1748-1772 (2009).

the mechanisms of heat and mass transfer associated with material interfaces, phase-change phenomena, surface phenomena and thin films relevant for developing new high-efficiency energy conversion technologies.

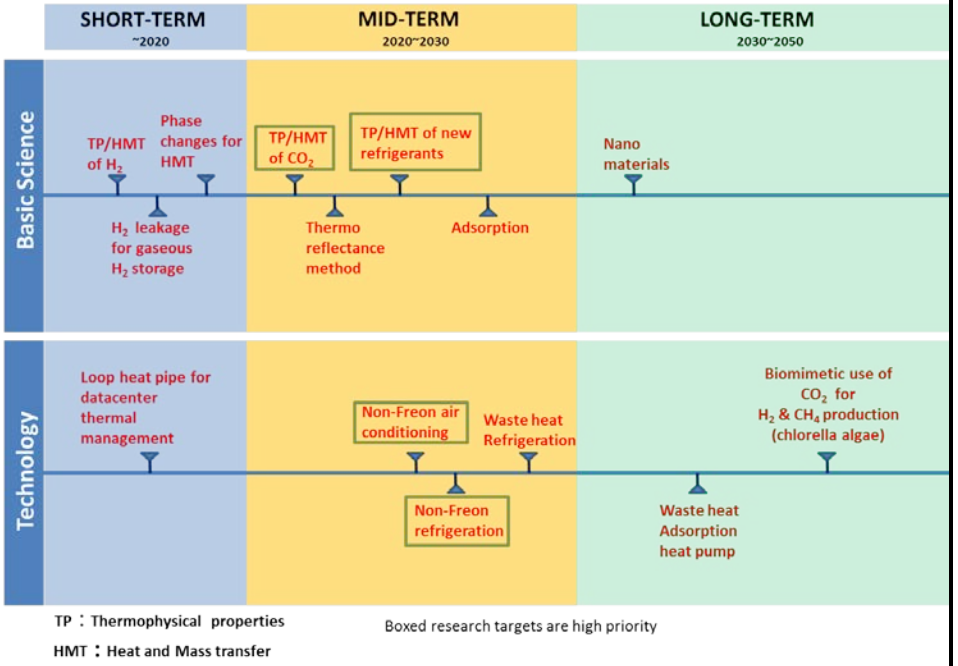


Fig. 13. Thermophysical Properties Division Roadmap

Research Highlights

The PVT property, viscosity and thermal conductivity of hydrogen up to 100MPa and 500°C has been measured. In addition, a compact curved wire vibrating method for viscosity measurement has been developed. We have succeeded in measuring the thermal conductivity of multi-walled carbon nanotube(CNT) and in the in- and out-of –shell thermal conductivities. Pump-probe optical technique has been applied to generating and detection GHz frequency surface acoustic waves. Innovative T-type method was used to detect thermoelectric properties of CNT.

Significant Accomplishments

Hayashi, H.; Ikuta, T.; Nishiyama, T.; and Takahashi, K. "Enhanced anisotropic heat conduction in multi-walled carbon nanotubes." Journal of Applied Physics, 113, 014301, 2013.

Description of Scientific Achievement:
Carbon nanotube (CNT) is a promising candidate as a supporting material for fuel cell catalyst. However, its thermophysical property is still unsolved, especially for multi-walled CNTs. By using our measurement technique of individual CNT, its anisotropic heat conduction is firstly unveiled. The determined in- and out-of-shell thermal conductivities of each CNT graphite shell show differences of more than four orders of magnitude due to the inter-shell gaps. The large range for the thermal conductivity reported for CNTs is caused by this enhanced anisotropy.

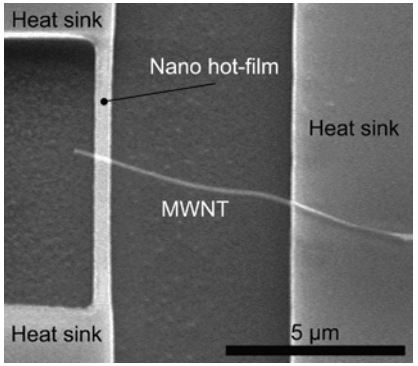


Fig. 14. SEM image of measurement of thermal conductivity of an individual CNT

Yusibani, E.; Woodfield, P.L.; Shinzato, K.; Takata, Y.; and Kohno, M. "A compact curved vibrating wire technique for measurement of hydrogen gas viscosity." Experimental Thermal and Fluid Science, 47, 1-5, 2013.

Description of Scientific Achievement:
Studies with the view to application of a curved vibrating wire method to measure hydrogen gas viscosity have been done. A fine tungsten wire with a nominal diameter of 50μm is bent into a semi-circular shape and arranged symmetrically in a magnetic field. The frequency domain response for forced oscillation of the wire is used for calculating the viscosity. Argon, nitrogen, helium and hydrogen viscosities have been measured at room temperature up to 0.7MPa. The deviations with respect to existing equations suggest that with more refinements it may be possible to take gas viscosity measurements with a precision of less than 1%.

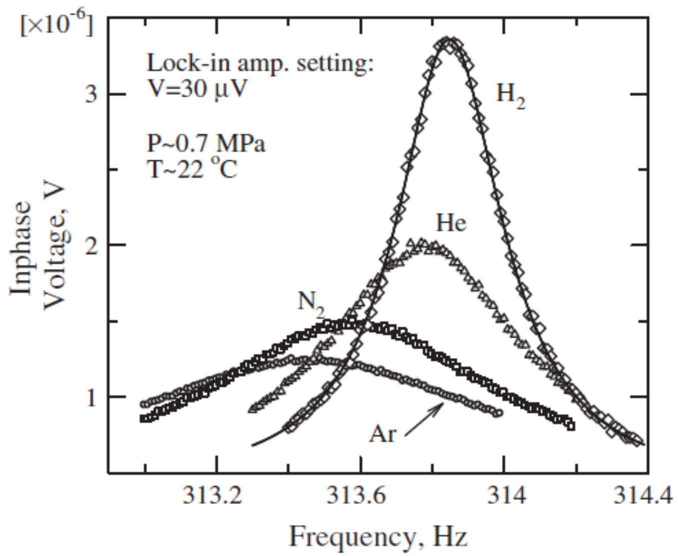


Fig. 15. Typical measurement and the corresponding least squares fit to the measured data with a 10mHz/step at 0.7 MPa

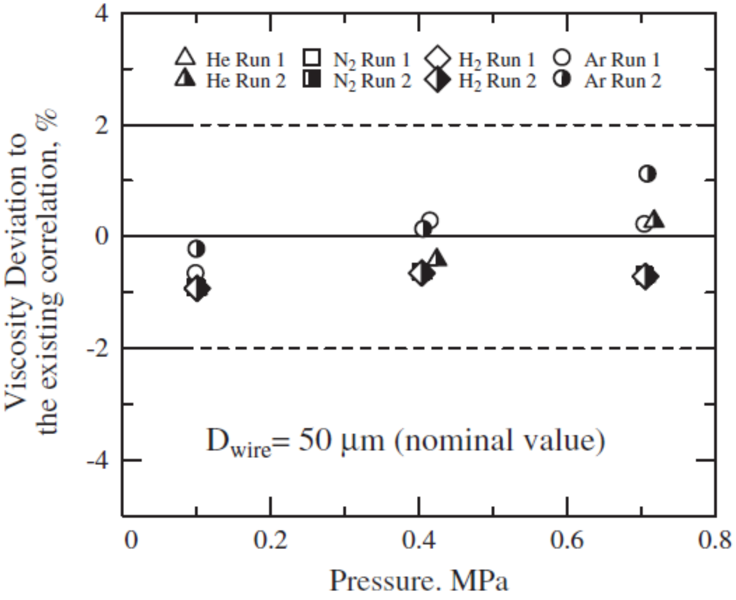


Fig. 16. Viscosity deviations versus pressure at room temperature

Future Directions

The Thermophysical Properties division will change its name to "Thermal Science and Engineering Division." This new name represents more accurately the research thematic areas of the division. Guided by the Division's roadmap, the Division's research in the future will focus on issues of: i) surface wettability in boiling and evaporation, ii) fundamental issues in nanoscale thermal transport; iii) low greenhouse potential refrigerants; iii) thermophysical property measurement by time-domain thermoreflectance; iv) low grade heat utilization systems; v) phase boundaries in fluid mixtures in the presence of hydrogen; vi) measurements of the viscosity, thermal conductivity and thermal diffusivity of carbon dioxide and its mixtures, vii) measuring in real-time of elastic constants of structural metals exposed to hydrogen using non-contact pump-probe optical methods, viii) efficient pump power use for hydrogen production (similar to chlorella algae).

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 mission of the Division is to carry out basic science research for the development of hydrogen storage materials for technology options that can significantly advance the realization of a carbon-neutral energy society. Applications include on board hydrogen storage, stationary energy storage in wide range of usage and capacity, electrochemical application such as the Ni-hydrogen battery, and others.

In the area of mobile applications, especially on board hydrogen storage for fuel cell vehicle, recent discussions with the Japanese automotive industry has guided the Division to focus on weight density, volume density, cost, and shape—Lead PI Professor Akiba is the chairperson of the national committee to revise the national hydrogen storage/transport target. At present, the research objectives of the Division for the on board hydrogen storage are identical to the national targets as shown in the roadmap of Fig. 17.

For the stationary applications, after the East-Japan earthquake energy storage from fluctuating renewable energy stably and compactly for a short to long term has become increasingly important. Storage of electricity in the form of hydrogen is a promising solution pathway. The volume energy density of hydrogen is higher than existing batteries by

Reference

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

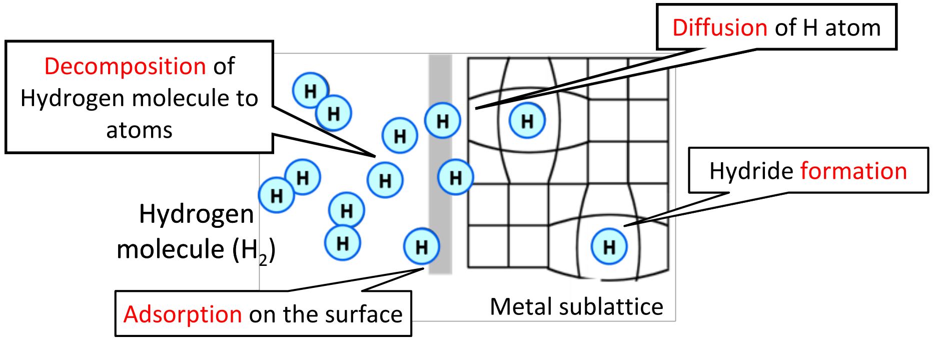


Fig. 5a. Fundamental processes at the surface of hydrogen storage materials

more than one order. Also, hydrogen storage materials can store hydrogen at much higher density than compressed gas of 70 MPa and liquefied hydrogen. For stationary applications, there are no Japanese national targets at present. One of the reasons is that this application is dispersed in scale, purpose, location of installation, etc. The Division's research is focused on volume density, cycle ability, and cost, as they all constitute key important targets for the development of materials for stationary usage.

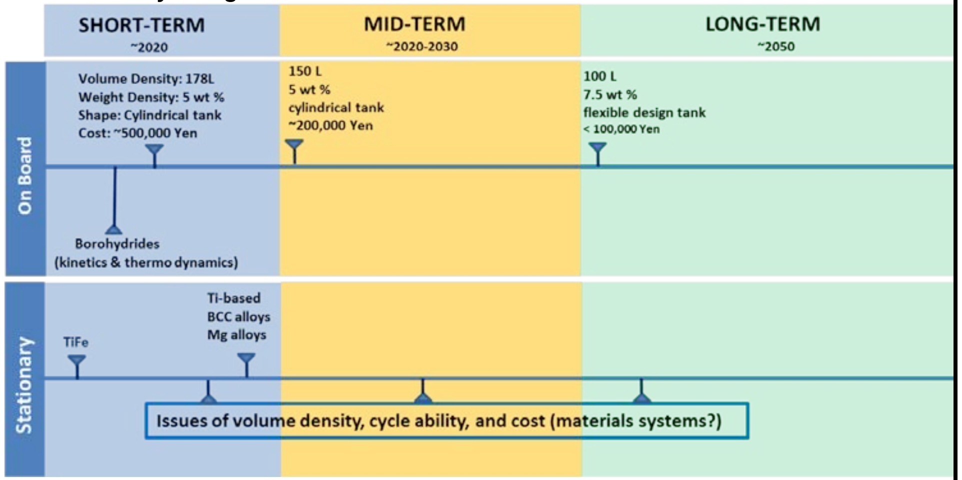


Fig. 17. Hydrogen Storage Division Roadmap

Research Highlights

TiFe is a low price ideal hydrogen storage material for stationary storage. It absorbs and desorbs hydrogen at room temperature under ambient hydrogen pressure in a more compact form than liquefied hydrogen. Although it has been reported as a storage system in late 1970s, it was abandoned for decades because activation (hydrogen absorption/desorption) requires heating at temperatures higher than 400°C under 30 bar (or higher) of hydrogen. In an ongoing collaboration, PIs Akiba and Horita targeted this issue of activation by using high-pressure torsion (HPT) techniques. Surprisingly, it was found that severely strained TiFe readily absorbs and desorbs hydrogen without activation.

For the study of Ti-based BCC systems, the microstructural changes of V-Ti alloys after hydrogenation were identified; twin boundaries introduced into the hydrogenated V-Ti alloys result in degradation of the effective absorbing capacity. Hydrogenation/dehydrogenation properties and microstructure of other Ti-based BCC alloys, which are one of the most promising candidates for hydrogen tanks in fuel cell vehicles, have also been investigated.

An important research focus point of the Division is to elucidate the hydrogenation mechanism of Mg/Ni films in order to improve kinetics and thermodynamics of Mg-based materials. Optimizing the composition of these films will help develop materials with higher performance. The relationship between microstructure and Mg/Ni ratio in Mg-Ni films has been elucidated by means of TEM.

