The 1st Symposium for Collaborative Research on Energy Science and Technology (SCREST-1st)

January 10th-11th, 2019, National University of Singapore, Singapore

Main theme of SCREST-1st: Energy Materials and Devices for Innovation

Topics of SCREST-1st include, but not limited to:

- Energy materials
- Hydrogen energy
- Hydrogen production
- Fuel cells
- Biofuels
- Solar energy
- Alternative energy
- Photocatalysis
- Supercapacitors
- Photovoltaics
- Nanomaterials
- Nanoenergy
- Geothermal Energy

Organized by

National University of Singapore
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Functional Materials Society

Sponsored by

Department of Mechanical Engineering, National University of Singapore
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INVITATION

Dear Colleagues,

To solve global problems, interdisciplinary collaboration is being required. The innovative energy materials would be created by collaborating among various researchers in the field of physics, chemistry, materials, mechanical, and electrical engineering, because such collaboration can promote effective acquisition of state-of-the-art technology in each field. The SCREST-1st (The 1st Symposium for Collaborative Research on Energy Science and Technology) will be held at National University of Singapore from January 10th to 11th, 2019. The International Advisory and Organizing Committees cordially invite you to attend the symposium and participate in its scientific programs. In this symposium, we aim to construct a novel consortium between the two universities, having many researchers related intensively to energy materials. Presentations will consist only oral presentation. The official language of the symposium will be English.

Important Deadlines

Deadline of Abstract Submission; Dec. 10, 2018

Congress Date; Jan. 10-11, 2019

January   9: Reception

January 10: Presentations/Banquet

January 11: Lab. tour

Advisory and Committee members
Organizing committee
Chairperson:

Li Lu   National University of Singapore

Co-chairperson:

Mitsunobu Sato   President of Kogakuin University

Committee member

Kaiyang Zeng	National University of Singapore
Jun Min Xue	National University of Singapore
Daniel Chua	National University of Singapore
Hua Chun Zeng	National University of Singapore
Ichiro Takano	Kogakuin University
Toshinori Okura	Kogakuin University
Tohru Honda	Kogakuin University
Hiromitsu Takaba	Kogakuin University

■Language

English will be the official language during the symposium.

■Symposium Venue

The symposium will be held at National University of Singapore.

CORRESPONDENCE

If you have any inquiry, you can contact with the general secretary via e-mails in the URL.

Hiroki Nagai (KU)

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ORAL PRESENTATIONS:

This symposium has only oral presentation.

Keynote Talk: Speaker has 25 minutes for their presentation. With approximately 20 minutes given for the presentation followed by 5 minutes for questions and answers.

Oral Presentation (Full Prof.): Speaker has 20 minutes for their presentation. With approximately 15 minutes given for the presentation followed by 5 minutes for questions and answers.

Oral Presentation: Speaker has 15 minutes for their presentation. With approximately 13 minutes given for the presentation followed by 2 minutes for questions and answers.

Standard facilities for PC presentations will be available at the symposium site.

GUIDELINES:

Abstracts should be prepared according to the abstract template. The abstract should be sent via e-mail (nagai@cc.kogakuin.ac.jp). The deadline for abstract submission would be **December 10, 2018**. The authors are encouraged to submit a camera-ready abstract (A4-size with 25 mm margins on all sides, or within a frame of 17 cm x 24 cm.) in Word or PDF format. Use Times New Roman font. In the PDF file case, all fonts should be embedded in the file. The font size should be boldfaced 14 point for the title and 11 point for the remaining. The abstract should be completed within 2 pages with figures and tables.

References

[1] A. Author and B. Author: "Title of paper," Journal Name, vol., startpage-endpage (year).

[2] A. Author, Title of book (Publisher), Chapter, (year).

The abstract should be completed within 2 pages.

Papers in the form of electronic file should be submitted by **e-mail** to the following address: nagai@cc.kogakuin.ac.jp

January 10: Presentations

Venue: E4-04-04, Faculty of Engineering, National University of Singapore

9:00-9:10   Opening Remarks   Prof. Li Lu, Prof. Mitsunobu Sato

Chair; Prof. Li Lu

9:10-9:40   Keynote 1   Prof. Mitsunobu Sato (KU)

Fabrication of functional thin films from the metal complexes for the SDGs

9:40-10:10   Keynote 2   Prof. Hua Chun Zeng (NUS)

Design Made Nanocatalysts for Green Fuel Production

10:10-10:30   Coffee Break

Chair; Prof. Chua Daniel

10:30-10:50   Lecture 1   Prof. Toshinori Okura (KU)

