

## Center Director's Vision

International Institute for Carbon-Neutral Energy Research  
— The Grand Highway for a Carbon-Neutral Energy Fueled World —  
Multi/Inter-disciplinary research on the interface between hydrogen/CO<sub>2</sub> and matter

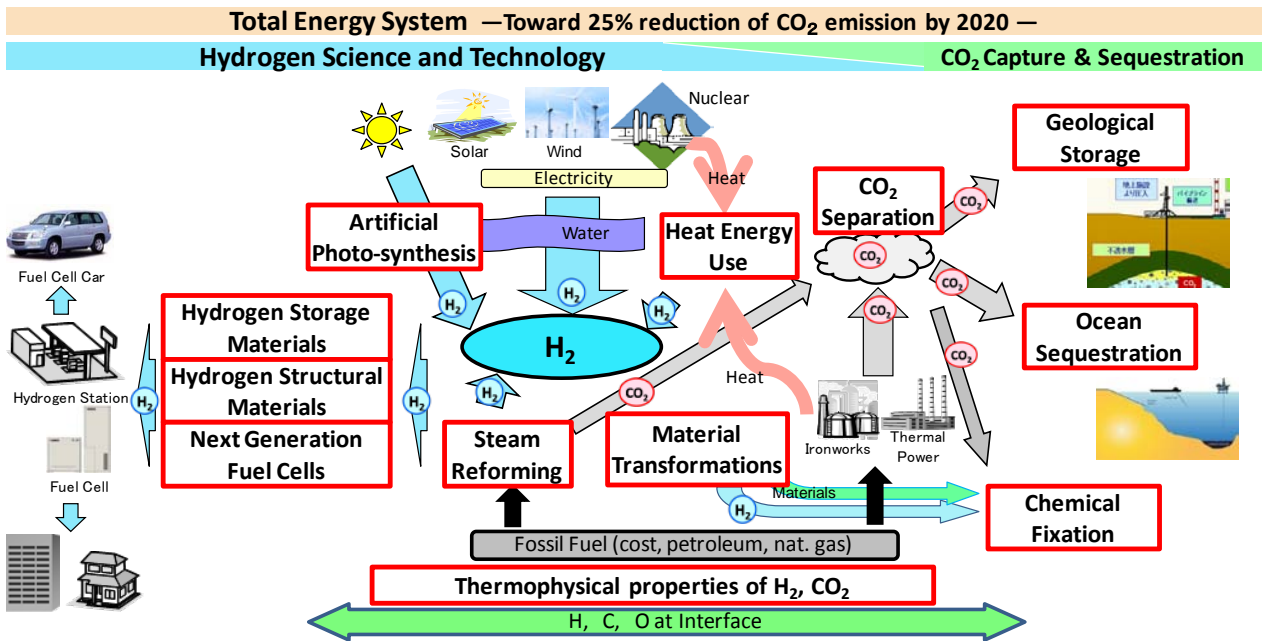
April 23, 2010  
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### <Summary>

Achieving and even exceeding CO<sub>2</sub> emission reduction targets requires not only strategies for capturing and either sequestering or converting CO<sub>2</sub> to a useful fuel but also developing high efficiency and effective methodologies for producing an alternate energy carrier such as hydrogen gas. The challenges require a paradigm shift in our approach to research that bridges not only multiple spatial, molecular to miles, and temporal scales, nanoseconds to decades, but it also necessitates bringing together scientists and engineers from disparate disciplines such as chemistry, materials and geoscience to work cooperatively and synergistically. The International Institute for Carbon-Neutral Energy Research will provide the foundation, environment and framework to stimulate novel research endeavors between leading experts in diverse research fields such as chemistry, physics, materials science, mechanics, geoscience, oceanic science and biomimetics. The Institute activities will lead to fundamental science discoveries underlying the development of innovative, safe, and reliable systems for the production, storage and utilization of hydrogen as a fuel in a hydrogen-based economy as well as for either capture and storage of CO<sub>2</sub> or its conversion to a useful product. In addition, it will provide the nation and the international community with the next-generation of scientists and engineers needed to address such complex and critical technological and societal challenges.

The approach that will be adopted will be integrative multi- and inter-disciplinary that focuses on physical chemistry and dynamics to discover, control and manipulate the interactions between materials and hydrogen or CO<sub>2</sub>, which will lead to hydrogen production and material transformation with no CO<sub>2</sub> emission; hydrogen storage materials; hydrogen embrittlement resistant materials; high efficiency fuel cells; and safe carbon capture, ocean sequestration and geological storage or efficient conversion of CO<sub>2</sub> to CO and O. The ultimate vision for the Institute is to create and use hydrogen as a fuel that enables the realization of a carbon-neutral energy fueled society through Green Innovation.