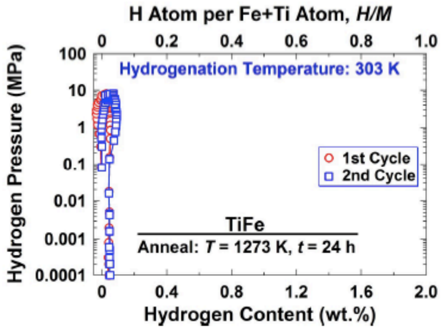
Significant Accomplishments

Edalati, K.; Matsuda, J.; Iwaoka, H.; Toh, S.; Akiba, E.; and Horita, Z. "High-pressure torsion of TiFe intermetallics for activation of hydrogen storage at room temperature with heterogeneous nanostructure." International Journal of Hydrogen Energy, 38, 4622-4627, 2013.

Description of Scientific Achievement:

TiFe is a low price ideal hydrogen storage material for stationary storage. It absorbs and desorbs hydrogen at room temperature under ambient hydrogen pressure in a more compact form than liquefied hydrogen. Although it has been reported as a storage system in late 1970s, it was abandoned for decades because activation (hydrogen absorption/desorption) requires heating at temperatures higher than 400°C under 30 bar (or higher) of hydrogen. In an ongoing collaboration, PIs Akiba and Horita targeted this issue of activation based on their complementary background, ideas, and techniques. Using high-pressure torsion (HPT) techniques, Professor Horita and his co-workers introduced enormously large strains in TiFe samples and measured their hydrogen storage and cycle life properties. Surprisingly, TiFe after the HTP treatment, readily absorbs hydrogen without activation at high temperature and high pressure as was required before. In addition, even though Ti and Fe are easily oxidized, TiFe exposed to air for a few months after several cycles of hydrogenation/dehydrogenation still readily reacts with hydrogen without activation.

In Figure 18 below, it is clearly shown that severely strained TiFe reacts with hydrogen without activation. It is also shown that no degradation has been observed after 4 cycles.



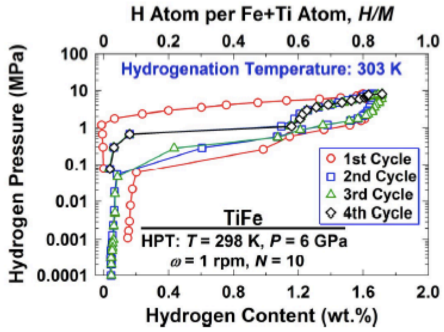


Fig. 18

Hydrogen absorption without straining   Hydrogen Absorption after severe straining

Future Directions

Advanced materials for on board application will be developed under a NEDO funded project (proposal under review) with three major Japanese carmakers and other stakeholders.

Hydrogen storage in severely deformed TiFe using the HPT (High Pressure Torsion) technique will be pursued further for mass production development and applications.

As the road-map indicates, first generation materials for on board storage are aimed for late real application in 2020s to 2030s. For early application they Division will also focus on high performance storage systems. Borohydrides have hydrogen capacity of over 10 wt %, but reaction speed and hydrogen release temperature are serious roadblocks at present. To control the kinetics and thermodynamics of borohydrides work will be carried out on intermediates of hydrogen release/uptake process.

Hydrogenation properties are heavily influenced by morphology, in other words nanostructures. TEM (Transmission Electron Microscopy) is one of the most powerful tools to observe nanostructures. This technique provides shape of nano-grains, crystal structures, interfacial structure and chemical analysis. Professor Matsuda introduces in-situ hydrogen cell to her TEM to observe dynamic behavior of hydrides using TEM. The materials to be observed are along the targets both for mobile and stationary applications as well as model materials for deeper understanding of phenomena.

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

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

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

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

6. Advanced Materials Transformations

Goals

The mission of the Division is to contribute to the creation of innovative carbon-neutral technology by developing novel catalysts, underlining both aspects of basic science and engineering. The activities are focused on investigations of catalysis-related "New energy and Energy conservation", all of which will make dramatic impact on the hydrogen-based carbon-neutral technology. The Division's work is classified into three major research areas with a roadmap shown in the figure as follows.

1. The sub-groups of S. Ogo and T. Rauchfuss are concentrated in basic research for understanding catalytic mechanism and exploring "novel catalysts for hydrogen activation and production." Subsequently, the research will drive the ultimate goal for conducting the artificial photosynthesis, extracting electron from water to produce fuels (hydrogen, methane, or formate, etc) for Carbon-Neutral Economy.

2. The sub-group of T. Katsuki is to explore effective "asymmetric catalysts for energy-conserving and waste-free materials transformations."

3. The sub-group of M. Yamauchi is focused on developing "nanoalloy catalysts for carbon neutral energy cycle."

In short, research in this Division focuses on exploring "novel catalysts" that underlie two important research objectives of Energy Conservation and Renewable Energy.

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.

References

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

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

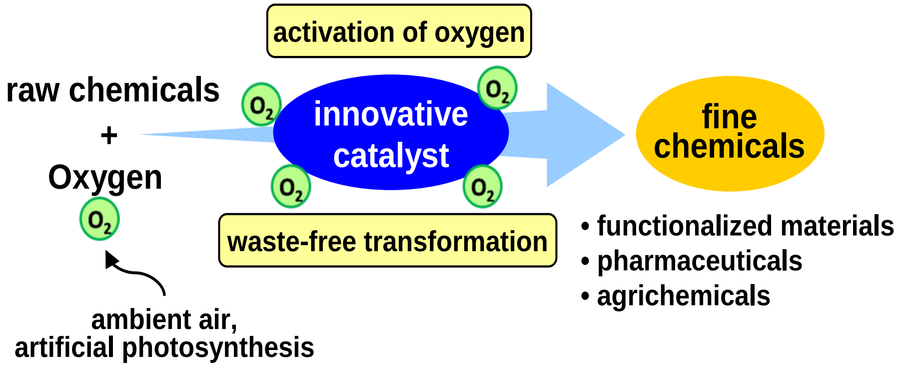


Fig. 6a. Concept of a catalyst process for a "zero-waste/no-carbon" reaction

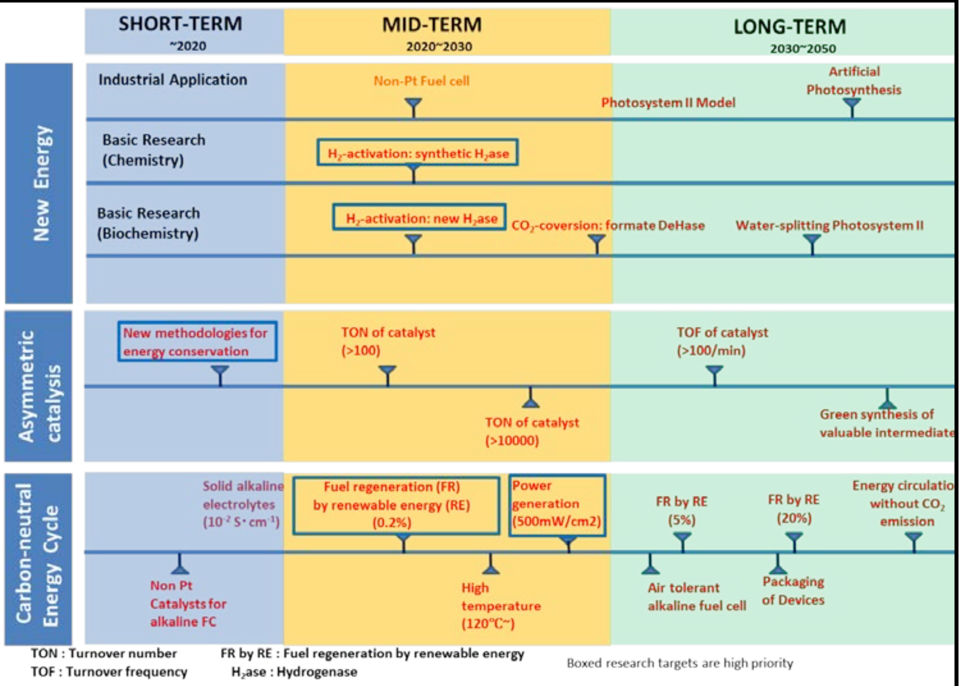


Fig. 19. Advanced Materials Transformations Division Roadmap

Research Highlights

As shown in the Division's roadmap (see Fig. 19), the main emphasis at this stage is the development of new synthetic hydrogenases (H_2ases). This fundamental but directed research is essential for our mid-term goals. Guided by biological designs, the S. Ogo group has described a potentially revolutionary approach to a functional [NiFe]hydrogenase mimic (Science 2013, 339: 682-684). Previous work by the Ogo group had led to a nickel catalyst that activated H_2, but it contained precious metals. Previous work by the Rauchfuss group had led to Ni-Fe catalysts but they lacked the ability to activate H_2. Ogo's breakthrough resolves both of the previous deficiencies, and the preliminary results suggest that the new catalysts exhibit properties useful for catalysis. For example, the catalysts transfer hydride to acceptor molecules, reminiscent of certain reactions in fuel cells. In parallel, the Rauchfuss group has completed related studies on a separately designed biomimetic catalyst, but with a focus on novel cofactors (Organometallics 2013, 32, 323). While the fundamental work by the Ogo and Rauchfuss groups is intrinsically interesting, it is of specific and practical value with respect to the evolution of new catalysts as described in our roadmap. Overall the combined, complementary efforts will help accelerate hydrogen fuel cell technology using a non-precious metal catalyst.

T. Katsuki and his group members have made good progress in developing routes for the synthesis of organic compounds with no or minimal waste. The range of opportunities for high impact are numerous. The breakthrough of the year entailed C-H amination under mild conditions (Angew. Chem. Int. Ed. 2013, 52(6), 1739-1742). This kind of transformation formerly required multiple steps and results in a substantial waste stream, the new shortcut is both more efficient and more selective. Clearly many opportunities exist in this theme (see roadmap), and current goals remain correspondingly broad within this context, including asymmetric epoxidation using air at room temperature, oxygen-driven dearomatization of hydroxy aromatic compounds, clarification of the mechanism for iron-catalyzed oxidation, asymmetric aziridination.

M. Yamauchi and her group succeeded in power generation by a direct ethylene glycol solid alkaline fuel cell using non-Pt catalysts, production of selective propylene synthesis catalysts and a high magnetization magnet (Nanoscale. 2013, 5(4), 1489-1493). In addition to the specific research accomplishment, I^2CNER is proud to have helped launch the independent research career of this dedicated and talented young woman.

Significant Accomplishments

Ogo, Seiji; Ichikawa, Koji; Kishima, Takahiro; Matsumoto, Takahiro; Nakai, Hidetaka; Kusaka, Katsuhiro; and Ohhara, Takashi. " A functional [NiFe]hydrogenase mimic that catalyzes electron and hydride transfer from H_2." Science, 339, 682-684, 2013.

Description of Scientific Achievement:

Chemists have long sought to mimic enzymatic hydrogen activation with structurally simpler compounds. We have reported a functional [NiFe]-based model of the active site of the [NiFe]-hydrogenase enzymes (Figure 20). This complex heterolytically activates hydrogen to form a hydride complex that is capable of reducing substrates by either hydride ion or electron transfer. Structural investigations were performed by a range of techniques, including X-ray diffraction and neutron scattering, resulting in crystal structures and the finding that the hydrido ligand is predominantly associated with the Fe center. The ligand's hydridic character is manifested in its reactivity with strong acid to liberate H_2.

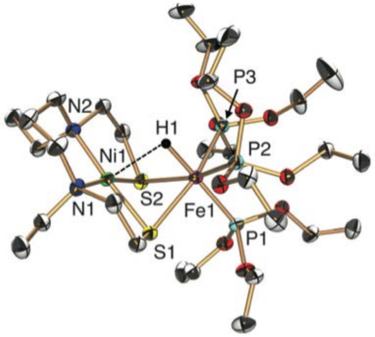


Fig. 20. Structure of the synthetic nickel-iron catalyst reported by Ogo et al.

Koya, Shota; Nishioka, Yota; Mizoguchi, Hirotaka; Uchida, Tatsuya; and Katsuki, Tsutomu. "Asymmetric Epoxidation of Conjugated Olefins with Dioxygen." Angewandte Chemie, International Edition, 51, 8243-8246, 2012.

Description of Scientific Achievement:
Biological oxidation, which is the most energy-conserving method for material transformation, is catalyzed by a sophisticated enzymatic system including oxidizing enzyme, electron transfer enzymes, and proton transfer and oxygen carrier proteins, and it is a long standing dream to design a catalyst that catalyzes biological-like oxidation using air as oxidant by itself. Water is obtained as byproduct in most biological oxidations. The authors designed a catalyst that can recycle water as proton source, undergo oxidation (that is, electron transfer process) twice in the catalytic cycle, and directly use air as oxidant (see Figure 21). This catalyst catalyzes biological-like epoxidation using air as oxidant at room temperature, without using electron and proton transfer and oxygen carrier systems (Figure 21). This is an unprecedented example that biological-like oxidation is conducted by a single catalyst.

