# Global Research GREETS ERSEELANT

Global Research Center for Environment and Energy based on Nanomaterials Science

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**Director-General of GREEN** Kohei Uosaki

### Making Breakthroughs in Materials Technology toward Solving Global Environmental and Energy Issues

Research and development of efficient energy conversion, storage, and transport are carried out intensively worldwide. To realize these systems, it is essential to develop new materials and devises that effectively utilize the newly developed materials but it is impossible to win the global competition if R&D is carried out via empirical approach.

In Global Research Center for Environment and Energy based on Nanomaterials Science (GREEN), leading scientists in fundamental science such as theory, simulation, and measurement, and in applied fields such as solar energy conversion, secondary batteries, and fuel cells, gather together from not only NIMS but also from universities and industries are carry out cutting edge research with close collaboration. GREEN also provides external scientists with most advanced equipments as well as knowledge and know-how of GREEN scientists through open-lab system so that GREEN will contribute to accelerate R&D in universities and industries.

### **MEXT Program for Integrated Materials Development**

GREEN was established in October 2009 with NIMS as the core host institution to carry out MEXT Program for Development of Environmental Technology using Nanotechnology and its aim is to promote nanotechnology in materials science research with the collaboration between industries and academia for achieving Green Innovation in Japan so that environmental and energy problems can be solved and a sustainable society can be realized.

In 2016, a new program "Integrated Materials Development" was started and in the new program, GREEN's research is significantly enhanced by the cooperation between "technology integration overviewing the entire social systems" and "material research integrated with theory, measurement and material creation", for properly matching the needs of future society and materials seeds in environmental technology.

### Collaboration of Computation, Characterization and Material in GREEN

**Director-General** 

Kohei Uosaki

**Managing Director** 

Yoshimi Kubo

Kenjiro Miyano

Deputy Director-General

Chikashi Nishimura

**Administrative Director** 

### **Solar Energy** Conversion

Coordinator

### Kenjiro Miyano

### Photovoltaics

Clarify the mechanism of photo-electron conversion Higher performance and

**Specially Promoted Research Team** Ad hoc Team on Perovskite PV Cells

### **Technology Integration** Unit

Unit Director

### Michihisa Koyama

 Technology integration toward Future Big Picture Transdisciplinary Research of Materials Science and System Engineering

### Member Institution

**Hokkaido University** Ichizo Yagi Nagova University Yasutoshi Iriyama **Toyota Motor Corporation** 

### Computational **Materials Science**

Coordinator Takahisa Ohno Dynamic analysis of atoms electron migration and ion diffusion

### **Research Group**

Green Computational Materials Science Interfacial Electron Transfer Theory Battery Materials Exploration Electrocatalysis Theory

Solutions for common issues associated with the utilization and flow of solar energy

### Collaboration and fusion of computation and experiments

Understanding and control of the phenomena at interfaces

### Nano-interface Characterization

Coordinator Kazutaka Mitsuishi In-situ observation of surfaces and interface: Operation environment, solid/liquid interfaces

### **Research Group**

Nano Interface Characterization Environmental Microscopy In-situ Interface Analysis Nanointerface Laser Spectroscopy Nano-Structure Analysis Solid/Liquid Interface Analysis

### **Batteries and Fuel Cells**

Coordinator

Kazunori Takada

### ·Rechargeable Batteries High capacity Safe operation (All solid)

### ·Fuel Cells

Higher performance of solid electrolytes and electrodes Longer lifetime

**Specially Promoted Research Team** All Solid State Battery Lithium Air Battery

### Research Group

Nanostructured Electrocatalyst Solid Oxide Fuel Cell Materials Design Polymer Electrolyte Fuel Cell Interface-Controlled Battery Materials Metal Negative Electrodes Innovative Polymer Electrolyte Design Electrocatalyst Precision Design

# Establishing a Research Center Involving Collaborations between Industries, Government and Academia

### **Promoting Overriding Themes with an ALL JAPAN Formation**

### **Open Laboratory**

Aiming to accelerate materials research for the solution of environmental and energy issues, GREEN invites researchers from universities and research institutes in Japan to work on the topics well linked to GREEN's mission through a public recruiting process. GREEN open-lab guest researchers have an opportunity to communicate with NIMS researchers from various fields, and jointly analyze the experimental results obtained by using the cutting-edge facilities at NIMS. This leads them to yield significant research results.

