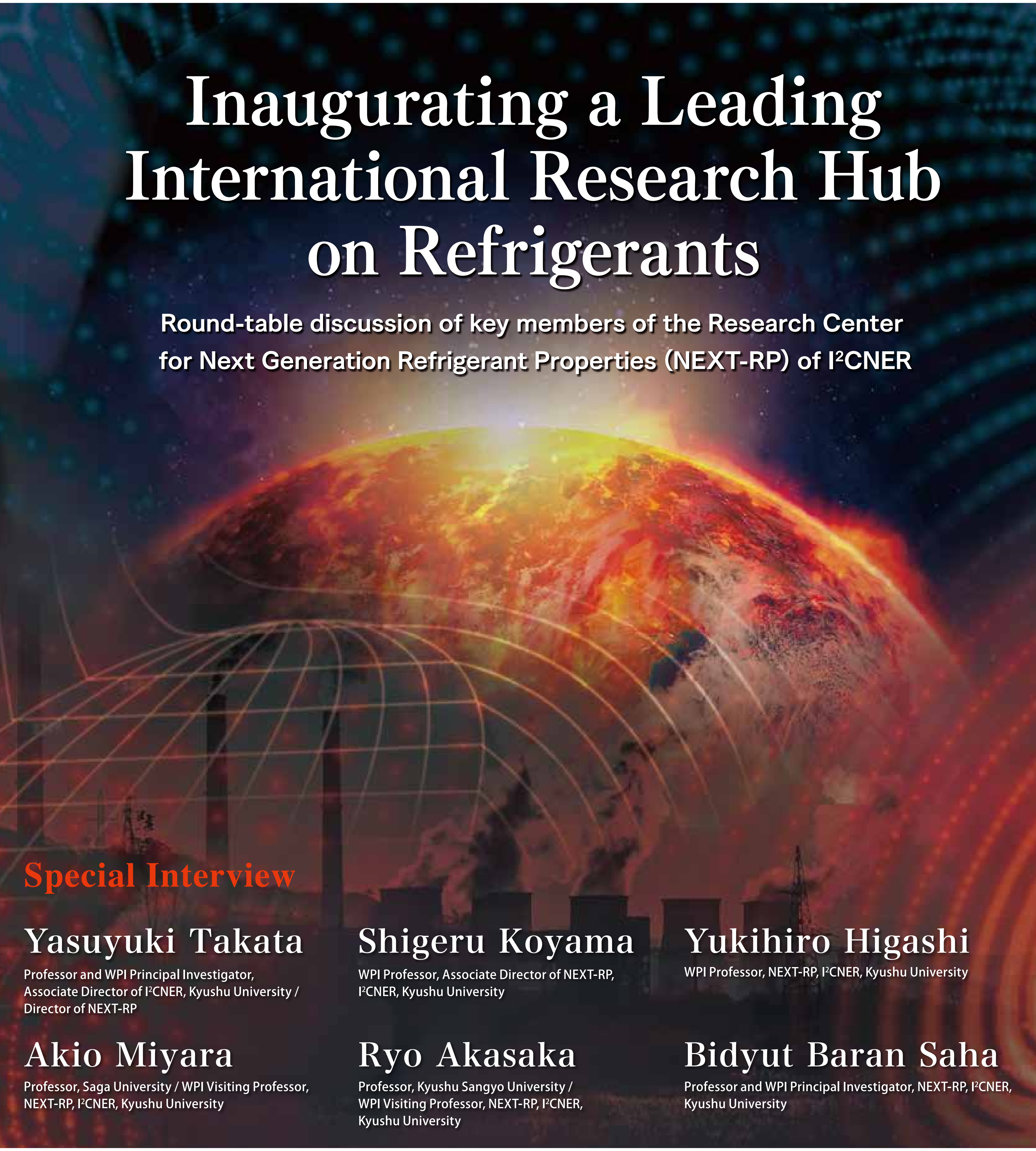
Energy Outlook

International Institute for Carbon-Neutral Energy Research

May 2017



Inaugurating a Leading International Research Hub on Refrigerants

Round-table discussion of key members of the Research Center for Next Generation Refrigerant Properties (NEXT-RP) of I²CNER

Special Interview

Yasuyuki Takata
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wpi World Premier International Research Center Initiative

I²CNER

KYUSHU UNIVERSITY

ILLINOIS UNIVERSITY OF ILLINOIS AT URBANA-CHAMPAIGN

NEXT-RP Kick-off Symposium @ I^{2}CNER

Six months after its inauguration, NEXT-RP held its kick-off symposium at I^{2}CNER on October 7, 2016. The large crowd of participants included numerous representatives from partner organizations and businesses, including refrigerant / air conditioning manufacturers. In an effort to further promote I^{2}CNER's broad-ranging research efforts, a lab tour for keynote speakers of the symposium was also hosted.