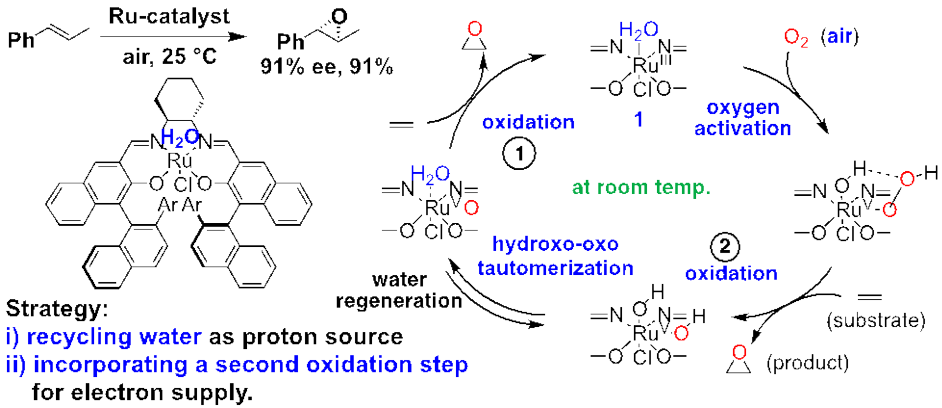


Fig. 21. Asymmetric epoxidation using air at room temperature and the mechanism proposed for this biological-like oxidation

Future Directions

In the area of energy conservation, research by the group of Prof. T. Katsuki has established the opportunities for I^2CNER-relevant catalysis that is unusually carbon-neutral. Because of the numerous opportunities, continued, careful consideration will focus on evaluating those transformation with the greatest impact, greatest relevance to the I^2CNER targets, shown in the roadmap of Fig. 19, and best leverage our collaborative atmosphere.

PIs S. Ogo and T. Rauchfuss are involved in area of New Energy. Guided by the roadmap, they will evolve and optimize synthetic hydrogenases at an accelerated pace. In view of breakthroughs in the Ogo group, the pace of this work is completely on course. Between the efforts of these two research groups, I^2CNER is in the position to lead the world in the elucidation of mechanism for biomimetic hydrogen activation. The coming year or two will witness integration of their new catalysts into fuel cell prototypes, as is being led by S. Ogo.

The group of M. Yamauchi has explored the nano alloy catalysis for carbon-neural cycle, linking the efforts of Energy Conservation and New Energy. Future work will be aimed optimizing these catalysts and integration with the efforts focused on fuel cells and hydrogen production.

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

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

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

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

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

7. CO_2 Separation and Concentration

Goals

To contribute to the mitigation of CO_2 emissions, the Division focuses on the fundamental science underlying the development of effective CO_2 separation and concentration technologies. In addition, since CO_2 is a by-product in current industrial H_2 generation, the Divisions research efforts on separation technologies are important for establishing a carbon-neutral hydrogen–powered society. Lastly the conversion of CO_2 to various value-added compounds, such as methanol, is also central to the Division's research objectives.

Research Highlights

In FY 2012, the Division revisited its research areas and in consultation with the Energy Analysis Division (EAD) refocused its efforts on capture, separation, and utilization technologies that hold promise for the future. The relevant scientific and technical challenges, which are outlined in the Division's research roadmap shown in Fig.22, are summarized as follows:

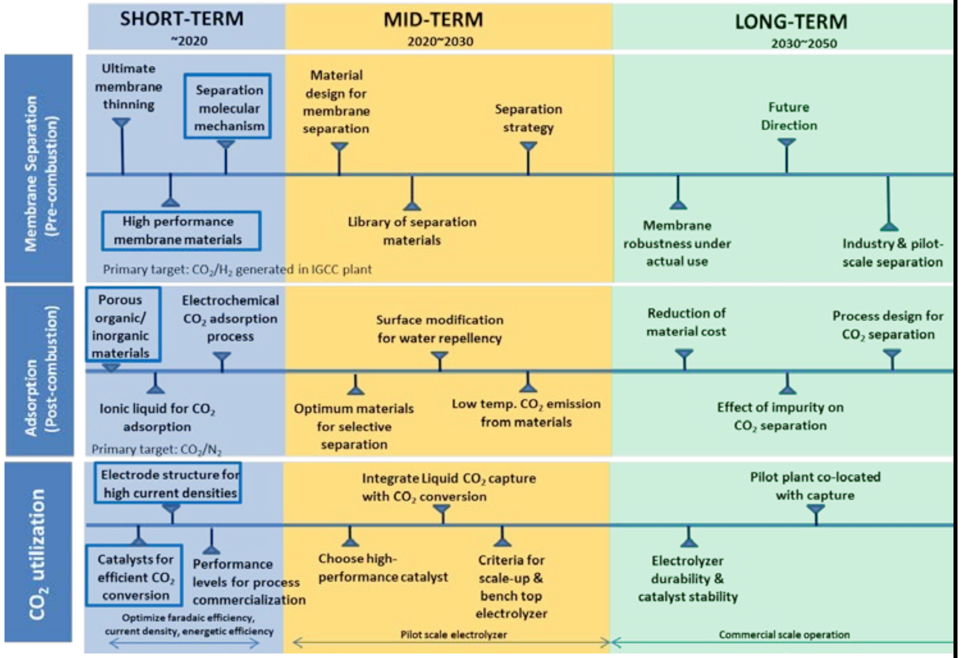


Fig. 22. CO_2 Separation and Concentration Division Roadmap

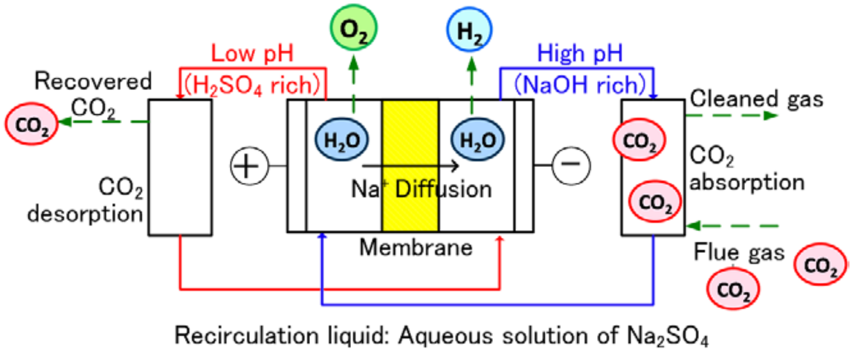


Fig. 6a. An advanced CO_2 separation and concentration system

CO_2 Capture and Separation

The CO_2 separation cost is a dominant feature of the whole process of carbon capture and storage (CCS). Among conventional CO_2 capture technologies, the solvent absorption method has been investigated and has gained current acceptance as the most accessible CO_2 capture technology. However, it requires heating or additional energy for CO_2 recovery after the absorption, which results in increased costs of CO_2 capture. Table 1 summarizes the present and targeted costs of each of the current CO_2 capture technologies.

Table 1. Separation technologies

Technology	Current Situation: Cost: JPY/t-CO_2	Current Situation: Energy: kWh/t-CO_2	Target cost: JPY/t-CO_2
Liquid absorption	4,900-5,800* ($54 - 64)	200-230	2,000 ($22)
Membrane	- (Not used)	- (Not used)	1,000 ($11)
Solid Adsorption	13,000-17,000** ($144 - 188)	640-680	1,500

* From METI's report 2010
** From National Petroleum Council Report 2012
Energy is calculated from 1 kWh = 25 JPY (1 USD = 90 JPY).

According to this table, the solvent absorption method is not the most efficient process and alternative and game changing separation technologies are needed. Membrane separation and adsorption are promising candidates with great potential for efficient CO_2 capture processes, at reduced cost. In order to fully understand and utilize the advantages of membrane separation and adsorption, we decided to aim at the separation and adsorption of pressurized CO_2 gas emitted in pre-combustion and liquid natural gas extraction, as these sources emit a pressurized gas stream.

By considering and surveying of the current state-of-the-art in membrane separation of CO_2, our priority target of source gas is a pressured mixture gas of CO_2 and hydrogen, since hydrogen is valuable as an energy carrier. This mixture gas is generally emitted from an Integrated Coal

Gasification Combined Cycle (IGCC) plant. In addition to the industrial aspects, such membrane separation presents serious scientific challenges. Because the CO_2 molecule is larger than hydrogen, conventional size-based separation and capture do not work well. Furthermore, there is a contradictory problem in membrane separation, i.e. effective gas separation leads to smaller gas permeance and vice versa. In order to tackle this problem, the Division's approach is based on membrane material design and ultimate thinning of the membrane, an approach that may also turn out to be useful for other gas separation technologies. Capture is also an issue. As part of the CO_2 capture process, we will make efforts to develop porous materials, including MOFs, zeolites, etc.

CO_2 Utilization

Underground carbon sequestration is likely to be part of the strategy utilized to curb the increase in atmospheric CO_2 levels. Sequestration is part of the now widely accepted "stabilization wedges" approach, introduced in a famous publication by Pacala and Soclow in Science in 2004 (Vol. 305, pp. 968-972). Many of the stabilization wedges, for example the capture and underground sequestration of CO_2, come with a substantial net cost, and many have absolutely no potential for economic gain. *In contrast,* utilization of CO_2 has also attracted much attention recently, since CO_2 is one of the carbon sources to be converted to valuable compounds Thus, *this project seeks to explore an approach (i.e., a potential additional stabilization wedge) that has the potential to earn back some of the cost of carbon capture through the electrochemical reduction of the captured and purified CO_2 into useful chemicals.* This process can be driven by the vast amounts of intermittent *excess* renewable power that is becoming available in many locations around the world. Furthermore, by utilizing CO_2 as the starting material for chemical production, our dependency on fossil fuels is reduced. We strongly believe that the research in CO_2 utilization is necessary to establish a whole scheme from CO_2 capture to its utilization as an alternative option instead of CO_2 storage. As mentioned above, CO_2 capture, separation and underground sequestration is a highly costly process, with no economic return. Instead, CO_2 capture, separation followed by chemical conversion (and no underground sequestration) has the potential to provide economic value!

Significant Accomplishment

Thorson, Michael R.; Siil, Karl; and Kenis, Paul J.A." Effect of cations on the electrochemical conversion of CO_2 to CO." Journal of the Electrochemical Society, 160, F69-F74, 2013.

Description of Scientific Achievement:

In this study we investigated the influence of electrolyte composition on the electrochemical reduction of CO_2 to CO. Specifically, we studied the effect of the size of alkali *cations* on the partial current densities of the two products: CO and H_2. We found that large cations suppress H_2 evolution, while increasing the partial current density for CO resulting in high Faradaic yields for CO production. We were able to rationalize these observations through a model that is described in the resulting publication.

Future Directions

The Solvent absorption approach is the most established technology. However, implementation and commercialization requires further cost reduction. In I^2CNER, the focus will be on CO_2 separation with membranes and adsorbents which are expected to lead to more effective technologies.

CO_2 Capture and Separation

Membranes (Taniguchi, Fujikawa)

The target of membrane separation is in an IGCC plant, where CO_2 is separated over H_2. A number of CO_2 separation membranes have been developed, however, only a few successful examples can be found. The dendrimer membrane developed by Prof. Taniguchi exhibits some of the highest CO_2 separation performance. The separation factor (ratio of permeability) and CO_2 permeance under pressurized condition are 30 and 1.0×10^{-10} m^3(STP)/(m^2 s Pa), respectively. However, for implementation, the CO_2 permeance has to be raised to 7.5×10^{-10} m^3(STP)/(m^2 s Pa), whereas the separation factor is qualified. It has been found that CO_2 permeance is inversely proportional to the membrane thickness (10-500 μm), which indicates that CO_2 permeation is diffusion controlled. Increase in CO_2 permeance would be achieved by reducing the membrane thickness. Considering these aspects and the milestones, efforts will focus on material design and membrane thinning.

Porous materials (Kusakabe)

Exploration of various classes of absorbent materials is important given that organic/inorganic composite materials have great potential for the design of porous structures absorbing CO_2. The purpose is to develop porous materials, including MOFs, and zeolites. In FY 2011, we have succeeded in preparing a large size MOF-5 which has porous crystal structure composed of organic ligands and metal ions. We will evaluate gas adsorption functions with this large MOF crystal and improve its CO_2 adsorption and desorption properties by re-designing the structure based on the initial experimental results. In addition, preliminary results to make a membrane from this porous material on a filtration support have been obtained. This porous membrane on a filtration support also has great potential as an efficient CO_2 separation membrane.

CO_2 Conversion

In FY 2012 Kenis, in close collaboration with collaborators from the fuel cell division, has identified three very promising catalyst materials for the selective conversion of CO_2 to CO: (1) polymer-wrapped, multiwall nanotube supported Au nanoparticles – with Nakashima and Fujigaya as well as Gewirth; (2) an organometallic catalysts – with Gewirth; and (3) a metal free carbonitride catalyst – with Lyth. These catalysts start to approach the metrics needed for development of a commercial process: a Faradaic efficiency (FE) of >95%, an energetic efficiency (EE) of >60%, and a current density (CD) of at least 200 mA/cm^2.

Considering these aspects and the research targets of the Division, our efforts in 2013 to 2014 will focus on three points: further characterization and optimization of these catalysts, and optimizing electrode structure, including implementation of these catalysts into these electrodes; and evaluation of the envisioned process with respect to its potential for commercialization.

8. Carbon Capture and Storage

Goals

The carbon capture and storage (CCS) Division of I^{2}CNER addresses the underlying science associated with the roadblocks for large-scale implementation of CO_2 storage, including risk of CO_2 leakage, risk of induced seismicity, and high-cost, that are intimately related to the highly

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

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

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

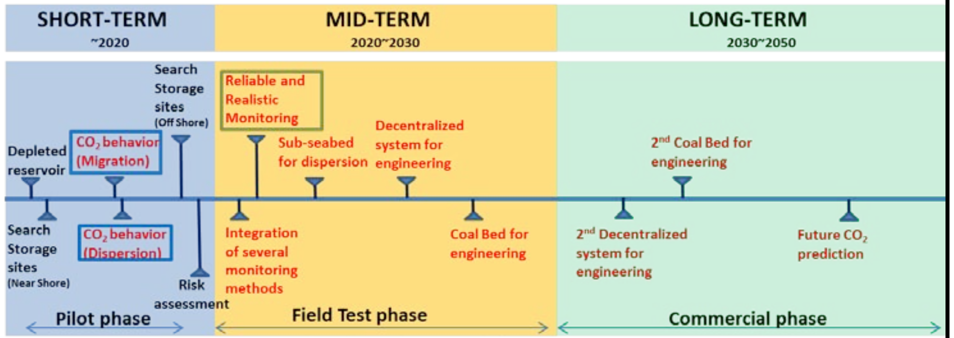
- Prof. Kyuro Sasaki has a notable research record on the study of the effect of SO_x on the CO_2 storage capacity and CO_2 phase behavior.