Development of Na^+-Superionic Conductor Narpsio Glass-Ceramics

10:50-11:10   Lecture 2   Prof. Tohru Honda (KU)

Carbon nanotube dispersed Ga_2O_3 films fabricated by molecular precursor method

Chair; Prof. Masato Morita

11:10-11:30   Lecture 3   Prof. Hiromitsu Takaba (KU)

Functional Materials Design using Machine-Learning and Computational Chemistry

11:30-11:45   Lecture 4   Mr. Mahendra B Chaudhari (Shimadzu)

Use of Advanced Characterization Technologies for High Performance of Functional Materials

11:45-13:15   Lunch

Chair; Prof. Hiromitsu Takaba

13:15-13:30   Lecture 5   Ms. Ting Xiong (NUS)

Defect Engineering of Oxygen Deficient Manganese Oxide to Achieve High Performing Aqueous Zinc Ion Battery

13:30-13:45   Lecture 6   Prof. Shiro Seki (KU)

Research and Development of Next-Generation Battery Systems: Lithium-Sulfur Batteries and All-Solid-State Batteries

13:45-14:00   Lecture 7   Ms. Minchan Li (NUS)

Advanced hybrid lithium-air batteries achieved by atomically iron sites anchored on N-doped carbon

Chair; Prof. Shiro Seki

14:00-14:20   Lecture 8   Prof. Jim Yang Lee (NUS)

Dual-band Electrochromic Windows/Electrochromic Batteries

14:20-14:35   Lecture 9   Prof. Tomohiro Yamaguchi (KU)

Toward fabrication of GaInN-based devices: Epitaxial growth and characterization of GaInN by RF-MBE

14:35-14:50   Lecture 10   Prof. Chua Daniel (NUS)

Study of 2D Materials for Energy and Device Applications Using High Resolution Transmission Electron Microscopy

14:50-15:20   Coffee Break

Chair; Prof. Toshinori Okura

15:20-15:35   Lecture 11   Prof. Masato Morita (KU)

Applications of a High Resolution Mass Imaging Microscope (FIB-TOF-SIMS)

15:35-15:50   Lecture 12   Ms. Serene Wen Ling Ng (NUS)

Embedment of Cu co-catalyst into TiO_2 for exceptionally active and stable photocatalysts

15:50-16:05   Lecture 13   Prof. Hiroki Nagai (KU)

Fabrication and Characterization of a Layered $LiCoO_2$ Thin Film on a Quartz Glass Spray-coated with an Aqueous Ammonia Solution Involving Metal Acetates

Chair; Prof. Tomohiro Yamaguchi

16:05-16:20   Lecture 14   Ms. Lei Zhang (NUS)

Mesoporous Mo_2C Microflower Supported Pt Single Atoms for Efficient Oxygen Reduction

16:20-16:40   Lecture 15   Prof. John Wang (NUS)

2D Layered, 2D Non-layered and 2D Non-layered Holey Materials for Energy Storage and Conversion

16:40-16:50   Closing Remarks   Prof.   Li Lu

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Fabrication of functional thin films from the metal complexes for the SDGs

Mitsunobu Sato[1, *]

[1] *Department of Applied Physics, School of Advanced Engineering, Kogakuin University, 2665-1 Nakano, Hachioji, Tokyo 192-0015, Japan*

Abstract

The 2030 Agenda for Sustainable Development, adopted by all United Nations Member States in 2015, provides a shared blueprint for peace and prosperity for people and the planet, now and into the future. At its heart are the 17 Sustainable Development Goals (SDGs), which are an urgent call for action by all countries - developed and developing - in a global partnership. They recognize that ending poverty and other deprivations must go hand-in-hand with strategies that improve health and education, reduce inequality, and spur economic growth – all while tackling climate change and working to preserve our oceans and forests [1].