Lab Tour: A sample of the laboratories that were visited

Prof. Yukihiro Higashi's lab
(NEXT-RP)

Prof. Yasuyuki Takata's lab
(Thermal Science and Engineering Division)

Prof. Seiji Ogo's lab
(Catalytic Materials Transformations Division)

Prof. Masanobu Kubota's lab
(Hydrogen Materials Compatibility Division)

— Messages from NEXT-RP Kick-off Symposium Keynote Speakers —

Prof. Koichi Watanabe
Emeritus Professor, Keio University

It is unnecessary to point out that our first priority should be a concerted effort to achieve a series of productive research results in strategic areas as quickly as possible. The creative and innovative research activities that have been established in NEXT-RP could be one of the best sources of information for the global community in this area. NEXT-RP is also likely to attract attention because it is ideally positioned to be able to address the global community's ever-increasing concerns about next generation refrigerants. Emphasis should be placed on developing a systematic, targeted roadmap within NEXT-RP.

Dr. Eric W. Lemmon (REFPROP developer)
U.S. National Institute of Standards and Technology

The NEXT-RP collaboration could be very valuable in coordinating research efforts. This could take two forms: (1) By bringing researchers together to discuss their current work, new collaborations will naturally form. (2) The preparation of assessments of research completed and remaining research priorities would be very helpful — both to avoid duplication of effort and also to secure research funding. NEXT-RP should not "assign" research to different groups, but allow these coordination efforts to result naturally in more effective research.

Prof. Anthony Jacobi
University of Illinois at Urbana-Champaign

NEXT-RP has an excellent reputation from the start, owing to the established excellence and impact of the faculty involved. One idea might be to consider leveraging that reputation with a series of conferences in which you bring together a relatively small group of the most influential researchers in the area to exchange ideas. My advice would be to decide what partnerships you wish to form, being mindful that a mix of academic, corporate, and other organizations would be most powerful, then seek to identify individuals in those organizations who will champion the partnership.

Research Highlights

1 Application to Photocatalytic H_2 Production of a Whole-Cell Reaction by Recombinant *Escherichia coli* Cells Expressing [FeFe]-Hydrogenase and Maturases Genes

Yuki Honda, Hidehisa Hagiwara, Shintaro Ida, and Tatsumi Ishihara

Angewandte Chemie - International Edition
DOI: 10.1002/anie.201600177

An inorganic photo/biocatalyst hybrid, e.g. TiO_2 + [FeFe]-hydrogenase (HydA), is of interest for an efficient H_2 production since HydA is an excellent H_2 forming biocatalyst. However, the low stability of purified HydA hampers practical applications. In this study, instead of applying purified HydA, the direct application of a whole-cell of *Escherichia coli* expressing HydA genes was applied to the hybrid system (Fig. 1). As shown in Fig. 2, the combination of TiO_2 with the whole cell formed H_2 under light irradiation, demonstrating that the whole-cell biocatalyst could be employed for the hybrid system. The new system is a promising approach for developing an efficient water splitting photocatalyst listed in I²CNER's roadmap, and contributes to realizing a clean and noble-metal-free H_2 production.

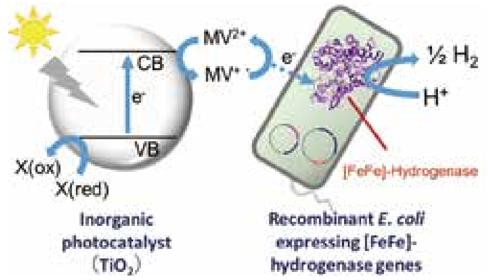

Fig. 1
Inorganic photo/biocatalyst hybrid system based on the combination of inorganic semiconductor (TiO_2), electron mediator, and the whole-cell biocatalyst.

