Current Status and Future Prospects of Research on Sustainable Energy Systems in NIMS

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1. Introduction

Since the first oil crisis in 1973, Japan has been working hard to improve the situation through various energy related national projects, because of the lack of natural resources including fossil fuels. The energy self-sufficiency rate of Japan, however, is still less than 10% and the demand to reduce the greenhouse gas (GHG) emission, i.e., the use of fossil fuels, is growing more and more. Thus, significant efforts are currently being made to establish energy systems based on renewable energy such as solar and wind. Here efficient processes for energy transport/carrier, storage, and generation/capture as well as saving/use are required. National Institute for Materials Science (NIMS), the only institute in Japan devoted to materials research, is committed to develop materials and devices for sustainable energy systems.

2. R&D activities related to clean energy technology

Since the foundation in 2001, the development of energy and environmental materials is always one of the most important research targets of NIMS. From October 2009 to March 2019, the Global Research Center for Environment and Energy based on Nanomaterials Science (GREEN), which was supported by the Program for the Development of Environmental Technology using Nanotechnology from the Ministry of Education, Culture, Sports, Science and Technology (MEXT), played the central role in R&D on energy and environmental materials with emphasis on the understanding and control of interfacial processes as common issues in energy flow from solar energy. As an extension of GREEN, the Center for Green Research on Energy and Environmental Materials was founded in 2016. Its activities include research on energy transport/carrier (liquid hydrogen technologies), storage (rechargeable battery and capacitors) and generation/capture (photovoltaic and thermoelectric materials). In the following section, representative results of energy transport/carrier, storage, and generation/capture are presented.