The metal complexes are used in various applications such as catalysts, luminescence, and medicine. In 1996, we focused on the thin film fabrication of various metal oxides and phosphate compounds using the coating solution including the metal complexes of stable [2]. This is the molecular precursor method (MPM). The method is based on the formation of excellent precursor solutions involving anionic metal complexes and the alkylammonium cation. The stability, homogeneity, miscibility, coatability and other characteristics of the precursor solutions which can be used for various coating methods, are practical advantages, in contrast to the conventional sol-gel method. This is because metal complex anions with high stability can be dissolved in volatile solvents by combining them with the appropriate alkylamines. The MPM, pertinent to coordination chemistry and materials science including nanoscience and nanotechnology, has been used to fabricate various high-quality thin films with appropriate film thicknesses. As a result, the MPM represents a facile procedure for thin-film fabrication of various metal oxides or phosphates, which are useful as electron and/or ion conductors, semiconductors, dielectric materials such as In_2O_3, ZnO, $LiCoO_2$, $Li_3Fe_2(PO_4)_3$, TiO_2, Cu_2O, Co_3O_4, $SrTiO_3$, ZrO_2, SiO_2, $BaTiO_3$, $Ca_{10}(PO_4)_6(OH)_2$ etc. One of the features related to this method is the low-cost manufacture involving the chemical process which can save both resource and production energy.

Recently, we reported many applications using the MPM such as a thin film lithium ion battery, and novel thin-film LIB (PV-LIB) which can be charged by light irradiation [3, 4]. The PV-LIB uses two active materials, TiO_2 (Titania) and $LiCoO_2$ (LCO) thin films, on conductive transparent glass electrode for the anode and cathode respectively, and an organic electrolytic solution involving Li ion. During the irradiation of 1-sun light from a solar simulator to the device for 1 min, the averaged voltage of 1.38 V was observed. After the charging operation, the self-discharge voltage was 1.37 V. However, the use of flammable organic liquid induces several problems based on the risk of liquid leakage *etc*. In order to fabricate the safely device, which has long cycle-life, low self-discharge, and high operating voltage, we attempted to fabricated the all-solid-state PV-LIB (ASS-PV-LIB) with $Li_{1.3}Al_{0.3}Ti_{1.7}(PO_4)_3$ (LATP) using MPM. LATP is one of the Li-ion conductive ceramics with NASICON structure and of a promising candidate as a solid electrolyte.

The repeated charge/self-discharge test was performed under light irradiation and in dark condition. The 1-sun irradiation was achieved using a solar simulator and the voltage change between the electrodes was continuously recorded with a DC voltage monitor. The irradiated area of the device was 4.6 cm². The charging and discharging cyclic was performed up to 600 cycles. The convergence at around 0.9 volt was obtained and indicates that the device can work as an excellent PV-LIB and the MPM is useful to fabricate the all-solid-state PV-LIB.
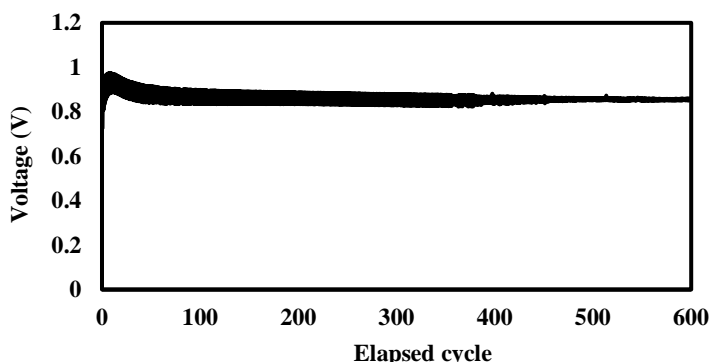
Fig. 1 One min Charge and discharge measurement cycles of ASS-PV-LIB by 1-sun light irradiation and under dark condition, respectively.

Keywords: molecular precursor method; thin film; lithium ion battery

Reference:

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[4] H. Nagai, T. Suzuki, Y. Takahashi, and M. Sato, Photovoltaic lithium-ion battery fabricated by molecular precursor method, *Funct. Mater. Lett.*, **9**, 1650046 (2016).

Short-biography:

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Biography; Prof. Dr. Sato is the president of Kogakuin University of Technology & Engineering (KUTE-Tokyo) from 2015 and a full professor at the Department of Applied Physics, School of Advanced Engineering. Dr. Sato research interests include the fabrication process of nanostructured materials, and functional thin films such as lithium ion batteries, semiconductor thin films and biocompatible coatings for implant materials etc.