References

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

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

uncertain local geological characteristics of potential storage sites. The relevant CCS technologies and research target areas are depicted in the Division's roadmap shown in Fig. 23. Thus, **reservoir characterization** as well as **monitoring and modeling of injected and leaked CO_2** are crucial steps in the development of CCS relevant to I^{2}CNER's short-term CCS objectives, as developed in parallel with the Energy Analysis Division, and have therefore received considerable research focus during FY 2012, with particular attention on the goal of monitoring and modeling of injected and leaked CO_2 in geological structures typical of Japan.



Boxed research targets are high priority.

Fig. 23. Carbon Capture and Storage Division Roadmap

With respect to **reservoir characterization**, efforts are directed at understanding rock heterogeneity in constructing geologic models and in designing monitoring surveys owing to the complicated nature of such formations in Japan compared to that in other countries (e.g., Australia). Furthermore, since it is difficult to find structural closure for CO_2 injection in the Japanese islands and around their continental margins (i.e., anticline structure), substantial research effort is focused on uncovering the physical mechanisms responsible residual, dissolution, and mineralogical trapping of CO_2 in porous formations. The current efforts involve collaborative experimental, modeling and simulation efforts to develop a comprehensive suite of tools that can be utilized in the future for robust prediction of CO_2 migration fate in the heterogeneous rock structure typical of Japan. An additional key focus area in this regard is the development of experimental capabilities that provide venues for studying the behavior of CO_2 in a range of contexts at pressures and temperatures relevant to actual CCS applications, including liquid CO_2 behavior in model and actual rock structures as well as CO_2 fate upon

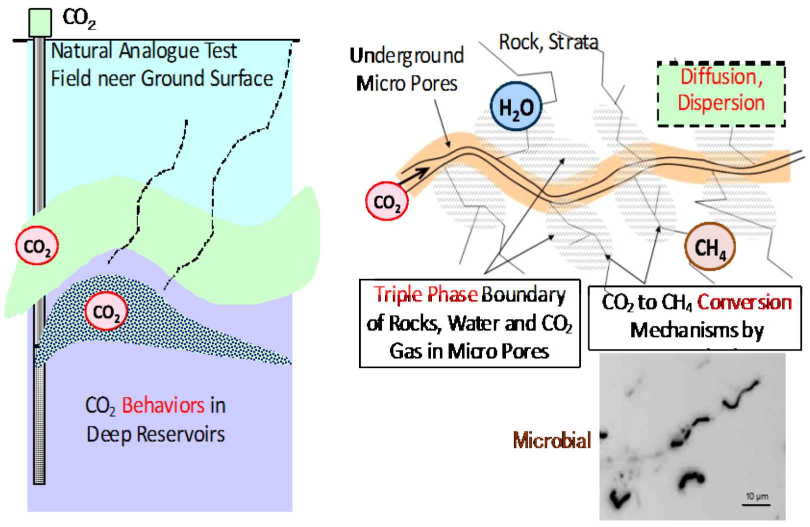


Fig. 8a. CO_2 geological storage

leakage into the ocean through compromised cap rock (using a new high-pressure water tunnel to be installed at Kyushu in FY2013). Finally, effort is directed toward developing reservoir characterization methods to construct geological models from limited geophysical/geological data.

With regard to **monitoring and modeling of injected and leaked CO_2**, efforts are directed to the development and deployment of monitoring methods that can address the very long time scales associated with permanent trapping of CO_2 in geological formations (which are much different than those utilized in CO_2-based enhanced oil recovery, for example). We are therefore developing a geophysical monitoring technique using the noise signal of ground tremors. To address potential leakage from sub-seabed storage sites, we are also developing monitoring techniques using seafloor-based acoustic tomography and pH/pCO_2 sensors mounted on an autonomous underwater vehicle (AUV) as well as on a remotely-operated underwater vehicle (ROV). Finally, since the water in many Japanese geological formations has low salinity, the dissolution rate, as well as chemical reaction rates, of injected CO_2 are being studied for successful prediction of CO_2 dispersion fate should it be leaked into the ocean.

Research Highlights

The CCS Division has undertaken a substantial refocusing of its short- and long-term research objectives during FY 2012, with wide-ranging accomplishments focused on the two main research foci of **reservoir characterization** and **monitoring and modeling of injected and leaked CO_2**.

In the first highlight, a monitoring method to estimate the variation of seismic velocity using ambient noise was developed. Since this method constructs virtual source signals from noise, we can conduct a time-lapse survey and extract subsurface information using only passive seismometer data. The low cost of this approach makes it particularly attractive for long-term monitoring of geological CCS projects. Minato et al. (2012) applied this method to the seismometer data in the Tohoku region and extracted the variation of seismic velocity of the crust during the 2011 earthquake. The variation of seismic velocity can be transformed to a pressure-stress variation and demonstrates that this method useful time-lapse information. We have recently applied this method to seismometer data acquired during fluid injection (injectivity

9. O_2 ocean sequestration: informing the public on ocean sequestration (Lead PI: Prof. Tetsuo Yanagi)

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

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

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

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

References

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

[2] G. Onitsuka, I. Uno, T. Yanagi and J. H. Yoon, "Modeling the effects of

test data for CO_2 injection). By improving this method, we have been able to resolve the variation of the P-wave velocity due to the fluid injection. This advance represents a crucial first step toward monitoring injected fluid using ambient noise because this velocity variation can be interpreted as pore pressure increasing due to fluid injection, thus allowing one to estimate pore pressure variation within an aquifer formation. These developments represent a critical underpinning for our CCS objective of long-term, reliable monitoring of formation stability during CCS.

The second highlight involves development of strategies for detecting and monitoring CO_2 leakage from the seafloor, using instrumentation and equipment that we have developed and tested. This development (Shitashima et al., *Applied Geochemistry*, 30, 14-124, 2012) culminated in a collective approach for detection and monitoring of CO_2 leakage in sub-seabed CCS via detection of CO_2 leakage using seafloor-based acoustic tomography, followed by mapping the distribution of the leakage points using a novel pH/pCO_2 sensor installed on an AUV, and then monitoring of the impacted area using a remotely operated underwater vehicle. This development is ground-breaking as it represents the first published work describing a comprehensive approach for effectively monitoring of CO_2 leakage in sub-seabed CCS and represents a critical advance toward another of our CCS objectives, specifically long-term, reliable monitoring of leaked CO_2.

The final highlight addresses the fate of CO_2 within porous rock structures leveraging the fact that the physical properties of rocks are controlled by the fluid state in the pore space, meaning property variations extracted from geophysical monitoring can be exploited to understand CO_2 behavior in the reservoir. In seismic approaches, the change in seismic velocity can be used to evaluate the distribution of injected CO_2, since the P-wave velocity decreases dramatically with increasing as CO_2 infiltration. To construct these relationships from geophysical monitoring, extensive laboratory experiments have been previously conducted (Kitamura et al., *Journal of MMIJ*, 128, 511-518, 2012), though these relationships are strongly influenced by pore geometry as well as by pressure and temperature (PT) conditions. Therefore, in order to generate a quantitative description of CO_2 migration in porous media and to construct relationships between CO_2 saturation and field-derived properties, we developed a digital three-dimensional rock model using a discrete-element method and applied a two-phase Lattice Boltzmann Method (LBM) implementation to

atmospheric nitrogen input on biological production in the Japan Sea", *J. Oceanography.*, **65**, 433-438 (2009).

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

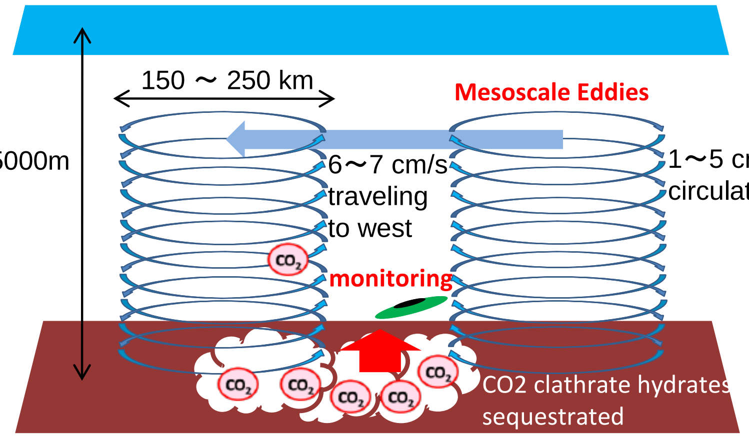


Fig. CO_2 ocean sequestration

compute supercritical CO_2 distributions within the pore space (Tsuji et al., *Geophysical Research Letters*, 39, L09309, 2012; AGU fall meeting, GC51A-1176, San Francisco, December 3-7, 2012). These results were then used to calculate elastic and electrical properties using a finite-element method, as a means of constructing a relationship between CO_2 saturation and survey-derived properties (i.e., seismic velocity and electric resistivity). These relationships are crucial for accurate estimation of CO_2 behavior from time-lapse geophysical surveys. This on-going work therefore represents a crucial component of our CCS objective to understand and eventually model CO_2 fate in geological formations and the viability of pore-space trapping mechanisms, particularly residual trapping.

Significant Accomplishments

Shitashima, K; Maeda, Y.; and Ohsumi, T. "Development of detection and monitoring techniques of CO_2 leakage from seafloor in sub-seabed CO_2 storage." Applied Geochemistry, 30, 114-124, 2012.

Description of Scientific Achievement:

In this work, an approach to detect and monitor CO_2 leakage from the seafloor in sub-seabed CCS, using instrumentation and equipment that we have developed and tested, is reported (Fig 24). The relevant strategy includes the following steps: i) detect CO_2 leakage using seafloor-based acoustic tomography, ii) map the distribution of the leakage points using the pH/pCO_2 sensor installed on the autonomous underwater vehicle (AUV), iii) monitor the impacted area using a remotely operated underwater vehicle, or the automatic elevator, or by towing the multi-layer monitoring system. This is the world's first paper to discuss monitoring of CO_2 leakage in sub-seabed CCS. The establishment of a reliable approach to monitor leaked CO_2 is one of the most important goals of the CCS Division. This study is directly related to the Division's long-term targets regarding reliable monitoring of leaked CO_2.

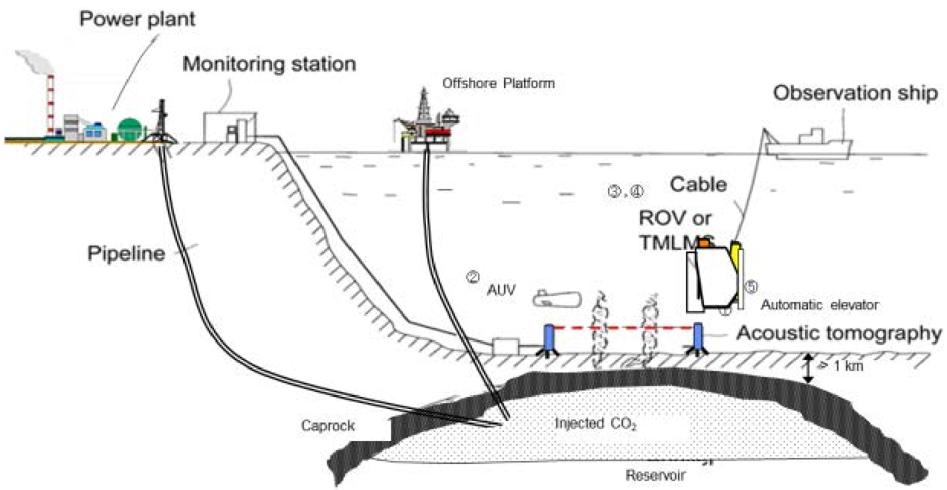


Fig. 24. Strategy for detection and monitoring of CO_2 leakage in sub-seabed CCS.

Minato, S.; Tsuji, T.; Ohmi, S.; and Matsuoka, T. "Monitoring seismic velocity change caused by the 2011 Tohoku-oki earthquake using ambient noise records." Geophysical Research Letters, 39, L09309, 2012.

This paper develops a monitoring method to estimate the variation of seismic velocity using ambient noise for the purpose of monitoring injected CO_2. Since this method constructs virtual source signals from noise, a time-lapse survey and extraction of subsurface information using only passive seismometer data can be conducted. The low cost of this approach makes it particularly attractive for long-term monitoring of CCS projects. The method was applied to the seismometer data in the Tohoku region and extracted the variation of seismic velocity of the crust during the 2011 earthquake. The variation of seismic velocity can be transformed to a pressure-stress variation. The method has already been applied to seismometer data acquired during fluid-injection (injectivity test data for CO_2 injection). By identifying the variation of the P-wave velocity due to the fluid injection the method can provide a robust first step toward monitoring the injected fluid through using ambient noise.

Future Directions

The CCS Division will continue focusing on its short-term objectives of **reservoir characterization** and **monitoring and modeling of injected and leaked CO_2**, as developed in collaboration with the EAD, are crucial steps toward the execution of CCS projects in Japan. Of particular focus will be the local heterogeneity when constructing geological models for modeling studies, as well as for the design of geophysical monitoring surveys. In parallel, we will continue our efforts toward understanding and modeling CO_2 injection using the mechanisms of residual, dissolution, and mineralogical trapping. We will also accelerate our efforts to develop a reservoir characterization method to construct geological models from the limited geophysical and geological data. A key aspect of overall mitigation is understanding issues of seismicity, so the CCS division will also develop new and novel tools to monitor and control the pore pressure variation due to CO_2 injection, in order to prevent generation of large earthquakes due to CCS, with specific focus on geological formations typical of those in Japan.