**Proposal Submission** 

**Review of Proposal** 

**Invitation Procedure** 

Research

Report

**Year Round Applications** 

Contact: GREEN Administrative Office E-Mail: GREEN@nims.go.jp



### **Short-term Research Assistant**

GREEN short-term research assistants, who are the students of the universities and the colleges of technology where GREEN open-lab guest researchers belong to, are expected to participate actively in the Open Laboratory while learning leading-edge study in NIMS. This program can be also applied flexibly to a certain technical training for young researchers and engineers in companies under the agreement between guest and host researchers.

◀ Various models of Open Laboratory and networking

### **GREEN Symposium**

GREEN symposium is regularly held as a forum for sending up-to-date information and exchanging views concerning GREEN's results and challenges. More than 200 people mainly belonging to companies have participated in this symposium held at Tokyo once a year.

### **NBCI-NIMS Joint Seminar**

NBCI and NIMS have held joint seminar since October, 2012 and GREEN plays a central role.

### **Battery Research Platform**

Battery Research Platform was established by a supplementary budget in fiscal year 2012 to accelerate the R&D of the next-generation batteries in our country, and started service in 2014 with state-of-the-art equipment installed. It preferentially supports the JST-ALCA project "Specially Promoted Research for Innovative Next Generation Batteries". It also supports other projects for next-generation batteries being carried out by universities, research institutes and companies in Japan.

### **Analysis Forum for Battery Materials**

For the purposes of dissemination of GREEN's results on the next generation batteries to companies and offering opportunities for various collaborations, workshops as well as technical courses including practical training have been organized on a continuing basis.



Super Dry Room



### **Nurturing Young Leaders for the Future Generation**

We foster the promising young researchers actively for the next generation. At GREEN, young leaders themselves were assigned the responsibility of group leaders. Each floor of NanoGREEN building completed in 2012, has an open space for stimulating interactions between researchers of a variety of backgrounds under one roof. Corporate researchers can obtain a doctoral degree at GREEN from partner universities of NIMS. Postdoctoral researchers and doctoral graduate students can acquire necessary skills of working in the industry through their experience at NIMS.

### The GREEN Prize

The GREEN Prize was established in the FY2011 to encourage and recognize the contribution of young researchers who have made excellent achievements in terms of promoting green innovation and addressing the associated challenges.

## **Advanced Computational Science Field**

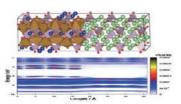


Computational Materials Science Field Coordinator

### Takahisa Ohno

Based on advanced computational science techniques we are aiming to analyze the structures, physical properties, and functions at nanoscale surfaces and interfaces and to elucidate physical and chemical phenomena occurring in energy conversion systems.

Green Computational Materials Science Takahisa Ohno



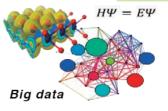
Structure and density of states at electrode/electrolyte interface of solid state secondary battery

Interfacial Electron Transfer Theory Ikutaro Hamada (Associate Professor, Osaka University) Yang Sun

Battery Materials
Exploration

Masanobu Nakayama
(Professor, Nagoya

Inst. Tech.)



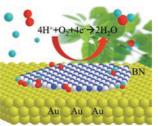
New material research based on materials informatics

We are developing in-situ nanocharacterization technologies for the surface and interface while controlling various environmental fields. We aim at clarifying the basic mechanism of the interfacial phenomenon which is the key of the functional manifestation of the environment and energy materials.