Design Made Nanocatalysts for Green Fuel Production

Hua Chun Zeng

Department of Chemical and Biomolecular Engineering, Faculty of Engineering,
National University of Singapore, Singapore 119260

Abstract

Our research is focused on design and synthesis of integrated nanocatalysts for green fuel technology such as hydrogenation of CO_2 to methanol. In preparing such new catalysts, various synthetic approaches have been developed in recent years [1-7]. Normally, the primary catalytic phases are synthesized into monodisperse nanoparticles through wet chemical routes, while the hosting matrixes are often prepared as porous and/or hollow supports through soft synthetic approaches with desired structural complexity and chemical functionality which are accessible to reaction constituents (Figure 1). In particular, integration of different catalytic components can be achieved in a step-by-step manner. Both *top-down* and *bottom-up* strategies have been employed in this type of synthetic architecture, benefiting from rapid advancement of nanoscience and nanotechnology as well as the maturing chemistry of materials. It is anticipated that structural and compositional requirements of such state-of-the-art nanocatalysts can be met at a higher level of sophistication and precision but at a much lower cost in future. Toward this goal, synthetic architecture of nanomaterials will continue to be an important field in future development of catalyst technology. Further investigation and invention of integrative methodology will lead to even more powerful catalysts, achieving an industrial scale of applications.

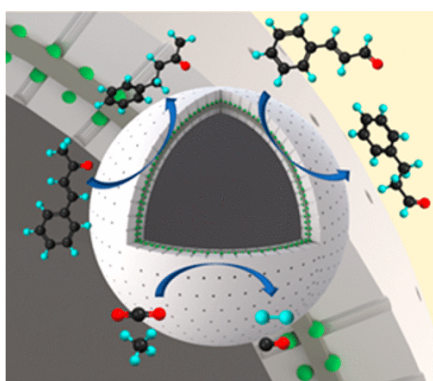**Keywords: Nanocatalysts; Catalyst design; Green fuels; CO_2 hydrogenation**

Figure 1. Intercalation of transition-metal nanoparticles within mesoporous silica for robust catalytic reactions.

Minister's Office, Singapore under its Campus for Research Excellence and Technological Enterprise (CREATE) program.

Reference

[1] H.C. Zeng, Integrated Nanocatalysts, Acc. Chem. Res. **46**, 226-235 (2013).

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Short-biography

Name: Hua Chun Zeng

Affiliation: Department of Chemical and Biomolecular Engineering, Faculty of Engineering, National University of Singapore, Singapore 119260

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Biography: Professor Hua Chun Zeng obtained his B.Sc. in Chemistry from Xiamen University in 1982 and Ph.D. in Physical Chemistry (with Professor Keith A.R. Mitchell) from University of British Columbia in 1989. Following postdoctoral work (with Professor John C. Polanyi, Nobel Laureate in Chemistry, 1986) at University of Toronto, he joined the faculty at National University of Singapore in 1991. His research interests are, at present, focused on the exploratory design and synthesis of inorganic nanostructures, with an emphasis on heterogeneous catalysis.

Development of Na$^+$-Superionic Conductor Narpsio Glass-Ceramics

Toshinori Okura[1, *], Koji Kawada[1], Naoya Yoshida[1] and Kimihiro Yamashita[2]

[1]Department of Applied Chemistry, School of Advanced Engineering,

Kogakuin University, Tokyo 192-0015, Japan

[2]Institute of Biomaterials and Bioengineering,

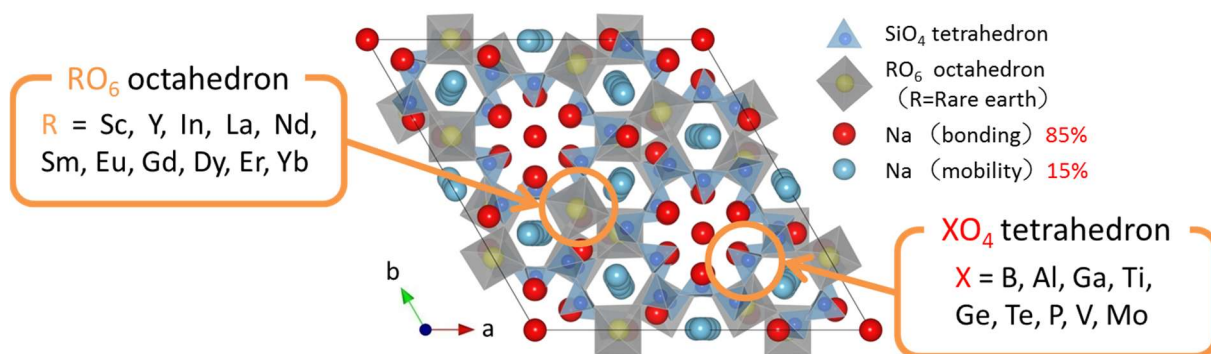*Tokyo Medical and Dental University, Tokyo 101-0062, Japan*