We have begun, and continue, to develop **new CCS concepts suited for geologic characteristics in Japan.** We focus on the decentralized, renewable, and deep-offshore CCS. In decentralized CCS, the primary trapping mechanism is dissolved trapping. Thus, we can safely inject CO_2 into a relatively shallow reservoir (~100 meters) at low cost. In renewable CCS, we propose to convert injected CO_2 into CH_4. This CCS approach will provide hydrocarbon fuel for Japan. In deep-offshore CCS, we can inject large amounts of CO_2 into deep-sea sub-seafloor reservoirs around the Japanese islands (e.g., Sea of Japan). These CCS approaches will allow us to inject large volumes of CO_2 at many sites in and offshore of Japan.

Finally, the CCS Division is committed to applying the techniques we have developed to ongoing CCS projects, and are planning to apply these techniques to future CCS projects that are being planned. For example, the I^2CNER-CCS Division is now officially collaborating with the Japan CCS Corporation on the Tomakomai CCS project, where we analyze geophysical and geological data from the Tomakomai CCS project for monitoring purposes.

9. Energy Analysis

Goals

The goals of the Energy Analysis Division (EAD) are to ensure that I^2CNER research is relevant to future low carbon or carbon-neutral energy systems for Japan, to ensure that I^2CNER research is informed of all relevant current and future energy options, and to take a lead role in defining an I^2CNER Vision and Roadmap for a carbon-neutral energy society for Japan.

In order to help define the vision, the EAD will identify the challenges and technologies that can lead to a carbon-neutral energy society for Japan. The EAD will provide guidance to the I^2CNER research divisions to help ensure their efforts are relevant with appropriative objectives and targets. It will also provide guidance as to other technologies not within the I^2CNER research portfolio as possible additions to I^2CNER research efforts.

In addition to these goals, the EAD will study potential Japan and international energy policy implications. Utilizing a system analysis approach, based on expertise inside and outside the division, the EAD will conduct original research in both natural and social science fields.

EAD analyses will include potential energy use and greenhouse gas (GHG) emissions as well as economic, social, and national security aspects of technologies and energy pathways. Target technologies will be analyzed on Cradle-to-Grave basis where activities, costs, and energy flows are tracked throughout the life cycles of energy source and technology infrastructure.

Research Highlights and Accomplishments

The EAD made significant progress this year in three areas:

- Initial study of technology options for a low carbon energy infrastructure for Japan in 2050. This is leading to a Vision for Japan's energy future.
- Improvements and use of the model for energy technology systems for quantification of the potential GHG and energy use reductions in Japan through the use of new low carbon energy technologies.
- An initial roadmap of I^2CNER's research projects including timelines with milestones as well as support to the research divisions to help establish clear objectives and targets.

Technology Options for a Low Carbon and Carbon-neutral Energy Society in Japan

The initial study of potential low carbon energy futures for Japan began with examining the current technologies, energy demand and supply, and carbon dioxide emissions associated with each of the major energy consuming sectors. The energy use in 2050 was then projected based on government projections for population and GDP growth. Then each sector was examined relative to the potential use of low carbon emission and more energy efficient technologies. The present perceptions from this initial work can be summarized as follows:

- Energy efficiency improvements on the demand side such as in manufacturing processes, appliances, lighter vehicles, lighting, insulation, a smart grid, and elsewhere can be significant in reducing carbon emissions.
- Electricity generation accounts for 46% of carbon dioxide emissions in Japan and should be a key focus for low carbon emission technologies. The future use of renewable energy resources in Japan (hydroelectric, wind, solar, geothermal, and biomass) and nuclear energy could be significant. The use of fossil fuels in combination with advanced more energy efficient technologies and carbon capture and sequestration (CCS) can also be an important part of the path to low carbon emission power production. Such use of fossil fuels that also permits adjustable power output along with electricity storage would enable use of significant amounts of intermittent wind and solar energy. The I^2CNER research on organic solar cells, hydrogen production, large-scale solid oxide fuel cells, and CCS can be key enablers for this sector to achieve low carbon emissions.
- The industry sector (excluding electricity use) accounts for 23% of carbon dioxide emissions. It is the need for heat that drives these carbon emissions in this sector. New chemistry technology such as that being researched in the I^2CNER material transformation division and other process technology developments could reduce the energy requirements. Some of the same advanced more energy efficient fossil fuel based energy technology and CCS being developed for electricity production could also enable low carbon emission heat for the industrial sector.

- The transportation sector accounts for 21% of carbon dioxide emissions and should also be an important focus for low carbon emissions. There are a number of attractive low carbon technologies being developed and improved for transportation. These are focused on vehicle transportation which account for the vast majority of the carbon emissions. The most promising new vehicle technologies are hybrid electric vehicles (HEV), plug-in hybrid electric vehicles (PHEV), battery electric vehicles (BEV), and fuel cell vehicles (FCV). The HEV could have very low carbon emissions if it used biofuel. PHEV and BEV technology requires an electricity grid with very low carbon emissions to be really attractive. There are some concerns with BEV technology relative to vehicle range, battery performance and cost. The FCV would be an excellent choice as long as there are sufficient resources for low carbon emission production of hydrogen and refueling infrastructure issues during the transition are addressed. I^2CNER research on polymer electrolyte fuel cells and low carbon hydrogen production technologies can play important roles for low carbon emission vehicles.
- Biofuels could play a very significant role for a low carbon energy future for Japan. They can replace fossil fuels in both current and advanced more efficient energy technologies. While Japan does not appear to have significant biomass resources, importing biofuels can be a topic to be examined.

  NOTE: It should be noted that the reported CO_2 emission shares by sector are calculated based on direct emission statistics. The corresponding emission shares based on statistics of indirect emission are 11% for electricity generation, 37% for industry, 22% for transportation, 16% for residential and 13% for commercial sectors.

There are many possible low carbon emission energy futures for Japan. The exact mix of technologies and fuels will depend greatly on the ultimate cost and performance achieved by the promising technologies being researched, the renewable and CCS resource capacity that can be tapped by Japan, and the social acceptance of technology options.

A Model Framework for Assessing Energy Technology Systems

It is necessary to develop a set of models for energy flows in Japan to evaluate the contributions of potential energy technologies to the realization of a low-carbon or carbon-neutral energy society quantitatively. We therefore adopted as a first step a model framework consisting of the demand-side energy flow model and the centralized power supply system model.

The demand-side energy flow model was developed on the basis of the comprehensive energy statistics of Japan supplemented by other statistical data as necessary. We implemented the model so that it could evaluate the contributions of demand-side technologies through the time horizon of year 2010 to 2050. Examples of demand-side technology impacts are efficiency improvement in energy appliances, residential photovoltaic cell and solar heating, cogeneration systems, insulation efficiency improvement, electrification (kitchen, boiler, and heating), membranes for distillation processes, low-temperature heat recovery, and future vehicles. Note that economic and social scenarios such as population decrease and demand increase associated with economic growth can be set as the model boundary. We can set input scenario parameters related with each technology option (efficiency, penetration ratio, etc.) to obtain the overall change of demand in Japanese society. Estimated power demand data are input to the centralized power supply system model.

The centralized power supply system model is developed on the basis of the traditional power generation dispatch model to optimize power generation from the Japanese centralized grid for the target period. Our model optimizes the centralized grid for minimum cost throughout year 2010 to 2050. The model incorporates nuclear, thermal combustion (LNG, coal and oil), hydro, pumped hydro, geothermal, photovoltaic, wind, and other potential energy technology options. We collected reference data from literature and published databases.

Preliminary analyses have been conducted to check the validity of the model algorithm using a set of tentative input data. The model is now ready to quantitatively study potential carbon emission and energy reductions scenarios for present and near future technologies.

Roadmap

After interviews with researchers in every research divisions in I^2CNER, the EAD has come up with an initial vision and roadmap as illustrated in Fig. 25. Draft timelines with key targets and milestones have also been generated with each I^2CNER research division and appear in their individual sections of this annual report.

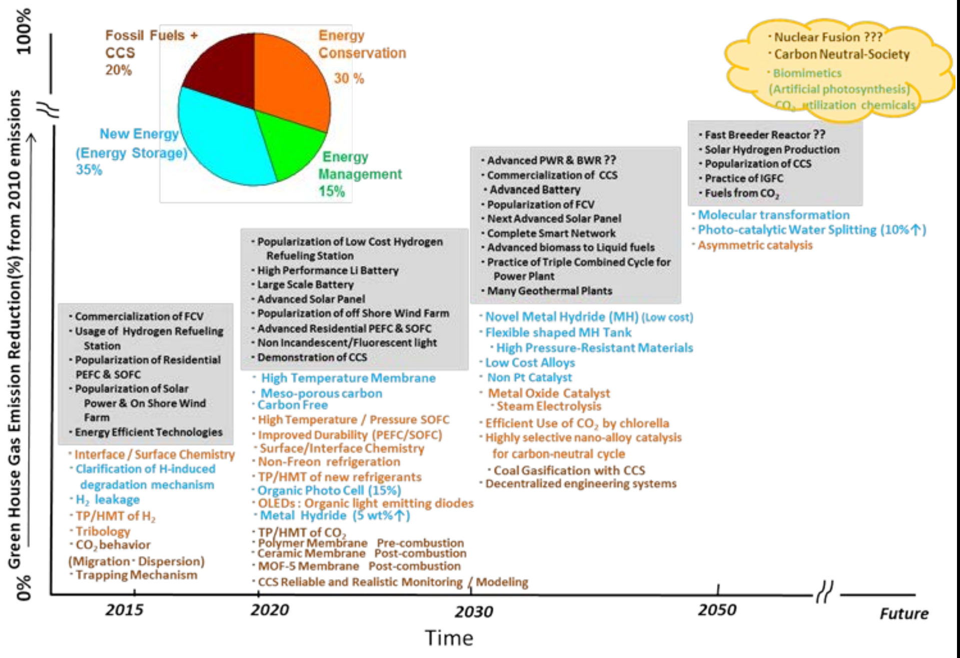


Fig. 25. I^{2}CNER Vision and Research Timeline

Future Directions

- Continue to work with the research divisions to help ensure their projects are relevant to a low carbon emission energy infrastructure for Japan's future and that they have appropriate performance and economic targets. This will include system modeling and analysis as appropriate.
- Analyzing and modeling I^{2}CNER technologies so as to incorporate them into the present model framework together with competing technologies.
- Quantifying the potential contribution of I^{2}CNER technologies to reduce carbon emissions and energy use in Japan by using the energy technologies systems model and other analytical tools that will be developed by the EAD.
- Develop an I^{2}CNER Vision for a low carbon emission energy infrastructure for Japan through the use of the of the technology options study, ETSS model potential scenarios, and other information and tools.

	• Define one or more national security metrics and incorporate them into EAD analyses. • Development of a computer based database system that will include the data required to quantify the cost, energy use, and GHG emissions for the current energy pathways in use in Japan. Extend this to include I^2CNER and other energy technologies being researched and developed. • Analyze and model the potential energy pathways that could utilize the I^2CNER research efforts, stressing analysis on vehicle system. • Conduct social science research to assess the social acceptability in Japan of key technologies and pathways that can reduce carbon emissions and characterize social aspects of these technologies. This can help inform the public and increase public awareness of these new technologies. • Study of the penetration process of energy technologies based on social choice theory.

4. Management

<Initial plan>	<Results/progress/alternations from 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	1) Composition of Administrative staff • Administrative Director, Prof. Hideyuki Tsunoda, resigned his position as of March 31, 2013. As of April 1, 2013, Prof. Kazuo Funaki took responsibility for the Administrative Office, as well as the other duties of the Administrative Director. • As of April 1, 2013, the administrative staff includes 19 members, and is divided into four groups: 1. General Affairs and Human Resources (6 members) 2. Accounting and Contracting (5 members) 3. Research Support and International Affairs (3 members) 4. Public Relations (3 members) These four groups act as a support system to the Institute's researchers and administration under the supervision of the Administrative Director and the Associate Administrative Director.

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 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:
  - 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.
  - 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.
  - 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.
  - 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 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.

2) Decision-making system

- In order to promote excellent communication and understanding amongst I^{2}CNER's administrators, regularly scheduled administrative meetings between the Director, the Associate Directors, and the Administrative Director have been established. This face to face meeting is intended to supplement the existing communication system which includes daily emails, telephone calls, video-conferencing, etc.

- Upon the resignation of I^{2}CNER's Vice Director, Yukitaka Murakami, effective January 31, 2013, the position of Vice Director within the Institute has been eliminated. The duties of the Vice Director have been absorbed by the two Associate Directors, beginning February 1, 2013.

- In order to specify the decision-making process in the Director's absence and to clarify the roles and responsibilities of the administrators of the Institute, document "22. Institutional Management and Administration" was written and officially added to the governing documents of the Institute in FY 2012.

- In consideration of the changes that occurred in FY 2012, the governing documents of the Institute were revised and updated. The full, current list of the Institute's governing documents is as follows:

1. Divisional And Personnel Structure for the Thematic Research Areas
2. Science Steering Committee
3. External Advisory Committee
4. Program Evaluation Committee
5. Faculty Recruiting Process
6. Faculty Excellence Process
7. Super Research Assistant (SRA) Program
8. Postdoctoral Research Associates for Foreign Principal Investigators
9. Roles and Responsibilities of Administrative Office
10. Organization and Sponsoring of Conference or Workshop
11. Start-up funding for Interdisciplinary Research
12. Rules on Indirect Cost of Competitive Funds
13. Guidelines for I^{2}CNER Project Funds

	14. Guidelines for Visiting Students Acceptance 15. Guidelines for WPI Visiting Researchers 16. Faculty & Postdoctoral Performance Evaluation Process 17. WPI-Funded I^{2}CNER Travel Expense Policy for Researchers 18. Faculty Promotion 19. Research Division Operation 20. Research Web Page Policy and Procedures 21. Treatment of Principal Investigators After Retirement 22. Institutional Management and Administration
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. Further details on the Director's authority are described specifically in I^{2}CNER Governing Document 22. Institutional Management and Administration, as mentioned above. • Compensation considerations are 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."