Electrocatalysis Theory

Tetsuya Taketsugu (Professor, Hokkaido University)

**Andrey Lyalin** 



Proposal of electrocatalytic reaction by theory

# Advanced Nano-interface Characterization Technology Field



Nano-interface Characterization Field Coordinator

Nano Interface

Characterization Group Nobuyuki Ishida Chikako Sakai Environmental Microscopy

Ayako Hashimoto

In-situ Interface Analysis

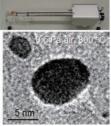
Kazutaka Mitsuishi Raman Bekarevich Nano-Structure
Analysis
Nanointerface Laser
Naoyuki Sugiyama

Spectroscopy
Hidenori Noguchi
Shuo Yang
Suresh Kukunuri

Solid/Liquid Interface Analysis

Takuya Masuda Ru<mark>tt</mark>ala Devivaraprasad

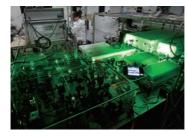




Gas environment heating specimen holder and obtained TEM image of Pt nanoparticles



Low temperature STM/AFM chamber for in situ observation of solar cell



Femtosecond laser system

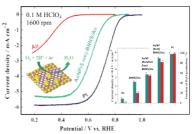
### Nanostructured Electrocatalyst Group



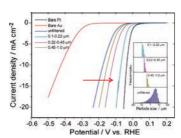
Kohei Uosaki

Kohei Uosaki Akihiro Okamoto Kentaro Tomita Yang Liu

Bottom-up fabrication of unique electrochatalysts and clarification of the mechanism of electrocatalitic reactions



Au nanoparticles decorated BN nano sheet on Au substrates and their oxygen reduction properties.



Hydrogen evolution from BN nano sheet on Au substrates. Inset: Size distribution of BN nano sheet

# All Solid State Battery Specially Promoted Research Team



Team Leader Kazunori Takada

Lithium-ion batteries are already used very widely for various applications. Much higher performance and reliability are, however, required for their future applications. This special team in GREEN is studying all solid state battery to achieve the high performance by dissolving the limitations originating from liquid electrolytes in the collaborative research among materials, computational, and characterization scientists.

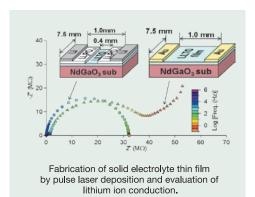
### Materials

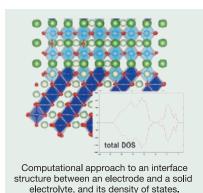
### Computation

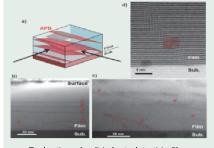
Characterization

Kazunori Takada, Tsuyoshi Ohnishi Narumi Ohta, Shogo Miyoshi Kazuhiro Kawashima, Yusuke Matsuki

Takahisa Ohno Yoshinori Tanaka Kazutaka Mitsuishi







Evaluation of solid electrolyte thin film by electron microscopy to relate the defect structure and the lithium ion conduction.

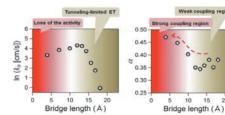
### **Electrocatalyst Precision Design Group**



Katsuyoshi Ikeda

Katsuyoshi Ikeda (Professor, Nagoya Institute of Technology)

Study on electrocatalyst models based on atomic and molecular scale control of electrode interfaces



Dependence of catalytic reaction rates on distance between the conducting surface and catalytic active sites

### Solid Oxide Fuel Cell Materials Design Group

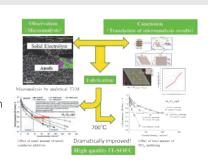


Toshiyuki Mori

### Toshiyuki Mori

To design of the active solid electrolyte/ electrode interfaces and the high speed ion diffusion pathway in the area of grain boundary and grain interior, the combination approach among micro-analysis, defect structure simulation and processing route design is used in our group. We believe that our approach will guide us to radical innovation in development of fuel cell and its practical use

Design of high quality fuel cell materials by combination of microanalysis, defect simulation and processing route design



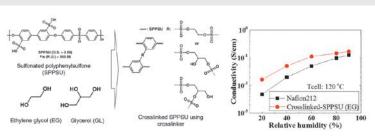
### Polymer Electrolyte Fuel Cell Group



Satoshi Matsushita

Jedeok Kim

Development of SPPSU membrane having high durability property



SPPSU polymer development and membrane conductivity (II)

# Lithium Air Battery Specially Promoted Research Team



Team Leader Yoshimi Kubo

In order to promote the widespread use of electric vehicles and renewable energy towards the low-carbon society, dramatic downsizing and price reduction of secondary batteries are required. We are developing basic technologies of Lithium-air battery that has the highest theoretical energy density, by conducting a wide range of R&D from materials science to prototyping of the cell.