Abstract

This paper describes a series of studies on the Na$^+$ superionic conducting glass-ceramics with Na$_5$YSi$_4$O$_{12}$ (N5)-type structure synthesized using the composition formula of Na$_{3+3x-y}$R$_{1-x}$P$_y$Si$_{3-y}$O$_9$ for a variety of rare earth elements, R, under the appropriate composition parameters (Narpsio) [1]. The possible combinations of x and y became more limited for the crystallization of the superionic conducting phase as the ionic radius of R increased, while the Na$^+$ conduction properties were more enhanced in the glass-ceramics of larger R. The meaning of the composition formula can be signified in the thermodynamic and kinetic study of crystallization and phase transformation of metastable to stable phase in the production of N5-type glass-ceramics. It was demonstrated that the medium value of content product as [P]×[R] is important in the crystallization of N5 single phase. Conduction properties of these glass-ceramics were strongly dependent upon the crystallization conditions as well as compositions. Not only complex impedance analysis but also TEM observation confirmed that this dependence was attributed to the conduction properties of grain boundaries which were glasses condensed at triple points enclosed by grains.

The Narpsio family has great potential, and is one of the most important groups of solid electrolytes, not only because it is practically useful for advanced batteries, but also because it is a three-dimensional ionic conductor, which comprises 12-(SiO$_4$)$^{4-}$-tetrahedra membered skeleton structure, from which or by analogy with which various kinds of solid electrolyte materials can be derived. It is a solid solution in the Na$_2$O-R$_2$O$_3$-P$_2$O$_5$-SiO$_2$ system. A variety of modified Narpsios have been synthesized by replacing R with Sc, Y, In, La, Nd, Sm, Eu, Gd, Dy, Er, Yb, and/or by substituting tetra (Ti^{4+}, Ge^{4+}, Te^{4+}), tri (B^{3+}, Al^{3+}, Ga^{3+}), penta (V^{5+}), and hexa (Mo^{6+}) valent ions for P or Si [2]. The use of glass-making processing is favorable for the fabrication of various shaped electrolyte, and the microstructure of glass-ceramic electrolyte is possible to control by changing of crystallization condition.

Keywords: Glass-ceramics; Narpsio; Solid electrolyte.

Reference

[1] T. Okura, H. Monma and K. Yamashita, *J. Electroceram. (Review)*, **24**, 84-90 (2010).

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RO$_6$ octahedron

R = Sc, Y, In, La, Nd, Sm, Eu, Gd, Dy, Er, Yb

SiO$_4$ tetrahedron
RO$_6$ octahedron
（R=Rare earth）
Na（bonding）85%
Na（mobility）15%

XO$_4$ tetrahedron

X = B, Al, Ga, Ti, Ge, Te, P, V, Mo

Crystal structure of Na$_5$RSi$_4$O$_{12}$-type (R=rare earth) solid electrolyte.

Short-biography

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Prof. Dr. Toshinori Okura completed his doctorate in glass materials science at the Tokyo Metropolitan University, Tokyo, Japan, in 1990. He is serving the Kogakuin University as a professor from 2010. He joined the Massachusetts Institute of Technology, Massachusetts, USA, as a visiting scientist in 1997-1998. Prof. Okura won the scientific prizes from the Japanese Association of Inorganic Phosphate Chemistry in 2008 and the Society of Inorganic Materials, Japan in 2010, and the International Association of Advanced Materials in 2017 (IAAM medal), respectively, for his great success.

Carbon nanotube dispersed Ga$_2$O$_3$ films fabricated by molecular precursor method

Tohru Honda[1,*], Yuki Takahashi[2], Ryosuke Yoshida[1], Chihiro Mochizuki[3], Hiroki Nagai[1],

Takeyoshi Onuma[1], Tomohiro Yamaguchi[1] and Mitsunobu Sato[1]

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Abstract

UV light-emitting diodes (LEDs) have an much attention for display application [1]. For their improvement in high quantum efficiencies, development of UV transparent electrodes is a crucial issue. The materials used in UV transparent electrodes requires high bandgaps and conductivities. Transparent conductive oxide (TCO) is one of the candidates. In this case, very wide bandgap (VWBG) oxides are required for its realization. On the other hand, VWBG oxides are known as insulator. This means that these materials selection is limited in sense of conductivity. Thus, we consider the separation of roles in TCOs. In other words, conductive materials are dispersed in UV-transparent base-materials. Carbon nanotube (CNT) has a good electric conductivity and its diameter is several nanometers. This means that a transparency in CNTs depend on Rayleigh scattering and a high light transparency will be expected for CNT dispersed VWBG oxides. In this paper, the fabrication of CNT dispersed Ga$_2$O$_3$ films by molecular precursor method [2], which is one of the chemical solution methods, is reported.