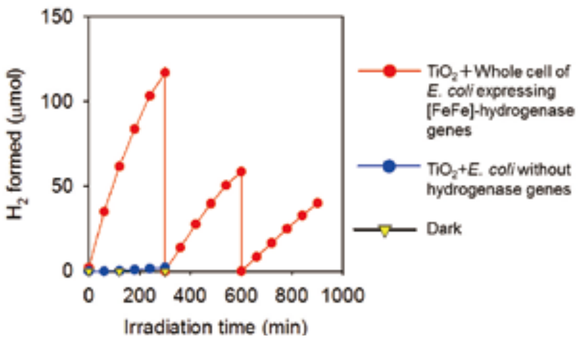

Fig. 2
Amounts of H_2 formed under light irradiation by the combination of TiO_2 and the whole-cell biocatalyst of recombinant *E. coli* expressing [FeFe]-hydrogenase genes.

2 Macroscale Superlubricity of Multilayer Polyethylenimine/Graphene Oxide Coatings in Different Gas Environments

Prabakaran Saravanan, Roman Selyanchyn, Hiroyoshi Tanaka, Durgesh Darekar, Aleksandar Staykov, Shigenori Fujikawa, Stephen M. Lyth, and Joichi Sugimura

ACS Appl. Mater. Interfaces 2016, 8, 27179–27187
DOI: 10.1021/acsami.6b06779

Despite studies showing superlubricity or ultra low friction (COF ~ 0.005) in nano and atomic scale, realizing it in macroscale (real-world applications), is always a challenge. We show that multilayer polyethylenimine/graphene oxide thin films prepared via a highly scalable layer-by-layer (LbL) deposition technique, can be used as solid lubricants (Fig. 1a). The tribological properties are investigated in air, under vacuum, in hydrogen, and in nitrogen gas environments. Fig. 1b (COF graph) shows that the superlubricity (COF <0.01) was achieved in dry N_2 with macroscale loading conditions while ambient air shows 20 times higher friction (COF ~ 0.2). Therefore, it can be assumed that superlubricity conserves the energy wasted by friction by 20 times. This superlubricity will have impact on the machines with sliding parts such as cars, trains etc., which will have a huge impact on our lives as we depend on machines for everyday life.

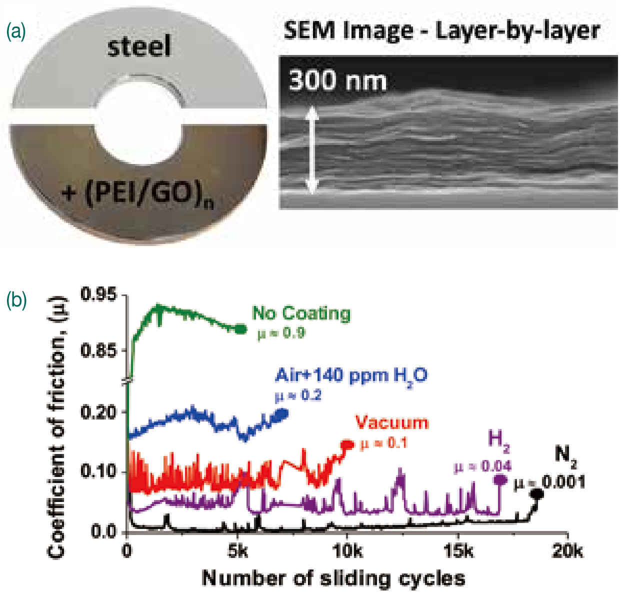

Fig. 1
(a) Digital photograph of bare steel and coated specimen (left). (a) Cross-sectional SEM image of coating on steel (right).
(b) Coefficient of friction (COF) vs Sliding number of cycles plot.

3 Determination of hydrogen compatibility for solution-treated austenitic stainless steels based on a newly-proposed nickel-equivalent equation

Setsuo Takaki, Shigenobu Nanba, Kazunari Imakawa, Arnaud Macadre, Junichiro Yamabe, Hisao Matsunaga, and Saburo Matsuoka

International Journal of Hydrogen Energy, Volume 41, Issue 33 (2016) 15095–15100
DOI: 10.1016/j.ijhydene.2016.06.193

The Hydrogen Materials Compability Division targets the development of low-cost and high-strength austenitic stainless steels with excellent resistance to hydrogen embrittlement (HE). With the current domestic regulation, the hydrogen compability of such stainless steels is determined based on a nickel-equivalent content, which is an indicater for the stability of the austenitic phase. However, the current nickel-equivalent equation does not contain nitrogen, which effectively contributes to the stability of the austenitic phase. Substituting nitrogen for nickel is an important direction to take for improving a new stainless steel with excellent resistance to HE. This study presented a newly-proposed nickel-equivalent equation, which contains nitrogen. The newly-proposed equation is expected to have the capability to contribute to the establishment of a hydrogen-based energy society, via the development of new low-cost and high-strength stainless steels with excellent resistance to HE.