### Materials

Yoshimi Kubo, Kimihiko Ito Akihiro Nomura, Ken Sakaushi Shoichi Matsuda, Xin Xing Arghya Dutta

### Computation

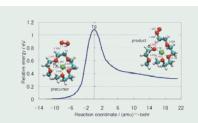
Ikutaro Hamada (Associate Professor, Osaka University)

### Characterization

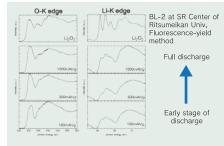
Osami Sakata Avako Hashimoto Chulho Song



Schematic and 10-cell stack of lithium-air battery The highest theoretical energy density is because it uses oxygen in air. Cell stack technology is developed to realize high energy density in practical applications.



Ab initio study of electrolytes Ether-based electrolytes are stable against the attack of superoxide anion produced by ORR during discharge.



XANES spectra for cathodes The Li<sub>2</sub>O<sub>2</sub> structure is already formed even at the early stage of discharge.

### Interface-Controlled Battery Materials Group

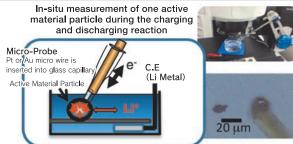
Kiyoshi Kanamura



Kiyoshi Kanamura

(Professor, Tokyo Metropolitan University) Chunyan Li

The development of single particle measurement technique and the understanding of reaction mechanism of new materials for next-generation



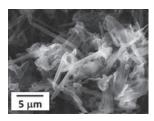
### Metal Negative Electrodes Group



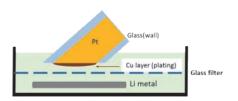
Kei Nishikawa

Kei Nishikawa

Fundamental study of metal negative electrodes for next-generation batteries



SEM image of typical Li metal dendrites



Schematic diagram of experimental set-up for the morphological variation study of Li metal

### Innovative Polymer Electrolyte Design Group



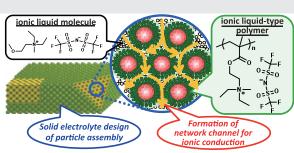
Takaya Sato

Takaya Sato (Professor, National Inst. Tech., Tsuruoka College)

Yoshinobu Tsujii (Professor, Kyoto University) Takashi Morinaga (Associate Professor, National Inst. Tech., Tsuruoka College)

Chaofu Zhang

Development of safety multiuse electrolyte using functional ionic liquids



Solid electrolyte using hybrid particle decorated with ionic liquid-type polymer brush

### Ad hoc Team on Perovskite PV Cells



Team Leader Kenjiro Miyano

Photovoltaic cells with lead halide compounds with perovskite structure as the light harvesting layer have been attracting attention due to their relatively high energy conversion efficiency despite their ease of fabrication. We aim at understanding the photo-electronic properties unique to this class of materials in order to reach a guiding principle in application. The ionic chemical nature is emphasized while the physical characterization capacity of GREEN will be fully utilized.

### Materials

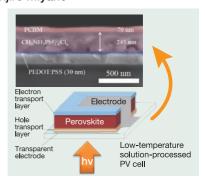
Masatoshi Yanagida Yasuhiro Shirai B. Dhruba Khadka (ICYS)

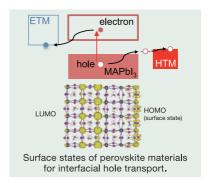
### Computation

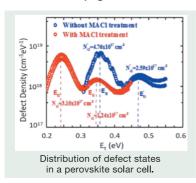
Yoshitaka Tateyama

### Characterization

Kenjiro Miyano Hidenori Noguchi James William Ryan Xiaoqing Chen





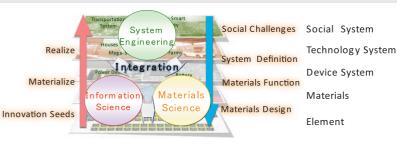


### **Technology Integration Unit**



Michihisa Koyama (Unit Director) Yasunori Kikuchi, Gen Inoue Takahisa Ohno, Tsuyoshi Ohnishi Karina Vink, Baber Javed Eriko Ankyu

Integrated Approach Bridging Materials, Technology, and Society



### Michihisa Koyama

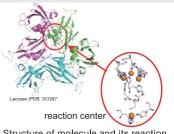
### **Hokkaido University**



Ichizo Yagi (Professor, Faculty of Environmental Earth Science) Masaru Kato (Assistant Professor)

Ichizo Yagi

Development of bio-inspired non-platinum electrocatalysts for fuel cell



Structure of molecule and its reaction center of Laccase which is natural catalyst for oxygen reduction reaction.