Their transparent properties and conductive properties are also discussed. The Ga$_2$O$_3$ precursor solution was prepared as follows [2]. The 3.65 g (12.5 mmol) of ethylenediamine-N, N, N', N'-tetraacetic acid (EDTA) and 5.00 g (12.5 mmol) of Ga(NO$_3$)$_3 \cdot n$H$_2$O (n = 7–9) [calculated as Ga(NO$_3$)$_3 \cdot$8H$_2$O] were added to 30 mL of pure water at 80°C, and the solution was stirred for 1 hour, and then cooled to room temperature (RT). The white powder (abbreviated as Ga-edta complex) precipitated from the solution was collected on a paper filter under reduced pressure and air-dried. The precursor solution was prepared by a reaction of 1.34 g (3.55 mmol) of Ga-edta complex with 0.51 g (3.91 mmol) of dibutylamine in 10 g of ethanol. The solution was refluxed for 0.5 h, and then cooled to RT. The Ga concentration for the precursor solution was adjusted to 0.3 mmol g^{-1}. Single-wall CNT solution of ethanol solvent (CNT; 0.0583 mmol g^{-1}). The solutions were then mixed with the CNT solution. The 100 μL of solution was coated
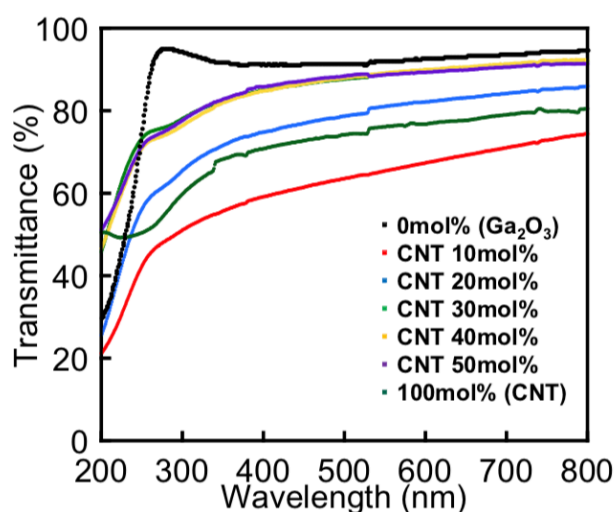

Fig.   *Transmittance spectra of CNT doped Ga$_2$O$_3$ thin films at RT.*

on quartz glass substrate by spin-coating method, and the films were dried in air at RT for 10 min and were then thermally treated using a tubular furnace in an Ar gas flow of 1.0 L min^{-1} at 600°C for 30 min. Thickness of the resultant CNT doped Ga_2O_3 films were 0.1 μm. The transparencies of the films are over 80% in UV spectral regions longer than a wavelength of 300 nm. The typical resistivity of a CNT-dispersed Ga_2O_3 film is 2 x 10^{-2} Ω·cm. The results indicate that the CNT-dispersed Ga_2O_3 film have a potential for the application of UV transparent oxides.

Keywords: UV light-emitting diodes; Molecular precursor method; CNT-dispersed Ga_2O_3

Reference

[1] T. Honda, T. Yamaguchi, N. Sakai, S. Fujioka and Y. Sugiura, Fabrication of GaN-based electroluminescent devices on Al substrates and their application to red, green and blue pixels for flat-panel displays, *Jpn. J. Appl. Phys.* **52**, 08JH12 (2013).

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Short-biography

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Biography; Prof. Tohru Honda graduated from the Interdisciplinary Graduate School of Science and Engineering, Tokyo institute of technology in 1993, and received Ph. D. in Engineering. Since 2006, he has been professor in Kogakuin University, and now dean of school of advanced engineering, Kogakuin University. He has been engaged in research in the fields of materials science and applied physics.

Functional Materials Design using Machine-Learning and Computational Chemistry

Hiromitsu Takaba[*]

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Abstract

Computational chemistry has been paid much attention in the field of materials research. On the other hand, inductive approaches such as machine-learning (ML), quantitative structure property relationship (QSPR), and chemo-informatics, have been used as a useful tool to obtain rational model could provide some relationship between materials properties and functionality from the accumulated data. Therefore a combination of computational chemistry and inductive approaches would be expected to be a powerful tool for materials design. This paper presents recent our researches regarding the application of computational chemistry integrated with deductive techniques to some functional materials, e.g. design of white light emitting diode (LED), heterogeneous catalyst, battery materials, separation materials.