The Institute will be launched by the Kyushu University in collaboration with the University of Illinois at Urbana-Champaign. Both institutions are internationally recognized centers for research in the area of hydrogen and materials. An agreement for student and faculty exchanges between the two universities was signed in 2008.



## 1. Preface

There is no more opportune time for the Kyushu University in collaboration with the University of Illinois at Urbana-Champaign to mount such an unprecedented international effort for an institute on carbon-neutral energy. The Kyushu University is a leading world institution on hydrogen research and fuel cell technology. Its institute for hydrogen industrial use and storage is the best equipped and funded laboratory in the world for research on hydrogen-induced degradation and materials for the next generation fuel cells. The prefecture of Fukuoka is well known for its strong support for sciences and its ability to move rapidly and put science in the use of society by developing new technologies. The University of Illinois research contributions to research on hydrogen embrittlement and materials over the past 30 years have won it international acclaim. Significantly there is an agreement already in place between the Kyushu University and the University of Illinois for student and research personnel exchange. All these factors warrant a sustained institutional and local government support for research at the planned International Institute for Carbon-Neutral Energy Research by a team of researchers with recognized research records and ongoing collaborations. Such a sustained research environment and commitment to quality research will enable the Kyushu Institute to attract and engage world-class researchers in all fields of its mission.

More specifically, success of the Institute requires that it:

- Has a well-defined vision and a strategic plan to achieve its mission and goal
- Attracts and supports world-class researchers, both nationally and internationally.
- Provides its researchers with the facilities and tools needed to achieve the research goals
- Establishes a management and administrative plan that fosters multi- and inter-disciplinary research.

The grand vision of the Institute is to produce and distribute efficiently and effectively a fuel that ultimately leaves no carbon footprint. To achieve this vision requires

addressing several grand challenges including the efficient production of hydrogen, ideally using energy sources and processes that generate no harmful emissions; capture and sequester or convert to fuel any CO<sub>2</sub> generated by the production or use of the fuel; delivery and storage systems to enable effective use of hydrogen as an energy carrier; as well as design and construction of high-efficiency fuel cells for applications in a hydrogen-based economy.

To address the technological challenges and to accomplish the mission, the Institute must provide the resources, facilities and environment to attract and retain top scientists and engineers, both nationally and internationally, from a wide range of science and engineering disciplines. Additionally, the Institute will establish collaborative programs, including joint research efforts with national and international research institutions and universities that will involve not only collaborative efforts but a two-way exchange of personnel.

The Director will provide leadership and overall management of the Institute. To assist the Director, Steering Committee and External Advisory Committees will be established. Key members of the Steering Committee will be program area leaders (science advisors) although the Director may invite additional members as deemed appropriate. The External Advisory Committee will be 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 will be the responsibility of the Director.

The Institute will promote the activities and achievements of the Institute through an annual progress report which will describe research highlights, significant accomplishments and future directions, newsletters to highlight achievements on a more regular basis, scholarly publications in internationally peer-reviewed journals, participation and organization of symposia at international meetings as well as a biannual workshop at Kyushu University or a partnering research institution.

A more detailed description of each of these topics is provided in the following sections.

## 2. Critical Research Initiatives

The impact of global warming, the rising cost of fossil fuels as well as the anticipated decline in supply provide societal, economic and technology driving forces for developing an alternate energy source or carrier. Although these issues are vital to the future well-being of Japan, success has global societal and economic implications. Moving to and implementing a non-fossil based energy carrier system, especially one in which the production is independent of foreign sources, is highly desirable. Hydrogen gas is a potential energy carrier that could address these issues provided that methodologies are in place for producing a sufficient hydrogen supply that utilizes an energy source that either does not involve generation of CO<sub>2</sub> (e.g., solar or next generation nuclear systems) or includes strategies for capturing and sequestering in the ocean or geologically or converting the CO<sub>2</sub> to a more useful form. To make a hydrogen-fueled economic system viable, the scientific and engineering challenges of delivering and using hydrogen will need to be overcome. This means that materials with a high tolerance to hydrogen-induced degradation will need to be developed for production, delivery and application systems; effective and efficient hydrogen storage media will need to be developed for a multitude of