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 2012	Results at end of April 2013
Researchers from within host institution	16	16	16 (March, 2011)	21	15
Foreign researchers invited from abroad	11	11	11 (March, 2011)	23	8
Researchers invited from other Japanese institutions	3	3	3 (March, 2011)	1	1
Total principal investigators	30	30	30 (March, 2011)	45	24

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 2012	Results at end of April 2013
Researchers	71 <21, 30%>	92 <36, 39%>	130 <54, 42%> (March, 2014)	132 <50, 38%> [10, 8%]	151 <71, 47%> [20, 13%]
Principal investigators	30 <11, 37%>	30 < 11, 37%>	30 <11, 37%> (March, 2011)	45 <23, 51%> [3, 7%]	24 <9, 38%> [1, 4%]
Other researchers	41 <10, 24%>	62 < 25, 40%>	100 <43, 43%> (March, 2014)	87 <27, 31%> [7, 8%]	127 <62, 49%> [19, 15%]
Research support staff	32	37	51 (March, 2013)	90	54
Administrative staff	23	23	23 (March, 2011)	20 (19, 95%)	21 (20, 95%)
Total	126	152	204	242	226

-"Results at end of April 2013" are calculated by including the total of 33 Illinois Satellite members (15 researchers, 16 research assistants and 2 admin. staff members)

ii) Satellites <Initial plan> Institution (1) -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> Institution (1) • As of March 31, 2013, all programs of the Illinois Satellite underwent a review by the Internal Programs Review Committee, chaired by Prof. Ian Robertson. The Director already notified those faculty members whose programs weren't fully integrated with Kyushu University, and an action plan for improvement is in place. If no improvement is shown by December 2013, funding for these programs will be terminated.
iii) Partner institutions <Initial plan> Institution (1) We envision engaging in collaborative research with distinguished scientists from internationally recognized institutions. This includes site visits to facilitate research by leveraging research capabilities. Key institutions are the following: • Tohoku University (JPN) • Atmosphere and Ocean Research Institute of the University of Tokyo (JPN) • National Institute of Advanced Industrial Science and Technology (JPN) • University of California, Berkeley (USA) • Massachusetts Institute of Technology (USA) • Sandia National Laboratories (USA) • University of Alberta (CAN) • Carbon Management Canada (CAN) • Imperial College of London (UK)	iii) Partner institutions <Results/progress/alternations from initial plan> The Participating Institutions, Personnel, and collaborating divisions are: • Imperial College London, Professor John Kilner, Hydrogen Production Division • Sandia National Laboratories, Dr. Brian P. Somerday, Hydrogen Structural Materials Division • University of Thessaly, Professor Nikolaos Aravas, Hydrogen Structural Materials Division • University of California at Berkeley, Professor Robert O. Ritchie, Hydrogen Structural Materials Division • National Institute of Advanced Industrial Science and Technology, Dr. Chao-Nan Xu, Hydrogen Structural Materials Division • Malaysia-Japan International Institute of Technology, Universiti Teknologi Malaysia, Professor Kanao Fukuda, Hydrogen Structural

• Swiss Federal Institute of Technology Zurich (SUI) • Tsinghua University (China) • Dalian Institute of Chemical Physics, Chinese Academy of Sciences (China)	Materials Division • University of Göttingen, Professor Reiner Kirchheim, Hydrogen Structural Materials Division • Massachusetts Institute of Technology, Professor Harry L. Tuller, Fuel Cells Division • Trinity College Dublin at Massachusetts Institute of Technology, Dr. Dario Marrocchelli, Professor Graeme Watson, Professor Bilge Yildiz, Fuel Cells Division • Swiss Federal Institute of Technology Zurich (ETH), Professor Ludwig J. Gauckler, Fuel Cells Division • Kitakyushu Foundation for the Advancement of Industry, Science and Technology, Dr. Toyoki Kunitake, Fuel Cells Division • Tsinghua University, Professor Xing Zhang, Thermophysical Properties Division • Dalian Institute of Chemical Physics, Dr. Ping Chen, Hydrogen Storage Division • Sojo University, Professor Katsuki Kusakabe, CO_2 Separation and Concentration Division • University of Bergen, Professor Tor Arne Johansen, Carbon Capture and Storage Division • Bandung Institute of Technology, Wawan Gunawan A. Kadir, Carbon Capture and Storage Division • Research Institute of Innovative Technology for the Earth (RITE), Dr. Ziqiu Xue, Carbon Capture and Storage Division • Pacific Northwest National Laboratory, Dr. Peter McGrail, CO_2 Separation and Concentration Division

6. Summary of center's research environment

<Initial plan>	<Results/progress/alternations from 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	1) Environment in which researchers can devote themselves to their research • It was decided that from FY 2012 on, each research division is provided with 1 technical staff member. Given that PIs have their own technical staff members, the total number of I^2CNER technical staff members as of April 1, 2013 is 19.

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.	2) Startup research funding • In order to encourage fusion research within I^2CNER, we implemented "Start-up funding for interdisciplinary research" in FY 2011. In FY 2012, there was a total of nine applications for Interdisciplinary Research Projects. A total of five projects were selected, of which one was a new project and four projects were renewed. The total budget allocated to these five projects is $85,500 USD (1USD=100 JPY). The five selected projects for FY 2012 will be required to give a research presentation in FY 2013. The five selected projects for FY 2012 are: o Hydrogen Adsorption on Graphene Nanofoam *(Profs. Lyth and Shao)* o Nano Processing and Properties of Mg-based Materials for Energy Storage *(Profs. Shao, Akiba, Takata, Bishop, Lyth, and Fujikawa)* o Investigation of proton conducting amorphous oxides for pre-combustion CO_2 separation *(Profs. Fujikawa and Bishop)* o Direct Investigation of physical characteristics of super critical CO_2 toward monitoring of CO_2 behavior in geological reservoir *(Profs. Kitamura and Fujikawa)* o A novel nanostructured electrode by combining nanotitania and mesoporous carbon *(Profs. Matsumoto and Hayashi)* • Start-up research funding up to 40,000 USD has been allocated to full-time faculty and post-docs (Total amount:

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 Britain, California, Washington D.C., Munich, Korea, Beijing, etc., at the Satellite Institute's web site in Illinois, and major international academic magazines and related magazines in Japan. The recruitment process will be supervised by the Institute Director in consultation with the Internal Advisory Committee. The corresponding recruitment practices at the University of Illinois will be used on all Institute research personnel hiring. • The Kyushu University has already carried out a recruitment campaign for its projects on "Young Researcher's Independent Research Environment Maintenance and Promotion Program" and "Next Generation Research Training Program." • The number of recruits will be 21 researchers and 5 research assistants in 2010; 23 researchers and 9 research assistants in 2011; 9 researchers and 5 research assistants in 2012; and 6 researchers in 2013, with the objective being to reach a net number of 204 researchers by the end of 2013.	565,000USD/1USD=100JPY). • In addition, competitive funding up to 30,000 USD has been allocated for full-time faculty based upon an application and review process. (Total amount: 291,830USD /1USD=100JPY). • A portion of the funds which were conserved through the budget cuts for the Interdisciplinary Research Projects has been allocated for a new initiative designed to help support young faculty. Beginning April 1, 2013, each of the young faculty members was automatically allocated 1.5 million JPY to support their research programs. • The Director has also set aside additional discretional funds. By way of example, we have set up "Competitive research funding" in FY 2013, which will be allocated at the Director's discretion to those faculty members who are productive and whose achievements are relevant to I^2CNER's fusion research (including papers, awards, external research funds, etc.). 3) Postdoctoral positions through open international solicitations • As of April 1, 2013, I^2CNER employed postdocs as follows: o Post-doc Lines for PIs: 8 o Open International Recruitment: 5 o Other: 2 o Illinois: 3 TOTAL: 18 • From March to June 2012, the fourth open international recruiting call was conducted, which was our first and only one during FY 2012. Advertisements were published in international academic magazines such as Nature and Science and yielded 29 faculty applicants and 12 postdoctoral applicants. The Faculty Recruiting Committee reviewed the applications and identified candidates for an on-site interview. As a result, 3 faculty members (1 professor, 1 associate professor, and 1 assistant professor, all Japanese) and 3 postdoctoral research associates (2 Chinese and 1 Japanese) joined the Institute on or before April 1, 2013. • In total, 13 researchers (8 faculty members and 5 post doctoral

- We also plan to recruit an international research assistant or a research administrator (RA) for the Institute's administration management department.

4) Administrative personnel who can facilitate the use of English in the work process

- We will adopt English as the primary language for work-related communications.

- In order to foster an English speaking environment in the Institute, we will employ in the administration department personnel from the Kyushu University who are fluent in English.

- We also plan periodically to provide training opportunities for the administration work force.

- The administration department will oversee the translation from 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.

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

research associates) joined the Institute in FY 2012.

4) Administrative personnel who can facilitate the use of English in the work process

- Kyushu University staff members have a good command of English, 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 held PhDs, which enabled them to better communicate with I^2CNER researchers.

- The Administrative Office is in close communication with the existing International Student and Researchers Support Center of Kyushu University, and offers full-time support to international researchers in the area of invitation procedures including visa application processing and accommodations on campus. 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. 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.

5) Rigorous system for evaluating research and system of merit-based compensation

- The Institute follows a special salary system (made possible by 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, as decided by the Director, in consultation with the two Associate Directors.

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.

6) Equipment and facilities, including laboratory space, appropriate to a top world-level research center

- The Kyushu University is relocating its campus to Ito on the western part of the City of Fukuoka. This relocation decision was made to serve our new strategic goal for an open university at the forefront of cutting edge research in an educational Institution.

- Currently, the Ito Campus houses the International Research Center for Hydrogen Energy, the Research Center for Hydrogen Industrial Use and Storage (HYDROGENIUS), and the Inamori Frontier Research 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.

- A salary increase for the following fiscal year has been given to I^2CNER full-time faculty members who were highly evaluated.

- The Institute provides a "site allowance" for jointly-appointed KU faculty members based on performance evaluation.

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, I^2CNER building 1 (approximately 4,873 m^2) was completed at the end of November, 2012. The Institute's members moved into I^2CNER building 1 in January 2013. A spacious lounge with a high ceiling and electronic black boards was designed in the lobby on the first floor in order to encourage impromptu meetings and exchanges of scientific views among I^2CNER members.

- In January 2013, an additional 7 labs, 15 researcher's offices, and a server room have been secured for I^2CNER's fuel cell researchers out of the space allocated to the Next-Generation Fuel Cell Research Center within the I^2CNER building. We also have secured labs for researchers of MIT and Imperial College London in order to promote exchange of researchers between KU and renowned foreign institutions.

- A 4-story building with a total floor space of 5,000 m^2 is being designed as the second I^2CNER building, funded by the FY 2012 supplementary budget from the Japanese government. Interdisciplinary research will be promoted by setting up primarily large-scale labs and common experimental space in the planned second I^2CNER building.

- Facility equipment such as fume foods and pneumatic piping has been installed in I^2CNER Building 1.

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.

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

International Symposia

1. I^{2}CNER Tokyo Symposium

   The I^{2}CNER in Tokyo Symposium was held on December 7, 2012 in Tokyo, Japan. The idea behind this event was to bring the research of I^{2}CNER to the attention of the citizens and energy stakeholders (i.e. academia, laboratories, and industry) of Tokyo, and showcase our Institute's efforts to innovate on fundamental science to support carbon-neutral energy technologies. The event was attended by 150 national and international attendees, including the following speakers:

   a. Daisuke Yoshida, Director-General, Research Promotion Bureau, MEXT
   b. John V. Roos, Ambassador Extraordinary and Plenipotentiary, the U.S. Embassy in Japan
   c. Monterey Gardiner, Technology Development Manager, Office of Hydrogen, Fuel Cells and Infrastructure Technologies, U.S. Department of Energy
   d. Katsuhiko Hirose, Project General Manager, R&D Management Division, TOYOTA Motor Corporation

e. Toshio Kuroki, WPI Program Director
f. Nobuhide Kasagi, WPI Program Officer
g. Setsuo Arikawa, President, Kyushu University
h. Petros Sofronis, Director, I²CNER
i. Kenneth Christensen, Satellite Associate Director, I²CNER
j. Kazunari Sasaki, Lead Principal Investigator, I²CNER
k. Mark Paster, WPI Visiting Professor, I²CNER

2. I²CNER New Building Completion Ceremony
The I²CNER New Building Completion Ceremony was held January 29, 2013 at Kyushu University's new I²CNER building. The event was attended by over 200 national and international guests. The following attendees offered congratulatory addresses:
a. Hiroo Imura, Chairperson of WPI Program Committee
b. Koichi Morimoto, Deputy Director-General of the Research Promotion Bureau, MEXT
c. Hiroshi Ogawa, Governor of Fukuoka Prefecture
d. Toshio Kuroki, WPI Program Director
e. Monterey R. Gardiner, Technology Development Manager, Office of Hydrogen, Fuel Cells and Infrastructure Technologies, U.S. Department of Energy
f. Peter Schiffer, Vice Chancellor for Research at the University of Illinois at Urbana-Champaign

3. I²CNER Annual Symposium 2013
The I²CNER Annual Symposium 2013 was hosted on January 29, 2013 and attended by more than 200 national and international guests. Four presentations were given by I²CNER researcher from the Hydrogen Production, Hydrogen Structural Materials, Fuel Cells, and Carbon Capture and Storage divisions, in addition to the keynote lectures which were given by Dr. Eiichi Harada, Kawasaki Heavy Industries, LTD, and Dr. George Crabtree, Argonne National Laboratory, who is the Director of a new DOE Energy Innovation Hub on batteries.