Data obtained from conventional computational chemistry is limited to that related to molecular orbital and atomic energy, or dynamical properties of atoms. These data are sometimes difficult to compare directly with observable functionalities of materials. To evaluate these properties, some numerical models, which could theoretically connect observables with computed data, is required (see Fig. 1). By combining computational chemistry with inductive approaches, however, it would be possible to estimate the functionalities without the construction of any numerical models.

One of the applications of our strategy is catalyst design. In the anode of fuel cells, alloy catalyst consists of two or more kinds of metals is used. The alloy catalyst is nanometer size, and the conformation of metal atoms determine the catalytic activity. We conducted the density functional theory (DFT), Monte Carlo simulations to determine the equilibrium atomic conformation of Pt_2Ru_3 alloy nanoparticles with diameters in the range from 1.0 to 3.5 nm at finite temperature [1]. Assuming that the binding energies from DFT could be correlated with some structural descriptors, multilinear regression equations to calculate the binding energy from structural descriptors were constructed. Using the constructed regression equation, MC simulations were successfully carried out to obtain the equilibrium conformation. The conformation change under the gas atmosphere is also investigated using the similar methodology [2]. This approach is possible to discuss the degradation mechanism and optimal conformation for high efficiency.

In the development of new secondary batteries, it is essential to discover better processing or materials that would enhance
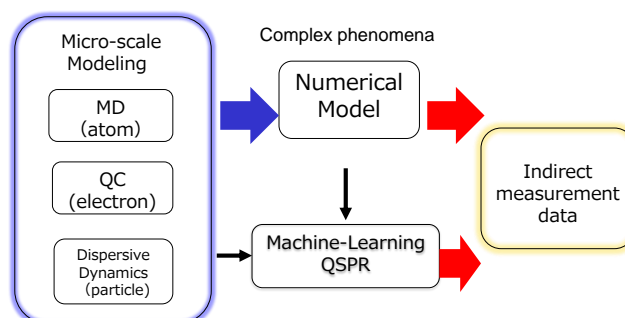

Fig. 1 Strategy of materials design using machine-learning and computational chemistry

the battery performance. The relationship between materials properties and battery performance could be obtained by comparing experimentally obtained data with the data from a numerical model, which considering electrochemical reaction and mass transfer in the cell. However, all parameters required for the numerical model those would be difficult to obtain in advance. Therefore, from the measured battery performance data, it is required to reverse infer the variables necessary for the numerical simulation. Here, we carried out machine-learning to induce the parameters necessary for a numerical model from the observable discharge capacity curve of lithium-air battery. Figure 2 shows the results of
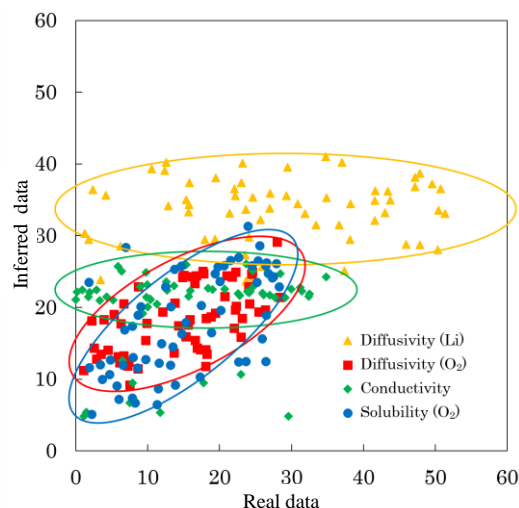
Fig. 2 Correlation of inferred values by machine-learning and the true values.

reverse estimation of several parameters by machine-learning. Except for some parameters, values close to the true value are predicted, and it is understood that reasonable accurate estimation is possible. The diffusivity of Li, however, was not predicted well. This is because this parameter has a small influence on the discharge capacity curve. The curves calculated using these parameters are almost identical. We also confirmed that it is possible to estimate multiple parameters. Estimation by machine-learning is considered to be applicable to a development where a computer instantly shows material properties from indirect measurement data.

The inductive approach with computational chemistry would be powerful tool for high efficient development of functional materials, and some other different applications will be presented.