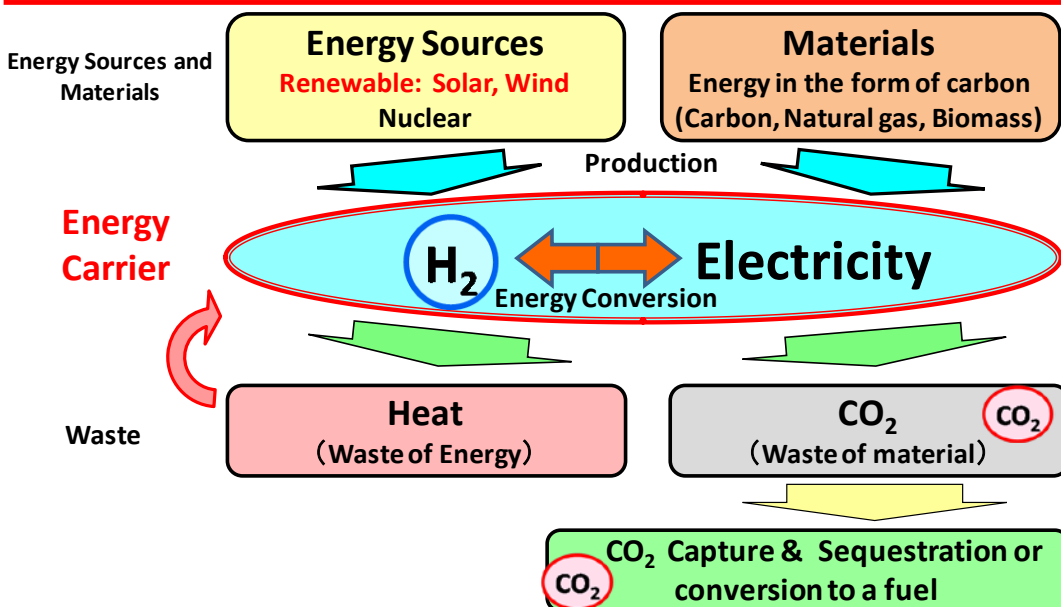
applications and the efficiency of fuel cells will need to be increased.

Hydrogen has several attractive features as an energy carrier that could remove our dependence on fossil fuels and at the same time reduce the levels of CO<sub>2</sub> that are being produced. For it to be a truly carbon-neutral energy source, methods for producing large quantities of hydrogen using energy sources that either generate no CO<sub>2</sub> or are used in conjunction with CO<sub>2</sub> capture technologies need to be developed. The mission of the Institute will be to develop science-driven technological solutions to enable the realization of a hydrogen-based energy economy that is sustainable and environmentally friendly. Therefore the research agenda of the Institute emphasizes critical issues in the areas of: hydrogen production; solid-state hydrogen storage; hydrogen tolerant materials; efficient and reliable fuel cells; material transformation; CO<sub>2</sub> capture, ocean sequestration and geological storage as well as energy-efficient conversion to more useful forms.

Furthermore, it is essential to understand the various phenomena occurring at the interface between materials and hydrogen, oxygen, and CO<sub>2</sub> (and their underlying mechanisms) to enable the scientific and engineering breakthroughs needed to realize a carbon-neutral energy fueled society. The Institute activities must be broad based, bridging multi-dimensional spatial (atoms to molecules to crystals, to geological formations and to oceanic systems) and temporal (nanoseconds to many tens of years and beyond) scales.

## Carbon-Neutral Energy Fueled Society

- Burning of fossil fuels and biomass produces CO<sub>2</sub> and waste of energy as **heat**
- **Hydrogen** is an **energy carrier** that can be produced from various sources (e.g., solar, carbon)
- Non-fossil based energy system as a solution to global warming, rising costs, declining of oil supplies, energy security, and independence by converting hydrogen to electricity with **minimum CO<sub>2</sub> production and waste of energy**