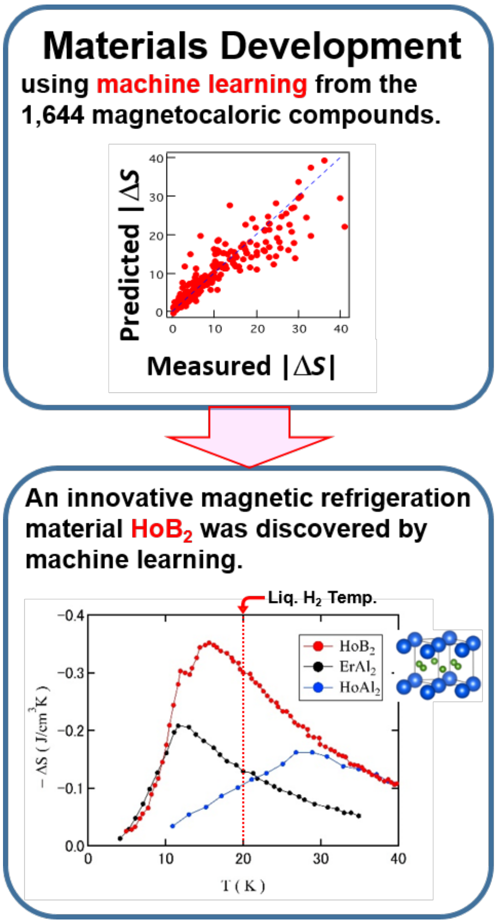


Fig. 1. Discovery of HoB_2

3. Specific research activities on sustainable energy systems

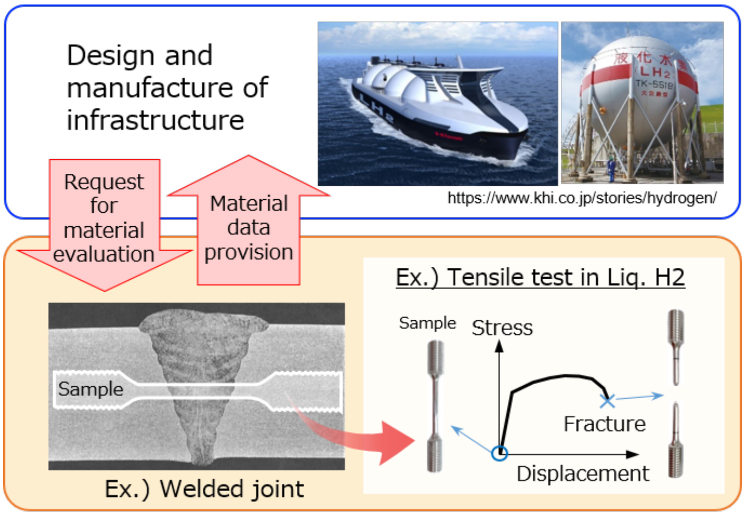
3.1 Liquid H_2 for Energy Carrier

The importance of hydrogen as an energy carrier is increasing. The technology for a hydrogen infrastructure consists of the production, transportation, storage and utilization of hydrogen. For transportation, it is desirable for hydrogen to be in a liquid form because a volume of liquid hydrogen is 800 times smaller than that of gaseous hydrogen.

There are two major issues for liquid hydrogen to become a popular energy carrier: (1) The cost of liquid hydrogen is too expensive, (2) the safety of materials reliability in cryogenic hydrogen is unknown for many materials.

The reason why liquid hydrogen is expensive is that the efficiency of the conventional liquefaction process based on gas compression and Joule-Thomson (J-T) effect is only 25%. In order for hydrogen to be a competitive carrier, hydrogen liquefaction efficiency should be above 50%. To conquer this issue, NIMS has started in 2018 a project supported by JST "Development of an advanced hydrogen liquefaction system and a zeroboiloff subcooler system by using magnetic refrigeration technology." Magnetic refrigeration uses the magnetocaloric effect, where the temperature of a magnetic material increases or decreases by applying or removing a magnetic field, respectively. Magnetic refrigeration doesn't need compressors, instead being a combined system of magnetic materials and a high field magnet. The development consists of synthesizing magnetic materials and optimizing the system including a superconducting magnet. We use a machine learning technique to explore new magnetic refrigeration materials. The discovery of HoB_2 is a successful example (Fig. 1). We use numerical analyses to optimize the particle size of magnetic materials and superconducting magnet design.

In order to ensure the safety of materials reliability in cryogenic hydrogen, NIMS is planning to establish a test facility in which we make materials reliability evaluation in cryogenic hydrogen (Fig. 2). Evaluation of strength properties, durability and hydrogen compatibility of materials are vital to manufacturing products provided for liquid hydrogen supply chain. An investigation of the reliability data would also give a chance to develop new materials suitable for the use in cryogenic hydrogen.



https://www.khi.co.jp/stories/hydrogen/

Fig. 2. Materials reliability evaluation in cryogenic hydrogen

3.2 Energy Storage/ Rechargeable Batteries

Although lithium-ion batteries (LIBs) have been supporting the development of modern society as the key mobile power source for smart phones, personal computers, and electric vehicles (EVs), etc., they do not meet all the new demands in the coming sustainable society. EVs require batteries with much higher energy density. Introduction of large scale renewable energy, in which temporal fluctuation is inevitable, must be associated with much durable stationary batteries. Research on innovation batteries in NIMS is focusing on lithium/air and solid-state batteries for high energy density and high reliability, respectively.

Lithium/air batteries (LABs) have an extremely-high theoretical energy density, but the observed value has been moderate. By employing air cathodes made of carbon nanotubes, we have demonstrated for the first time that the actual energy density can reach 600 Wh kg^{-1}. The module structure is important for the practical performance. We have developed a module structure with a 10-cell stacking

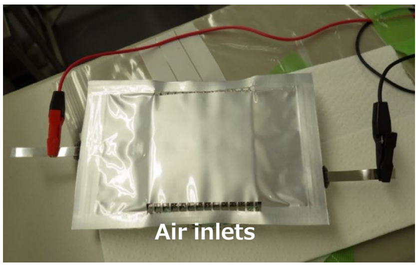


Fig. 3. 10-cell module with Li-air batteries stacked in parallel.

and passive air intake to deliver a practical discharge capacity (Fig. 3). Based on our achievements, we established a collaborative center with Soft Bank Corp in April 2018 to develop LABs for high altitude platform stations (HAPS) where light weight batteries are essential to be used in flying objects including drones.