4. I²CNER International Workshop 2013
The I²CNER International Workshop 2013 was hosted on January 31, 2013 and attended by 150 national and international attendees. The event was held in conjunction with the International Hydrogen Energy Development Forum 2013 on January 30, 2013. Three

workshops, each with a focus on an individual research field, including CO_2 Separation and Concentration/Carbon Capture and Storage, Hydrogen Storage, and Advanced Materials Transformations, were held at Kyushu University's Ito Campus.

5. HYDROGENIUS & I^2CNER Joint Research Symposium
   The HYDROGENIUS & I^2CNER Joint Research Symposium was held over two days (January 28 & 31, 2013) at Kyushu University's Ito Campus in Fukuoka, Japan. On January 28, 14 lectures with a focus on the Fuel Cell and Hydrogen Production fields were given. The lectures on January 28 were attended by 80 national and international guests. On January 31, four research symposia on Hydrogen-Materials Interactions, Hydrogen Polymers, Hydrogen Tribology, and Thermal Issues for Hydrogen Energy Systems were hosted, and 220 national and international guests attended.

International Seminars

- The I^2CNER Seminar Series was launched in March 2011 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, thus enhancing I^2CNER's global visibility. Seminars are being held regularly.

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:

a. 2012 Japan-Taiwan Bilateral Polymer Symposium (JTBPS'12)
   (organizer) Professor Atsushi Takahara
   Date: Sep. 6-7, 2012

b. 2012 International Hydrogen Conference
   (co-organizers) Dr. Brian Somerday and Professor Petros Sofronis
   Date: September 9-12, 2012

c. International Symposium on Metal-Hydrogen Systems, 2012 (MH2012)
   (vice-chair) Professor Etsuo Akiba
   Date: Oct. 21-26, 2012

	d. 11th International Conference on Green Gas Control Technologies (GHGT-11) (booth exhibition) Professor Tetsuo Yanagi Date: Nov. 18-22, 2012
8) Other measures, if any • We have four university facilities to accommodate invited national and international researchers. We have also arranged for private apartments designated for university use. We will provide comfortable and fully-furnished accommodations for the invited researchers so that they will be able to concentrate on their research activities.	8) Other measures, if any • Currently, we have introduced university facilities to accommodate for invited national and international researchers, or have made arrangements for fully-furnished private apartments with easy-access to Kyushu University. • “Ito Guest House,” an on-campus housing accommodation facility for short-stay researchers from overseas, was newly built on Ito campus, where I^{2}CNER is located. • International initiatives such as a 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, are in place for the convenience of foreign researchers. • A new bus stop on the Ito Campus Loop bus has been established in front of the I^{2}CNER building as of February 1, 2013. • A new bus stop on the Campus Shuttle bus has been established in front of the new I^{2}CNER building as of April 1, 2013. • In order to facilitate a comfortable exchange environment, two volumes of *Fuse News* were published in FY 2012. *Fuse News* is an internal publication of I^{2}CNER which is intended to help the researchers become familiar with one another’s research programs, as well as the cultures and campuses at Kyushu University and UIUC. • A new networking event, I^{2}CNER CO^2 (Coffee and Collaboration) was established in January 2013 upon the inauguration of the new building. I^{2}CNER CO^2 gives the Institute’s researchers the opportunity to meet casually over coffee to discuss basic science issues, the details of their collaborations in front of electronic blackboards, etc.

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

<Initial plan>

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

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

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

<Current assessment>

- In FY 2012, a new ad-hoc committee, the Internal Programs Review Committee, was introduced. The committee is made up of 3 Japanese members and 3 Illinois members of the Institute. It is chaired by Professor Ian Robertson, who is currently the Dean of Engineering at the University Wisconsin-Madison. This committee is called by the Director to assist with program reviews when needed. In the future, this committee may become a standing committee.

  Using the indicators on the left, we assessed our activities from April 2012 to March 2013 as noted below:

1. **WPI-Affiliated Publications** (January- December 2012)
   In calendar year 2012, there were 213 publications indicating WPI affiliation (76 in FY 2011). The Institute's researchers published 415 papers related to WPI (total number of citations in 2012: 559).

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 2012 (20 in FY 2011).

3. **Invited Lectures**
   The Institute's researchers were invited to give a total of 184 invited lectures in FY 2012 (79 in FY 2011).

4. **Symposia organization in international conferences by Institute Researchers**
   The Institute's researchers contributed to the organization of a total of 33 symposia in FY 2012 (21 in FY 2011).

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 12 trend-setting workshops in FY 2012 (5 in FY 2011).

6. **Organization of International Conferences**
   The Institute's researchers participated in the organization of a total

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.

of 9 International Conferences (21 in FY 2011).

7. **Participation of the Institute's researchers in international conferences (e.g. Gordon Research Conferences)**
The Institute's researchers participated in a total of 191 international conferences (88 in FY 2011).

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 18 government panels in FY 2012 (14 in FY 2011).

9. **Patents and technology accomplishments**
The Institute's researchers contributed to a total of 16 patents (22 in FY 2011).

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 were invited to and visited foreign institutions such as the Illinois Satellite Institute. In particular, there were 42 visits made to I^2CNER by international WPI PIs. Among them, 20 visits were made by Illinois Satellite PIs. By way of comparison, in FY 2011, 32 visits were made to I^2CNER by international researchers, of which 15 were made by Illinois researchers.

8. Securing competitive research funding

<Initial plan>

A. Past Record

- Research funding acquired by Japanese PIs in the past 5 years is as follows:
    - Fiscal 2005: 3.7 million dollars
    - Fiscal 2006: 21.7 million dollars
    - Fiscal 2007: 24.6 million dollars
    - Fiscal 2008: 29.2 million dollars
    - Fiscal 2009: 28.5 million dollars

<Results/progress/alternations from initial plan>

In FY 2012, KU researchers of the center have acquired a total amount of 31.56 million US dollars (3.16 billion yen), which amounts to a 93 % increase compared to FY 2011.

The breakdown for FY 2012 is listed below.

- Grants-in Aid for Scientific Research:2.79 million USD(279 million yen)
- Other grants from government :13.20 million USD(1.32 billion yen)

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.

- Commissioned research projects : 9.03 million USD(903million yen)
- Collaborative research funds from industry: 1.74 million USD(174 million yen)
- Donations :1.26 million USD(126 million yen)
- Other government subsidies :1.12 million USD(112 million yen)
- Funds from KU :2.42 million USD(242 million yen)

Past records are listed below

- FY 2010 11.86 million USD (1.19 billion yen)
- FY 2011 16.36 million USD (1.64 billion yen)
- FY 2012 31.56 million USD (3.16 billion yen)

In addition to direct costs, total amount of indirect costs acquired by KU researchers of the center for FY 2012 are 3.31 million USD (331 million yen).

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

<Initial plan>

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

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

- This Institute is the first example of a foreign researcher to be selected as the Institute Director. It is expected that other units and organizations of the Kyushu University will benefit from the academic administration system of this Institute, which will be morphed according to the academic

<Results/progress/alternations from initial plan>

- I^{2}CNER has been embraced by Kyushu University as a permanent institution (unit) and the I^{2}CNER Director participates in the Education and Research Council that is administered by the KU President.

- The Institute Director has the authority to make decisions on all matters of the Institute.

- The KU President has allocated additional 4 tenure track positions to I^{2}CNER in FY 2012 (5 total).

- The Grainger Engineering Library Information Center at the University of Illinois (Profs. William H. Mischo and Mary C. Schlembach) has been working closely with the Kyushu University Library (Profs. Eriko Amano and Takeshi Omura) to develop a set of scholarly information services that provide enhanced access to a myriad of online information resources available to I^{2}CNER researchers. In particular, work has focused on the development of a custom Group Information Productivity Tool (GRIPT) that offers access to I^{2}CNER researcher

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.	publications by group and author, key subject journals, specific known item journal articles, pre-stored customizable topical search results, highly cited articles and papers, and articles citing a specific article. This tool is customized for on-campus and remote access by both Illinois and Kyushu researchers. This project involves visits by the Illinois Librarians to Kyushu University. On February 1, a presentation was given entitled “Scholarly Information Tools for I^{2}CNER Researchers” on the newly developed search tools named ‘GRIPT (Group Information Productivity Tool)’. URLs: http://hades.grainger.uiuc.edu/guy/pip7j.asp?i2cner http://hades.grainger.uiuc.edu/sarina/i2cner_scopus/i2cner_search.asp • With the help of Energy Analysis Division (EAD) Member Mark Paster, the Director initiated contact and brainstorming sessions between I^{2}CNER research groups and US DOE programs (managers and grantees). The first such meeting focused on photoelectrochemistry and took place during the ECS Annual Meeting in Honolulu, Hawaii October 7-12, 2012.

10. Host institution’s commitment

<Initial plan>	<Results/progress/alternations from 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: o 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.” o Mid-term strategy plans for this goal are: “To promote the research	-Provision in host institution’s mid-to-long-term plan • No modification

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, 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.

(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

-Concrete Measures

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

- I^{2}CNER's Administrative Director, Prof. Hideyuki Tsunoda, was also a professor of the Office for Strategic Research Planning and was actively engaging in gathering information regarding research grants, providing strategic advice on grant applications, etc. As of April 1, 2013, Prof. Funaki has taken over as Administrative Director, as mentioned above. In addition, two of the administrative staff members with a doctoral degree had taken charge of research support and international affairs. These staff members provided support and assistance, including applications, for substantial competitive research grants.

(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 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.

(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 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.

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 has been given the authority to recruit new faculty 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.

- Please see Section 6.5 for more information on the special salary system that is used within the Institute.

(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 parent departments, such as requests for cooperation and arrangements with the head of his/her department.

- In order to enable flexibility in allocating faculty within the University while further improving the standards of education and research conducted at Kyushu University, KU new established rules on the Intra-University Transfer system, which went into effect December 1, 2012. These rules enable researchers to safely and easily transfer their affiliations from their home departments to I^2CNER.

- As mentioned in Section 1. Summary of Center Project, 9 faculty members have transferred to I^2CNER from the Faculty of Engineering. -This process has improved the relationship between I^2CNER and the Faculty of Engineering, which is an advantage for securing tenure-track positions jointly with the Faculty of Engineering. Most importantly, this relationship between I^2CNER and the Faculty of Engineering has positively impacted PI mindset.

(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 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

(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, other matters will be changed by establishing new and revising current rules and regulations.

- Please see Section 6.5 for more information on the special salary system that is used within the Institute.

(5) Accommodation of center's requirements for infrastructural support (facilities, e.g., laboratory space; equipment; land, etc.)

- For details on the new I^{2}CNER building, including laboratory facilities, plans for a second I^{2}CNER building, please see Section 6.6.

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.	(6) Support for other types of assistance • The two Associate Directors, Professors Ishihara and Takata, have stepped into the role formerly fulfilled by Professor Murakami, which entails working in tandem with and on behalf of the Director to meet the objectives of the Institute, as well as coordinating with related departments of the university. When the Director is in Illinois or traveling, Professors Ishihara and Takata maintain daily communication with him in order to relay and implement 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 FY2012 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. <u>Science and PIs:</u> • There is still a need for the mindset and incentive of PIs to be improved to meet the general mission of the WPI program as recommended by the Program Committee. • It seems that the research subjects are somewhat fragmented. There are missing subjects that are indispensable to materialize the carbon neutral society.	1. Science and PIs: - PIs: • As mentioned in Section 1, as of April 1, 2013, the number of PIs became 24 (15 KU, 2 Illinois, 7 Others), from the previous year's 45 (21 KU, 13 Illinois and 11 Others). • As mentioned in Sections 1 & 10.3, as of April 1, 2013, 9 Kyushu PIs transferred from the Faculty of Engineering to I^2CNER, which has now

- Publications are not sufficient as an internationally competitive center supported by sizable funding. I^2CNER should take any possible actions to encourage the members to make their utmost effort to increase quantity and quality of their publications. They should note the WPI affiliation and acknowledge WPI in their publications.

- The efforts should be prioritized to recruit first-class scientists globally, while replacements must be sought to increase the level of science with new perspectives.

- At least 10% of full-time staying foreign PI's at KU should be achieved.

- The EAD needs to produce a road map with milestones, to identify the main difficulties to overcome, and to describe a quantitative or at least qualitative strategy to solve them. The EAD should hopefully be a scientific adviser for Japanese and US energy policy makers.

2. Administration:
- Director's strong leadership should be a key for I^2CNER's success

become their main affiliation. This brings the total number of full-time PIs to 11.

- We continue to utilize the Faculty Excellence Program in hopes of recruiting permanent-staying foreign PIs, and aim to achieve 10% of them at Kyushu.

- In consideration of the above measures, the personnel expenses will comprise about 70% of the FY 2013 budget, excluding the Satellite expenses and the rent of lab/office space. The Satellite expenses are all personnel expenses.

\- Mindset:

- Due to the increase in the number of full-time PIs starting April 1, 2013, the PIs' sense of belonging (to I^2CNER) has been reinforced. To further increase this sense of belonging, regular PI meetings and extended faculty meetings have already begun to take place.

- As for the issue of "disorganized and fragmented research topics," each individual division carried out a retreat and consulted with the Energy Analysis Division to focus its thematic research areas and establish research targets and a roadmap. These retreats were carried out in close collaboration between Kyushu and Illinois faculty, and international collaborators. Each division summarized its newly focused research plans, targets, milestones, and roadmap in a report submitted to the Director March 31, 2013, as mentioned in Section 1.

- We promote communication among researchers, including post-docs, by organizing networking events on a regular basis (e.g. photoelectrochemical hydrogen production (PEC) Retreat at the Electrochemical Society (ECS) conference in October 2012, PEC Retreat at Kyushu in February 2013, daily tea time, etc.). These networking events are organized at a division level.

- We raised the quality of science by promoting fusion and converting a portion of the research budget into competitive funds, as was mentioned in Section 6.2.