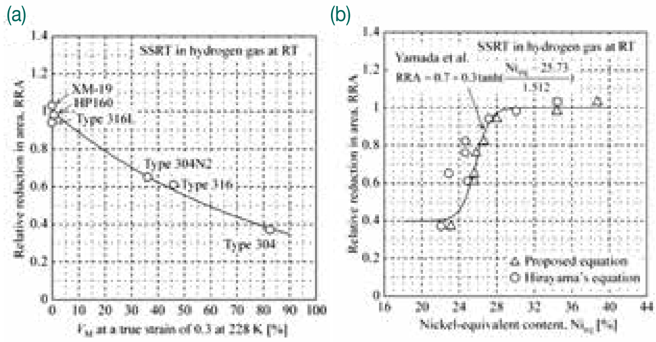

Fig. 1
Relationship among RRA, ΔV_M and Ni_{eq}: (a) RRA as a function of ΔV_M at a true strain (ε) of 0.3 and a temperature of 228 K; (b) RRA as a function of Ni_{eq} based on the proposed and Hirayama' s equations. RRA is the relative reduction in area, which is the ratio of reduction in area (RA) in hydrogen gas to RA in inert gas. ΔV_M is the net strain-induced martensite content. Ni_{eq} is the nickel-equivalent content. Fig. 1 contains the RRAs for the steels with nitrogen and the experimental result is successfully reproduced based on the newly-proposed nickel-equivalent equation.

4 Metal-Free Nitrogen-Doped Carbon Foam Electrocatalysts for the Oxygen Reduction Reaction in Acid Solution

Jianfeng Liu, Shundo Yu, Takeshi Daio, Mohammed. S. Ismail, Kazunari Sasaki, and Stephen M. Lyth

Journal of the Electrochemical Society
DOI: 10.1149/2.0631609jes

Hydrogen fuel cells could eventually replace combustion engines. However, the platinum catalyst is expensive and degrades over time, therefore Pt-free alternatives such as Fe/N/C are being investigated. Here, metal-free, nitrogen-doped carbon foam is utilized as a model electrocatalyst to investigate the role of nitrogen in the oxygen reduction reaction (ORR) in the absence of iron. Relatively high activity for the ORR in acid is obtained after graphitization, with an electron number of 3.6, revealing that a 4-electron pathway to H_2O can occur even in the absence of Fe-coordination sites. The activity is attributed to a large surface area, improved conductivity after graphitization, and the high proportion of tertiary nitrogen. This work will lead to improved design of non-precious fuel cell catalysts.

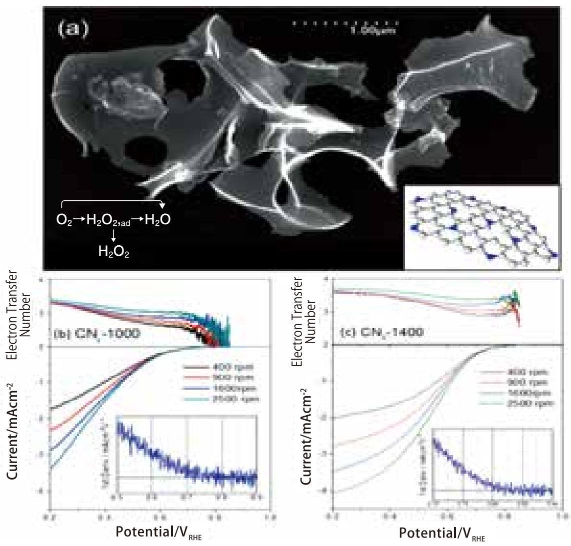

Fig. 1
(a) Scanning electron microscopy of nitrogen-doped carbon foam (CNx), showing the oxygen reduction reaction (inset left) and schematic chemical structure (inset right). Linear sweep voltammograms showing the oxygen reduction current density, electron transfer coefficient, and onset potential for CNx catalysts pyrolysed at (b) 1000˚C and (c) 1400˚C.