Data-driven experimental design is one of the most promising approaches to identify suitable electrode compounds, combined with high throughput experiments. Actually, such approaches are effective for the screening of liquid electrolytes compositions, which consist of complex multi-component mixtures, such as combinations of lithium salts, solvents and additives. We developed a combinatorial high-throughput system with a screening rate of more than 1000 samples/day, specialized for the evaluation of battery components. Using this system combined with Bayesian optimization techniques, a specific combination of five chemical compounds was identified that improved the performance of LABs. Our results revealed the utilization of the automated robotic experiments with AI/MI can accelerate the discovery of improved electrolyte compositions. While it is time-consuming or even unrealistic to find ideal combinations of multiple additives using a traditional bottom-up approach, our developed technique efficiently identifies complex electrolytes that can lead to superior rechargeable battery performance.

One of the most important features of solid-state batteries is high reliability. Replacement of combustible organic electrolytes with non-flammable solid electrolytes makes the batteries free from fire. Single-ion conduction in the solid electrolytes suppresses side reactions leading to the performance degradation. Despite these advantages, the development of solid-state batteries was not significant because of the low ionic conductivity of solid electrolytes leading to a low power density until the recent finding of sulfide based solid electrolytes with a conductivity higher than 10^{-2} S cm^{-1}, which is even higher than that of liquid electrolytes used in the current LIBs. Since even such a high ionic conductivity does not lead to the high power-density without reduction of interfacial resistance between the battery materials, we have been focusing our research effort on the interfacial phenomena in solid-state batteries. Our fusion study among computational science, advanced characterization, and material development has revealed that cathode interface in sulfide-electrolyte systems is highly-resistive due to the lithium depletion and thus rate-determining, and we have successfully developed a unique interfacial structure to reduce the resistance. Now, we put a major effort on solid-sate batteries based on oxide-electrolytes, which is more reliable and safer but has many issues to be solved. We have started research on processes involved in all solid battery under “Materealize Project” supported by MEXT in October, 2019 and initiated joint collaborative research on oxide based all solid state batteries with a group of companies in May, 2020.

NIMS operates NIMS Battery Research Platform, which is equipped with the facility for battery fabrication and materials characterization, to support R&D of next generation batteries in Japan in collaboration with ALCA-SPRING project, which is supported by Japan Science and Technology agency (JST), since 2013. NIMS was awarded competitive fund for a new facility on battery research by supplementary budget in FY2019.

Other research activities in NIMS on energy storage include a graphene based super capacitor, which is now being developed by a spin-out venture company.

3.3 Sustainable Energy Generation

(i) Photovoltaics

Major efforts of photovoltaics research in NIMS have been done on emerging PVs such as dye sensitized solar cells and metal halide perovskite solar cells. We have been carrying out

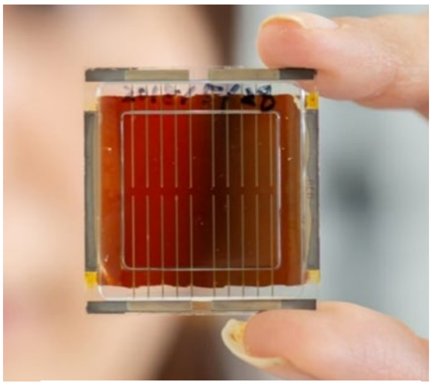


Fig. 4. Perovskite module for practical applications.

not only the development of solar cells with high efficiency and low manufacturing cost, but also fundamental research on photo-electric conversion mechanism. We have achieved the world's highest efficiency for a dye-sensitized solar cell and the highest stability with over 4,000 hours of power generation for a metal halide perovskite solar cell. The latter effort resulted in the development of large area perovskite solar cells (Fig. 4). Development of lead-free halide perovskites with low environmental impact has been also promising, recently achieved high efficiencies (>11%) and stability at the same time. Other research activities on photovoltaics in NIMS include Si-based nanowires and quantum dots.