8980

Molecular structure of bi-copper complex inspired by Laccase and in situ XANES spectra of the complex under electrochemical environment.

### Nagoya University



Yasutoshi Iriyama

Yasutoshi Iriyama (Graduate school of Engineering, Professor) Munekazu Motovama (Graduate school of Engineering, Lecturer) Takayuki Yamamoto (Graduate school of Engineering, Assistant Professor) Takavoshi Tanii (Emeritus professor / Green Mobility Research Institute /

Takashi Ishida (Institute of materials and systems

Probable factors on interfacial resistance at electrode/solid electrolyte interface Institutes of Innovation for Future Society) Matual diffusion layer (resistive layer) for sustainability, Assistant Professor) Space charge layer structural relaxation

Fundamental studies on electrode/solid electrolyte interface for advanced all-solid-state LIBs, and development of in-situ analysis technology of interface structure, potential, and electric field in SOFC

### **Toyota Motor Corporation**





NanoGREEN/WPI-MANA Bldg. (Opened in 2012)

# GREEN is registered as a project of TIA.

The new building is equipped with a rich research environment including the shared advanced facilities of NIMS. Further, it is an eco-friendly laboratory featuring solar panels, LED lightings and photocatalyst glass watering systems, etc., and aiming at effective utilization of renewable energy.

### History of GREEN

866?".N87/ · Foundation (October)

Consists of 6 research areas

8676".N88/
The 1st symposium (February)

The 2nd symposium (March)
Reorganization into 4 research areas
Became a core project of TIA Nano-Green

8678".N8:
The 3rd symposium (February)
Relocation to new research building (May)
The 4th GREEN Symposium (June)
The 5th GREEN Symposium (December)

8679".N8;
New Director-General and Deputy Director-General
were appointed from the researchers (February)
Inauguration of two Specially Research Teams (April)

· The 6<sup>th</sup> GREEN Symposium (June) 867: ".N8</ · The 7<sup>th</sup> GREEN Symposium (December)

· ICYS-GREEN (January)

· The 1st Tohoku Univ. & GREEN Joint Symposium (June) (The 8th GREEN Symposium)

• The 1st Workshop for Battery Materials Analysis (September) • Inauguration of ad hoc team of Perovskite PV Cells (October)

· GREEN Engineer Training Program (December)

867; ".N8=/ · The 9th GREEN Symposium (January)
· The 10th GREEN Symposium (June)

• The 2<sup>nd</sup> Tohoku Univ. & GREEN Joint Symposium (October) (The 11<sup>th</sup> GREEN Symposium)

· The 2<sup>nd</sup> Workshop for Battery Materials Analysis (November)

867<".N8>/ · The 12th GREEN Symposium (January)

· Foundation of Center for Green Research on Energy and

· Environmental Materials (April)

· The 13<sup>th</sup> GREEN Symposium (June)

· The 3<sup>rd</sup> Workshop for Battery Materials Analysis (November)

867=".N8?/ · The 14<sup>th</sup> GREEN Symposium (February)

· The 15th GREEN Symposium (June)

· The 4th Workshop for Battery Materials Analysis (November)

 The 3<sup>rd</sup> Tohoku Univ. & GREEN Joint Symposium (December) (The 16<sup>th</sup> GREEN Symposium)

867>".N96/ · The 17th GREEN Symposium (January)

### Logomark▶

The logo mark represents the objective of GREEN; to see, i.e., to observe and to understand, the world of nano-scale and the phenomena of nano-surface and nano-interface by fully exercising computational science and characterization technology.



# Global Research Center for Environment and Energy based on Nanomaterials Science (GREEN)

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**National Institute for Materials Science (NIMS)**