5 Heat Transfer through a Condensate Droplet on Hydrophobic and Nanostructured Superhydrophobic Surfaces

Shreyas Chavan, Hyeongyun Cha, Daniel Orejon, Kashif Nawaz, Nitish Singla, Yip Fun Yeung, Deokgeun Park, Dong Hoon Kang, Yujin Chang, Yasuyuki Takata, and Nenad Miljkovic

Langmuir, Vol. 32, pp.7774-7787, 2016
DOI: 10.1021/acs.langmuir.6b01903

Understanding the fundamental mechanisms governing vapor condensation on nonwetting surfaces is crucial to a wide range of energy and water applications. In this paper, we reconcile classical droplet growth modeling barriers by utilizing two-dimensional axisymmetric numerical simulations to study individual droplet heat transfer on nonwetting surfaces (90 °< θa < 170 °). It is found that the majority of heat transfer occurs at the three phase contact line, where the local heat flux can be up to 4 orders of magnitude higher than at the droplet top. We studied condensed water droplet growth using optical and environmental scanning electron microscopy on biphilic samples consisting of hydrophobic and nanostructured superhydrophobic regions, showing excellent agreement with the simulations. Our results demonstrate the importance of resolving local heat transfer effects for the fundamental understanding and high fidelity modeling of phase change heat transfer on nonwetting surfaces.

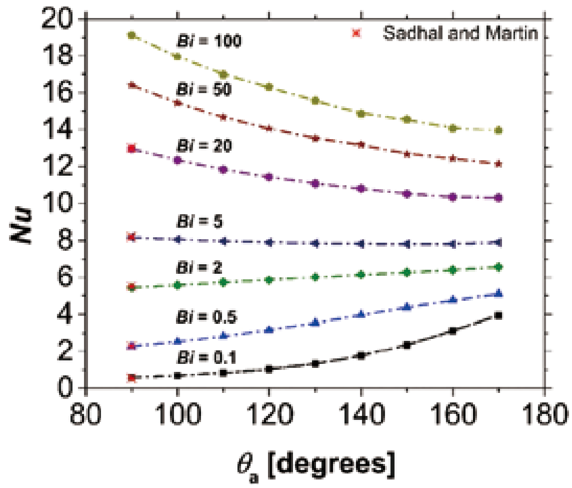

Fig. 1
Droplet Nusselt number as a function of apparent advancing contact angle for different Biot numbers.

6 Experimental and Quantum Chemical Approaches to Develop Highly Selective Nanocatalysts for CO_2-free Power Circulation

Miho Yamauchi, Naoki Ozawa, and Momoji Kubo

Chemical Record
DOI: 10.1002/tcr.201600047

We have proposed a new concept involving CO_2-free electric power circulation systems via highly selective electrochemical reactions of alcohol/carboxylic acid redox couples. We achieved the preparation of Fe-group nanoalloy catalysts to generate electric power from an alcohol, which is a highly storable and transportable liquid fuel, and TiO_2 catalysts which enable reproduction of an alcohol via electroreduction of a carboxylic acid, which is an oxidized waste of an alcohol. Design concepts for nanocatalysts able to catalyze highly selective electrochemical reactions are provided from both experimental and quantum mechanical perspectives. Our results are expected to greatly contribute to the effective use of renewable electricity and realization of a sustainable society, and contributes to the realization of carbon-neutral energy circulation, one of the final targets in the Catalytic Materials Transformations Division.

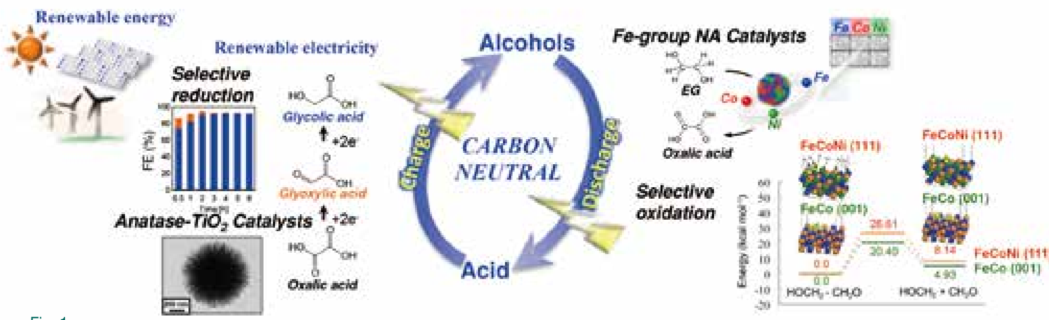

Fig. 1
Highly selective catalytic reactions of alcohols/carboxylic acid redox couples on the well-designed catalysts enable CO_2-free power circulations.