(ii) Thermoelectrics

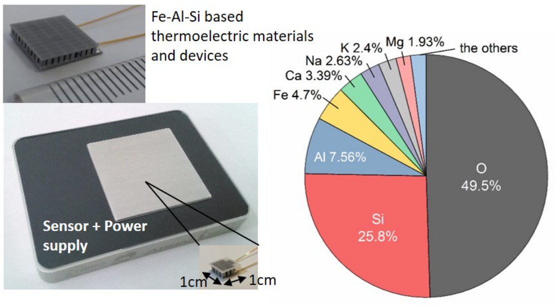


Fig. 5. Fe-Al-Si-based thermoelectric module and prototype device for IoT applications.

As the center of excellence for thermoelectric energy conversion research and development in Japan, NIMS carries out materials discovery, advanced thermal measurements, and module development to construct core technologies for future applications. Thermoelectric power generation, which can convert waste heat (with a temperature difference ΔT) into electrical energy, could contribute to develop the technology required to construct a sustainable energy supply. The need to establish a local-production-for-local-consumption-type autonomous power supply technology has emerged. It can provide the electric power necessary to drive a variety of sensors to support a society built around sensing networks. Although coin cell batteries are currently the main power supplies for sensors, the replacement cost and recyclability require alternative types of power supplies with longer lifetimes. Recently, NIMS succeeded in the development of high-integrated thermoelectric modules (~100chip/cm^2) with a power density of 100μW/cm^2 (ΔT = 5K at room temperature). These power generation modules can operate in the low-temperature region from room temperature to 473 K with a small temperature difference by using only earth-abundant and non-toxic elements of Fe, Al, and Si (FAST materials). We established a mass-production process (~1kg/batch) for FAST materials. Figure 5 shows the prototype of the thermoelectric modules and devices for sensing environment information such as temperature and humidity using a temperature difference at room temperature. The cost of constituent materials can be reduced by 1/5 from that of the conventional Bi-Te thermoelectric materials. In the mid-temperature applications, $FeSi_2$- and Mg_2SiSn-based thermoelectric modules are developed for waste heat recovery in various systems such as biomass boiler.

4. Related programs/projects conducted by NIMS

- NIMS operating subsidy project "Basic Research on Energy-Conversion & Storage" / Research on materials maximizing energy efficiency in the new energy value chain (MEXT, 2016-2022)
- Innovative hydrogen liquefaction technologies desired in future society / Development of advanced hydrogen liquefaction system by using magnetic refrigeration technology (JST project, 2018-2027)
- Advanced Low Carbon Technology Research (ALCA)/ Development of next generation solar cells based on the combination of perovskite and silicon photovoltaic technologies (JST project, 2016-2018)
- Autonomous Power Supply for IoT Devices using Small Temperature Difference Project / Research and development of low-cost and non-toxic Fe-Al-Si-based

thermoelectric materials and modules for driving IoT wireless sensors based on power generation technology that uses small temperature difference (NEDO project, 2018-2020)

- Advanced Low Carbon Technology Research and Development Program - Specially Promoted Research for Innovative Next Generation Batteries (ALCA-SPRING) / Acceleration of R&D of the next generation of the existing lithium-ion batteries (JST project, 2013-2022)
- SOLiD-EV project / Development of all-solid-state lithium-ion batteries for electric vehicles (NEDO project, 2018-2022)
- Element Strategy Initiative for Catalysts and Batteries / Developing high-performance automotive catalysts and secondary batteries through the interplay between experimental ant theoretical studies (MEXT, 2012-2021)
- Materealize Project / Establishment of process science for realizing all-solid-state batteries (MEXT, 2019-2026)
- Material Open Platform for All Solid State Batteries / Development of oxide-type all-solid-state batteries (MEXT, 2020-)

5. International collaboration

5.1 International alliance/networking development

NIMS has been encouraging its researchers to collaborate internationally. In fact, more than 50% of papers published by NIMS in recent years were internationally co-authored. Such papers tend to gain a significantly higher number of citations. Since its inception in 2001, NIMS has concluded a number of MOUs with high-level research institutions and universities in the world. 18 inter-institutional and more than 90 divisional MOUs are active now. In order to facilitate actual exchange of researchers and collaboration with foreign institutions, we have programs to support organizing international conferences and workshops, to invite prominent researchers to NIMS, and to support graduate students from universities overseas. A unique approach of NIMS may be the NIMS Award which started in 2007. Every year truly innovative researchers who succeeded to make a breakthrough in materials science are selected and invited to give a lecture at the academic symposium held during the NIMS Week, the largest PR event of NIMS. This one-day open symposium featuring the NIMS award has been an excellent opportunity for the NIMS researchers to cultivate and strengthen their international network. Also the NIMS ability to act as a key player in the international field of materials science is presented to the local community.