2. Administration:

\- Strengthening of the Management System:

and also for a major reform in the KU's administrative system. It must be kept and made even more effective with more Associate Directors' supports and tight collaboration with all PIs.

- Director's stay in KU was considerably increased in FY2011. So far in FY2012, his stay at KU has just reached about 50% of his time, and this needs to be sustained if not increased.

- The budget and expense of each fiscal year should be more clearly written and explained in the I^2CNER progress report for evaluation.

- Administrative Director should much more proactively advise Director, PIs and President of KU on the establishment of I^2CNER as a WPI center.

3. Fostering young researchers:
- The number of post-docs still remains extremely small, counting only 8. While the WPI budget allows such funding, only 15% of the budget was spent for personnel including postdocs, compared to 60-70% in the preceding 5 WPI centers.

- Recruitment of top young scientists is to be continued by enforcing strategy to attract students and PDs.

- We have made institutional changes to enable the Director, two Associate Directors and Administrative Director to run the institute under the Director's initiative and strong leadership starting February 1, 2013, as mentioned in section 1, whereby the Director has direct access to every organizational and research unit in the Institute.

- Under the vigorous management and administration of the competitive funding allocation, we aim to vitalize research by increasing financial and personnel support (e.g. post-docs and SRAs) to productive research teams which achieve results such as publishing papers in high impact-factor journals.

- In an effort to encourage our researchers to publish co-authored papers, we have converted a portion of the budget for FY 2013 into competitive funding, which will be used to promote interdisciplinary research. Projects will be funded based on performance evaluation, as mentioned in Section 6.2 and above.

- We strengthened the support system for newly-hired faculty members in order to help them obtain external funds and achieve results. The support includes general administrative support and assistance with improving proposal writing skills.

- We have increased the quality and efficiency of the Administrative Office, partly because Professor Funaki, a former faculty member of Kyushu University, has taken over the leadership of the office.

- Regarding the rules about the institutional decision-making and management in the Director's absence, we have them documented in governing document 22, as mentioned in section 4.2.

3. Fostering young researchers:

- Full-Time Faculty:
- We started the process of hiring 2-3 full-time faculty members through our Faculty Excellence Program (targeting permanent-residing foreign faculty including PI(s), if possible).

- Employing Post-docs:
- Including the number of post-docs hired by Kyushu PIs by utilizing

• Much more must be done to assure the long term future of young faculty and to allow them build their own careers. They should be provided opportunities for teaching and supervising students.	post-doc lines for PIs, the number of post-docs as of April 1, 2013 was 19. In FY 2013, we have budgeted for this number to increase to 28, as mentioned in sections 1, depending upon the quality of the candidates that we are interviewing. Recruiting efforts are ongoing. • All faculty members have been given the option to hire post-docs on a regular basis by submitting a research proposal for the purpose of promoting interdisciplinary research activities, as well as collaboration with overseas institutes, as mentioned in section 1. - Securing Tenured Positions: • Concerning the appointment of world's top-level researchers, we have been given 4 tenured positions by the President of KU (5 total), as mentioned in section 9. The hiring process is ongoing. • We have already made efforts to obtain tenured faculty positions by submitting proposals to the Kyushu University Reform Revitalization Program. Having strengthened our collaboration with the Faculty of Engineering and other colleges, we will make a concerted effort to secure tenured positions during next year's cycle. - Teaching and Supervising Students: • Following the increase in the number of full-time PIs in April, 2013, we have already provided opportunities for the young faculty members to collaboratively teach/advise PhD students under the advisement of the PIs. • As for the Director Sofronis' teaching/advising students at Kyushu University, he will begin doing so to the extent possible with the assistance of Associate Director Takata. His first lecture will be delivered on April 19, 2013 on "Fracture Mechanics" in front of 70 students in the Department of Mechanical Engineering.
4. International collaboration: • For the linked development of KU and the Satellite Center at University of Illinois (UI), the exchange and lateral visits of PIs and other researchers should be more encouraged. The period of their stay should be long enough to produce substantial outcomes of collaborative research work.	4. International collaboration: - Kyushu–Illinois Collaboration and Researcher Exchange • We have established the framework for sending Kyushu Researchers to Illinois. This involves a research proposal that is discussed in the SSC and which is approved by the Director, along with travel expenses. By way of example, 1 young faculty member from KU (Prof. Kohno, Thermophysical Properties Division) visited Illinois for six months

• The mix of national and international recruited young researchers should be even more enhanced. • A joint (or split-side) PhD program between KU and UI should be considered, allowing Japanese PhD candidates to be exposed to the US systems early in their career. Conversely, KU actively responds to potential young international researchers.	beginning at the end of October 2012 through the end of April 2013, and was hosted by Prof. Cahill. Similarly, from the Hydrogen Production Division was approved (Prof. Staykov will visit Illinois to collaborate with Prof. Ertekin for 5 weeks beginning April 2013). To this end, we will seek external funding from national agencies such as JSPS. • In order to further promote this international collaboration, I^2CNER funding for Illinois faculty is predicated upon the frequency of student and faculty visits at Kyushu University. By way of example, joint meetings between Professors Robertson, Horita, Sofronis, postdoc Edalati, and graduate students Megan Emigh and Kelly Nygren have already taken place in January 2013. As a result of this meeting, both Megan and Kelly will spend 2 months at Kyushu this summer. • Toward the goal of encouraging researchers to cross the Pacific (and thereby foster truly international researchers), we aim to further promote and publicize overseas exchange programs (primarily with the University of Illinois) in order to attract young researchers. • Director Sofronis has already met with Professor Wolfgang Schloer, Interim Associate Provost for International Affairs at the University of Illinois, to discuss a program for undergraduate student exchange between Kyushu and Illinois in order for those students to gain research experiences.
5. Commitment of KU: The WPI program offers a chance for KU to reform the existing academic structure and establish a world-leading research institute in KU. It must commit more proactively in guiding the institutional development of I^2CNER.	5. Commitment of KU: • Please see response in 11.-3 (Fostering young researchers) - Securing Tenured Positions. • As of April 1, 2013, KU allocated one additional experienced Kyushu University staff member to the Administrative Office. • Negotiations for further support from Kyushu University are ongoing.

12. Efforts to improve points indicated as requiring improvement by the Working Group	
-Points specified as needing improvement (extracted from the FY 2012 WPI Site Visit Report) 1. Increasing the number of researchers (4. Young researchers including postdocs and graduate students, under 7. Actions required and recommendations) • I2CNER needs continuous supply of able human resources. Recruitment of top young scientists is to be continued by enforcing strategy to attract students and post-docs. More WPI budget should be allocated for appointing and encouraging young researchers and graduate students.	-Efforts to improve them and results *If you have already described these in other parts of this report, please indicate where for reference. 1. Increasing the number of researchers a) Full-time faculty • 3 professors, 3 associate professors, and 2 assistant professors were hired during the FY 2012 (8 in total). • As of April 1, 2013, 13 professors, 6 associate professors, and 9 assistant professors are employed in the Institute (total of 28). By way of comparison, as of April 1, 2012, 2 professors, 3 associate professors, and 8 assistant professors were employed by I^2CNER (total of 13). b) Post-docs • One post-doc line has been allocated to each Kyushu PI, as mentioned in sections 1 and 11. • In addition, all faculty members (including junior) have been given the option to hire post-docs at any time by submitting a research proposal for the purpose of promoting interdisciplinary research activities, as well as collaboration with overseas institutions, as mentioned in sections 1 & 11. As a result, the number of post-docs has increased to 19 (including 3 females) as of April 1, 2013. By way of comparison, I^2CNER employed 6 postdocs as of April 1, 2012. c) Tenured faculty positions • As mentioned in section 9, in addition to one tenured position granted in FY 2011, which was used to recruit a very talented female researcher from Hokkaido University last year, I^2CNER has been given 4 additional tenured positions in FY 2012 by KU (5 total as of March 31, 2013). One of these positions is set aside so that we can hire a strong candidate who is currently under consideration. • With regard to the hiring of permanent-residing foreign PIs, our next international open recruitment call is to be administered in June. In order to optimize the outcome, extensive discussions intended to

	delineate the target area(s) of recruitment are being conducted by the Director, the division leaders, and PIs. • Continued efforts will be made to obtain additional tenured faculty positions by submitting proposals to the Kyushu University Reform Revitalization Program in collaboration with the Faculty of Engineering, etc., as mentioned in Section 9.
2. Strengthening of the management system (* *responded to PO Kasagi's recommendation/suggestion given to I²CNER during the administrative meeting held on January 28, 2013 @Hotel Okura)*	2. Strengthening of the management system a) Administration • Institutional changes have been made to enable the Director, two Associate Directors (both senior-level PIs and research division leaders) and the Administrative Director (newly appointed as of April 1, 2013) to run the Institute under the Director's initiative and strong leadership starting February 1, 2013, as mentioned in Section 4. • Decision-making and management in the Director's absence from the Institute has been clearly documented, as mentioned in Section 4. b) New Administrative Director • The new administrative director will get actively engaged to support our faculty, especially the newly-hired members, with applications for external funding and proposal writing skills (particularly to national agencies).
3. PIs' Mindset (2. Commitment of PIs, under 7. Actions required and recommendations) • Although the number of PIs has reached a sufficient level, there is a need for I²CNER to review all current PIs' degree of involvement and redefine the title and designation of PI from a viewpoint that a PI should play a substantive role in I²CNER by spending at least more than 50% of his/her time. They are core members leading and developing the I²CNER's research activities and cultivating younger scientists.	3. PIs' Mindset a) Screening of PIs • In an effort to keep only the committed and productive WPI PIs in the Institute, their number was reduced to 24 from last year's 45, as mentioned in Section 1. b) Intra-University Faculty Transfer Program • By utilizing the newly-established Intra-University Faculty Transfer Program of Kyushu University, 9 senior-level Kyushu PIs were transferred to the Institute from the Faculty of Engineering as of April 1, 2013, and as a result, their main affiliation is now with

	I^2CNER, which helps improve mindset, as mentioned in Section 1. c) Fostering PI participation in the Institute Research Administration • Under the above-mentioned new administration, two PI meetings were held during the FY 2012, and such meetings will be held on a regular basis so that PIs can exchange ideas and debate Institute issues. d) Competitive research funds • The process has been established to make part of the budget into competitive funds and allocate them to the members who are highly productive in their research (including co-authoring of papers), as mentioned in Section 6.2. This is incentive is expected to motivate our researchers to raise their level of science performance across the Institute. The Director will actively administer the fund allocation. e) Others • In addition, faculty meetings (including post-docs), divisional retreats, and other net-working events such as I^2CNER CO^2 (Coffee and Collaboration), have been launched in an effort to improve mindset, as mentioned in Section 6.8.
4. Kyushu-Illinois researcher exchange (2. Commitment of PIs, under 7. Actions required and recommendations) • For the linked development of KU and the Satellite Center at Illinois, the exchange and lateral visits of PIs should be more increased. In the last FY, the period of stay was too short to produce substantial outcomes of collaborative research work. (2. International collaboration, a recommendation for gaining competitiveness as an international research base) • The collaboration between young researchers of KU and UI should be more promoted.	4. Kyushu-Illinois researcher exchange • In order to promote continued collaborative research activities between the two universities, a system has been set in place for researcher exchange on a mid- to long-term basis. By way of example, one associate professor in the Thermophysical Properties Division stayed at Illinois for almost half a year and conducted research under the supervision of an Illinois Satellite faculty member, as mentioned in Section 1. • In total, Kyushu hosted 11 faculty members, 2 postdocs, and 5 PhD students from Illinois, and Illinois hosted 5 faculty members from Kyushu during FY 2012, as mentioned in Section 1.

13. FY 2012 funding

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

i) Overall project funding

Cost Items	Details	Costs (10,000 dollars)
Personnel	Center director and Administrative director	21
	Principal investigators (no. of persons):20	246
	Other researchers (no. of persons):65	273
	Research support staffs (no. of persons):20	54
	Administrative staffs (no. of persons):26	99
	Total	693
Project activities	Gratuities and honoraria paid to invited principal investigators (no. of persons):	13
	Cost of dispatching scientists (no. of persons):1	4
	Research startup cost (no. of persons):	94
	Cost of satellite organizations (no. of satellite organizations):1	203
	Cost of international symposiums (no. of symposiums):1	14
	Rental fees for facilities	88
	Cost of consumables	136
	Cost of utilities	10
	Other costs	164
	Total	726
Travel	Domestic travel costs	14
	Overseas travel costs	35
	Travel and accommodations cost for invited scientists (no. of domestic scientists): 56 (no. of overseas scientists): 40	25
	Travel cost for scientists on secondment (no. of domestic scientists): 7 (no. of overseas scientists): 1	3
	Total	77
Equipment	Depreciation of buildings	1
	Depreciation of equipment	526
	Total	527
Other research projects	Projects supported by other government subsidies, etc.	208
	Commissioned research projects, etc.	665
	Grants-in-Aid for Scientific Research, etc.	688
	Total	1,561
Total		3,584

Ten thousand dollars

WPI grant for FY 2012		1,324
Costs of establishing and maintaining facilities in FY 2012		16
Establishing new facilities (Number of facilities: , 0m²)	Costs paid:	0
Repairing facilities (Number of facilities: , 0m²)	Costs paid:	0
Others		16
Cost of equipment procured in FY 2012		1,604
Name of equipment: Fume foods Number of units:14	Costs paid:	63
Name of equipment: Audio and visual facilities Number of units: 1	Costs paid:	30
Others		1,511

ii) Costs of Satellites and Partner institutions

Cost Items	Details	Costs (10,000 dollars)
Personnel	Researchers (no. of persons): 17	
	Executive director (no. of persons): 1	
	Research support staff (no. of persons): 25	
	Others (no. of persons): 1	
	Total	121
Project activities		40
Travel		26
Equipment		16
Other research projects		
Total		203