### 3. Outline of research activities

The Kyushu Institute's approach to science necessary for the development of a

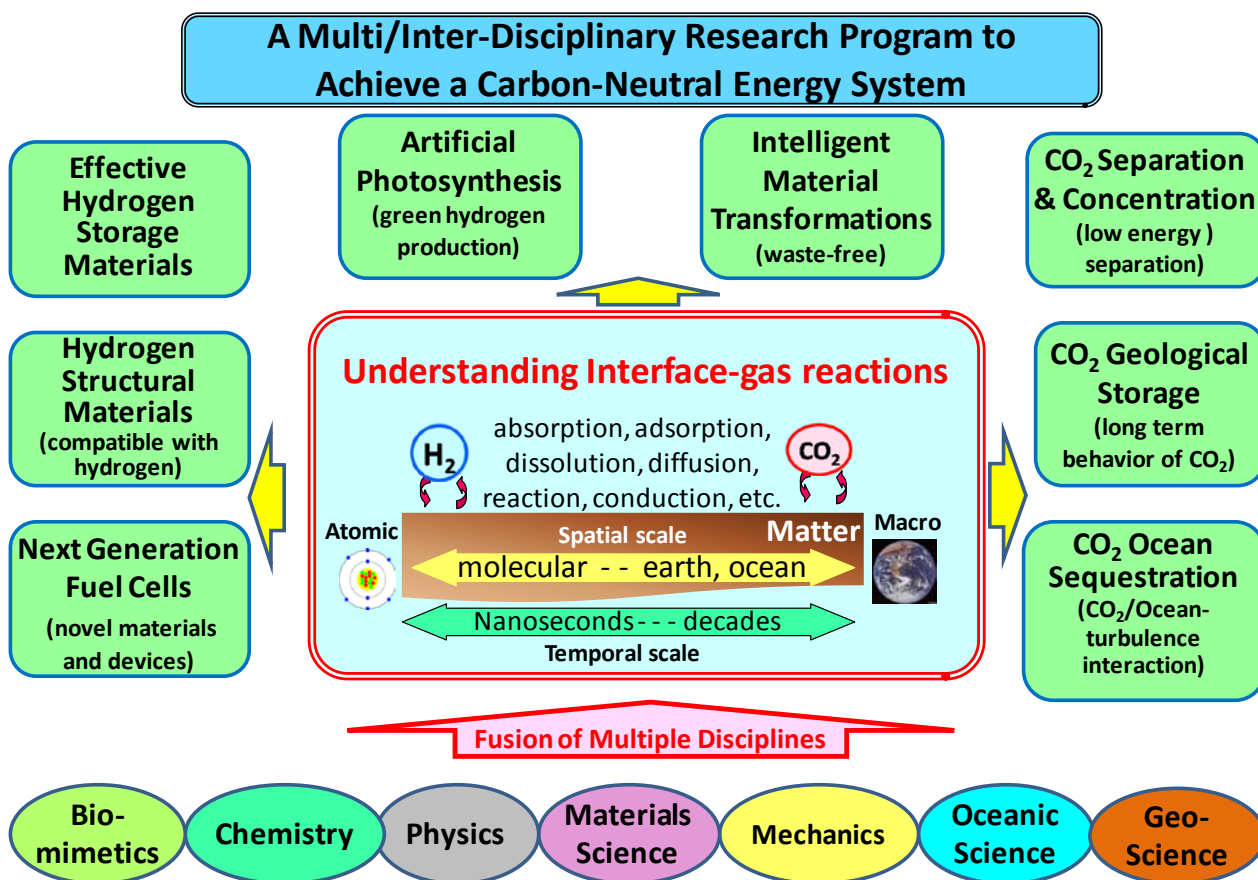
carbon-neutral energy fueled society will be to cross-cut disciplinary boundaries through a judicious integration of information from atomistic/microscopic/macrosopic time and length scales for phenomena occurring at the interface of chemistry, physics, materials science, mechanics, geoscience, oceanic science, and biomimetics. The global nature of this challenge is obvious and we will launch a “International Institute for Carbon-Neutral Energy Research” to work toward establishing it as the global leader for this work.

To achieve our mission of developing an carbon-neutral economy that is sustainable and at the same time is environmentally friendly – key criteria for addressing global warming and finding an alternate to fossil-based fuel systems – the following research themes have been identified. The concept of the interface between hydrogen/CO<sub>2</sub>/oxygen and matter is pervasive throughout all research themes. The research topics identified initially as being critical to the move toward a sustainable, earth-friendly hydrogen-based economy are:

- Artificial photosynthesis through autocatalytic water splitting.
  - Toward green hydrogen production.
- Structural materials compatibility with hydrogen.
  - Toward designing a safe and reliable hydrogen infrastructure.
- Materials for the next generation fuel cells.
  - Toward establishing the fundamentals for high efficiency energy conversion and the development of new devices.
- Fundamental thermophysical and flow properties of hydrogen, CO<sub>2</sub> hydrates, and carbon dioxide under extreme pressure conditions, e.g. 100MPa.
  - Toward elucidating the hydrogen/matter interactions over a broad range of temperatures and pressures and the stability of supercritical CO<sub>2</sub>
- Hydrogen storage materials
  - Toward designing an effective hydrogen storage system.
- Intelligent chemical transformations and catalysis.
  - Toward developing waste-free material transformation.
- Advanced CO<sub>2</sub> separation and concentration processes.
  - Toward the development of an efficient CO<sub>2</sub> separation and concentration technology.
- CO<sub>2</sub> geological storage.
  - Toward understanding the underground behavior of CO<sub>2</sub>, e.g. chemical interactions and stability among three phase of CO<sub>2</sub>, water and rock.
- CO<sub>2</sub>/Ocean-turbulenece interactions for ocean sequestration.
  - Toward understanding CO<sub>2</sub> behavior in ocean.
- Energy efficient and environmentally benign approaches to conversion of CO<sub>2</sub> to CO and O and then to a usable energy form.
  - Toward a carbon-neutral energy fueled society.

The research program must be multi- as well as inter-disciplinary. In addition, it must couple synergistically theory, computer modeling and simulation with experimental methodologies that utilize state-of-the-art approaches to explore solid-gas interactions at appropriate length and time scales. Here it is envisioned that the efforts will be coordinated such that the experiments inform model development and the predictions of the models are verified by appropriate experiments. Additionally, computer simulations and models will be employed to enhance the interpretation of experimental observations. For example, *ab initio* calculations might be used to determine the change in the electronic states on surfaces and in the interior to enhance our understanding of the initial adsorption and dissociation of hydrogen on the surface, which could accelerate development of a

solid-stage light-weight hydrogen storage medium or to ascertain the tolerance of internal interfaces to hydrogen, which could suggest how to create a microstructure with low sensitivity to high-pressure hydrogen environments.



#### 4. Research objectives

The overarching objective of the Institute is to establish the fundamental science underlying the technology of innovative, safe, and reliable systems for the production, storage and utilization of hydrogen (hydrogen production; hydrogen storage materials; hydrogen embrittlement resistant materials; fuel cells; material transformation), as well as for separation of CO<sub>2</sub>, carbon oceanic and geological sequestration and conversion to more usable forms. To reach this objective requires establishing a fundamental-science understanding at the atomic level of such phenomena as adsorption, absorption, dissolution, diffusion, reaction characterizing interaction of gases and matter in the framework of multi-phase fluid and solid systems. By publically disseminating our research findings we expect and aspire to contribute to the societal discourse on the scientific soundness of ocean sequestration and geological storage. Thus, the research objectives toward a carbon-neutral energy fueled society can be summarized as follows:

- Development of innovative and sustainable hydrogen production processes, such as photocatalytic water splitting.
- Development of hydrogen resistant alloys for the design of a safe and reliable hydrogen infrastructure.

- Development of the next generation fuel cells through research in novel materials and devices.
- Development of novel hydrogen storage materials with a storage capacity of over 6wt% H<sub>2</sub>.
- Development of high efficiency material transformation processes without any by-products such as waste and CO<sub>2</sub>.
- Development of low-energy carbon separation and concentration processes by investigating the mechanisms of CO<sub>2</sub> absorption.
- Educate the public about the scientific aspects of ocean sequestration and geological storage so that the society decides on the benefits of moving toward a carbon-neutral energy fueled world on the basis of sound scientific information.

## 5. Research organization and cooperation with related institutions

### (1) Research organization

The research organization will be theme based. Four broad-based divisions are envisioned initially: Hydrogen Production, Delivery and Utilization; Hydrogen Storage; CO<sub>2</sub> Capture, Sequestration and Conversion; and Energy and Society. Each will be lead by a science advisor who will be responsible for setting the scientific objectives and goals and for the day-to-day management. In addition, each division will be staffed by outstanding research faculty and staff who will be drawn from Kyushu University as well as other national and international universities and national laboratories. To drive the research mission and to ensure each program area/division has the needed expertise, the Director along with the Principal Investigators will invite periodically scientists and engineers from around the world to submit a white paper addressing how they could contribute to critical mission issues. The Director may seek input from the members of the External Advisory Committee as to the merits and value of these white papers to the overall mission of the Institute. This approach will ensure that the research environment remains dynamic and staffed with scientists and engineers that have the needed expertise.