5.2 International joint R&D activities

In NIMS, the Research Center for Energy and Environment focuses on materials science and technologies related clean energy. Currently the center has nine international MOUs (six of them with universities in G20 countries) and the subjects of collaborative research include new materials and technologies for solar cells, fuel cells, thermoelectric devices, and hydrogen energy. All these subjects are important to realize a low-carbon society. With national institutes in the G20 countries, NIMS has several important agreements. For example, with NIST (USA), we collaborate on data utilization and development of necessary technologies to expedite materials development. With EMPA (Switzerland), NIMS has been co-publishing an open-access journal "Science and Technology of Advanced Materials." With the Bredessen Center of the University of Tennessee, which is co-operated by the Oak Ridge National Laboratory (USA), we signed an agreement for cooperative graduate program last year. With ANSTO (Australia), we have a long history of collaboration in the field of neutron scattering and synchrotron X-ray research. We believe that collaboration with national institutions in the G20 countries in the research topics presented today is very important to accelerate materials research for clean energy as well.

6. Conclusion and future prospects

NIMS has been working hard to develop materials, which are required to realize a sustainable society based on renewable energy such as solar and wind. Our efforts are, however, not limited to materials for transport/carrier (hydrogen technologies as described above), for storage (rechargeable battery and capacitor) and for energy generation/capture (photovoltaic and thermoelectric materials). We put a great deal of effort to the development of materials for saving and efficient use of energy. For example, high temperature resistive alloys, which are essential for the high temperature operation of engines, and magnetic materials, which are required for highly efficient motors.

We continue to work on these materials but more efficiently and effectively with the aid of high-throughput screening of materials using MI/AI as well as advanced characterization tools. Furthermore, to accelerate the implementation of the materials we develop, we will be working on devices and systems utilizing these materials with the collaboration with industrial partners.

Dr. Kazuhito Hashimoto

Kazuhito Hashimoto accepted the appointment of President of National Institute for Materials Science in Tsukuba in 2016. He is also a professor at Institute for Future Initiatives of the University of Tokyo (UT) and serves as a senior counselor to the president of UT since 2016. He is a member of Board of Governors (BOG) of Okinawa Institute Technology (OIST) since 2016. As an executive member of Council for Science, Technology & Innovation (Cabinet Office, Government of Japan), he has also been contributing to the Science and Technology Policy of Japan since 2013.

After he received his BS (1978) and MS degrees (1980) of Chemistry from UT, he obtained a research position at the Institute for Molecular Science (IMS) in 1980. He obtained a Doctor of Science degree from UT in 1984. In 1989, he was invited as a lecturer at Department Applied Chemistry at UT, where he was promoted to Associate Professor in 1991. He was appointed a full professorship at the Research Center of Advanced Science & Technology (RCAST) of UT in 1997. He served as a Director of RCAST from 2004 to 2007. He was also appointed Professor at Department of Applied Chemistry at UT from 2003 to 2016.

His research interests are spread in a very broad area including photocatalysis, microbial electrochemistry, functionalized magnetic materials, artificial photosynthesis, and polymer photovoltaics, among many others. His contributions to science are described in more than 650 peer reviewed papers and more than 50,000 citations (h-index 110). He also wrote more than 200 reviews and book chapters. The truths he uncovered are the basis for many manufactured products. His contributions to technology and engineering are described in approximately 200 issued Patents, more than 20 of which are in use.

He received many awards including the Japan Prime Minister Award for Academia-Industry Corporation in 2004, the Japan Imperial Award for Invention in 2006, the Chemical Society of Japan Award in 2012, the Heinz Gerischer Award of ECS in 2017 and the Medal of Honor with the Purple Ribbon in 2019.