### (2) Cooperation with other institutions

To achieve success in our mission, collaborative and coordinated research efforts central to the mission of the Institute will be conducted in partnership with faculty and staff at other national and international institutions. This activity will involve not only research collaborations but also exchange of personnel. Regular meetings of all team members will take place through use of internet conferencing tools. This capability may also be used to deliver and broadcast important research meetings between partnering institutions. Broadening the research base from Kyushu University will further promote the Institute activities and help establish it as Center of Excellence in this area.

#### (Satellite Institution)

- University of Illinois at Urbana- Champaign, USA.

The Director of the Institute, Professor P. Sofronis, is a faculty member at the University of Illinois at Urbana-Champaign 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 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 to engage 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)
- High Energy Accelerator Research Organization (JPN)
- National Institute of Advanced Industrial Science and Technology (JPN)
- University of California, Berkeley (USA)
- Massachusetts Institute of Technology (USA)
- Sandia National Laboratories (USA)
- Imperial College of London (UK)
- Swiss Federal Institute of Technology (ETHZ)
- Tsinghua University (China)
- Dalian Institute of Chemical Physics, Chinese Academy of Sciences (China)

## 6. Research evaluation and visibility

The Director will organize a program review meeting on an annual basis and, in addition to the members of the External Advisory Committee, will invite leading scientists and engineers in each of the thematic areas to review the entire program, including the leadership and management of the overall Institute. This meeting will be convened at Kyushu University. It is envisioned that the science advisor of each theme will present an overview of the activities, highlighting specific achievements and challenges, as well as describing future research directions and activities. The Principal Investigators of each funded program will present the achievements of their program, describe synergistic activities with other members of the Institute and with partnering institutions, and conclude with planned future activities. The form of these presentations may be oral or in poster format. The program review committee will provide a written evaluation of the achievements and future plans of each effort. The Director, in consultation with the External Advisory Committee and Steering Committee, will use these evaluations to determine future funding for each program and theme. The final decision about program funding level will be made by the Director of the Institute.

Metrics of the Institute's visibility will be considered 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 and symposia that attract participation of national agencies such as MEXT, JSPS, US NSF, US DOE, European Commission; vi) 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.

## 7. Institute management

One of the goals of the Institute is to be a model for 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's Director whose duties will include the research team formation, the recruitment of the international research participants, the establishment of international collaborations and interactions with top research Institutions, the administration of the peer evaluation process of the Institute's research output, potential team reorganization and redirection of efforts in response to the feedback from the annual review of the Institute, review of the research personnel, and the observance of the research expenditures.

The Institute is established as an organization directly under the president of the Kyushu University. The structure of the organization is such that the Institute Director has the authority to make decisions regarding the planning and conduct of the research activities, the formation and composition of the research program areas or clusters, and the budget implementation related to the management of the Institute. On all these matters the Director consults the Steering Committee that is headed by the Director and its members (science advisors) are the program area leaders of the Institute.

A vital component of the Institute is the External Advisory Committee which is 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 will be the responsibility of the Director.

The Director is assisted by the Associate Director for the management of the Institute's research activities. The Office of the Director is supported by the Administrative Director, head of the office of the Institute's Administrative Office whose purpose is to provide administrative support to the research personnel of the Institute. The official language of the Institute's Administrative Office is English. To ensure efficiency and expediency of operations in the Administrative Office, 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.

## 8. Closure

We propose a research Institute with a mission to carry out fundamental science for the removal of the technical barriers toward a carbon-neutral energy fueled society. The

objective of the Institute is to develop the science required for the realization of a hydrogen economy and enable the technological breakthroughs required for efficient CO<sub>2</sub> capture and sequestration in both the ocean and the earth. Research topics include artificial photosynthesis for hydrogen production, efficient fuel cell catalysis, hydrogen storage and development of hydrogen resistant alloys, interaction of CO<sub>2</sub> with ocean turbulence and geological formations, and thermodynamics and chemistry of crystalline and supercritical CO<sub>2</sub>. The disparate length and time scales involved in these phenomena range from the electron to that for oceans and geo-formations and this necessitates approaches that judiciously bridge the temporal and spatial scales. The research will be interdisciplinary and will cross-cut the boundaries of chemistry, physics, materials science, mechanics, geoscience, oceanic science, and biomimetics. The effort will be international and will involve industry and national laboratories. The Institute will operate in accordance to the highest academic standards and through a rigorous peer evaluation and review process. We expect that the scientific discoveries of the Institute will result in the reduction of the societal carbon footprint and the removal of barriers to a carbon-neutral society.