Keywords: Catalyst; Secondary battery; Fuel cell; LED; Density functional theory

Reference

[1] Md. K. Alam, S. Saito, H. Takaba, Equilibrium atomic conformation of Pt_2Ru_3 nanoparticles under gas atmosphere of CO/H_2 investigated by density functional theory and Monte Carlo simulation, *J. Mater. Res.*, **32**, 1573-1584 (2017)

[2] Md. K. Alam, H. Takaba, Modeling of equilibrium conformation of Pt_2Ru_3 nanoparticles using the density functional theory and Monte Carlo simulations, *MRS Communications*, **8**, 562-569 (2018)

Short-biography

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Biography; His Ph.D. was completed from Tohoku University in Japan at 1998. After working in The University of Tokyo as Research Associate, and Tohoku University as Associate Professor, he becomes Professor at the current university from 2014. He has published more than 170 papers and was awarded from Japanese membrane society in 2006.

Use of Advanced Characterization Technologies for High Performance of Functional Materials

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Abstract

Full understanding of characteristics of materials' physical and chemical properties is crucial for synthesis of advanced functional materials. With better understanding, new materials with particular functionality can be achieved through engineering materials compositions, defects structure and electronic structures. We, Shimadzu, developed many types of advanced equipment to meet those needs, one of which is X-Ray Photo electron Spectroscopy (XPS) that allows elementals as well as chemical state analysis of the top few nanometer on material surface to be characterized. In this presentation, application of XPS technique will be overviewed, and particular applications for large sample analysis, LiPON electrolyte for microbatteries, and bioelectronic materials will be provided. For example, although LiPON is an old story, preparation routs will alter the electronic properties which can be monitored by XPS. Other examples will also be given.

Keywords: XPS; X-Ray Photo electron Spectroscopy; Solid electrolyte

Short-biography

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Defect Engineering of Oxygen Deficient Manganese Oxide to Achieve High Performing Aqueous Zinc Ion Battery

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Abstract: Zinc ion battery (ZIB) has recently gained significant research attention due to its use of aqueous electrolyte, high theoretical Zn capacity, high abundance, and ease of material handling.[1-2] Despite the abovementioned advantages, cathode component for ZIB is highly selective as only a handful of the materials such as manganese oxides, vanadium oxides, and Prussian blue, have been identified to demonstrate reversible Zn^{2+} storage. Among these materials, significant research interest has been focused on MnO_2. Despite the satisfactory electrochemical performances reported with the use of MnO_2, such progress has gradually decelerated due to the increasing challenge in enhancing the intrinsic MnO_2 capacity through modifying with different MnO_2 polymorphs or widening the interlayer spacing. This represent a bottleneck in enhancing Zn/MnO_2 electrochemical performance via structural enhancements, and hence alternative strategy such as modifying the material surface chemistry should be considered.
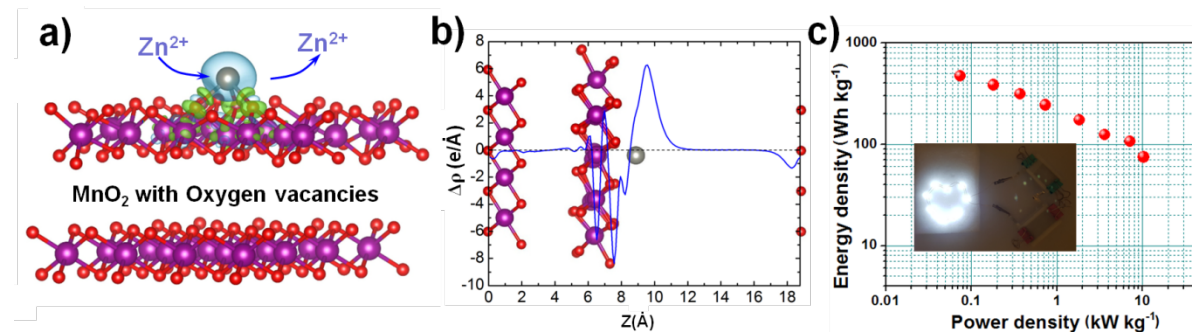
Fig. 1 a) The schematic illustration of Zn^{2+} adsorption/desorption for MnO_2 with oxygen vacancies, b) The charge transfer along z-direction between Zn and MnO_2 surfaces with oxygen vacancy, and c) the Ragone plots of Zn/oxygen deficient MnO_2.

Herein, for the first time, we propose the use of oxygen deficient σ-MnO_2 as a cathode material for ZIB. In this paper, we firstly evaluate the interaction of Zn^{2+} with both pristine and oxygen deficient MnO_2 surfaces, and secondly, we use experimental results to verify the theory derived from our simulation results. To the best of our knowledge, the as-assembled battery showed one of the highest specific capacities of 345 mAh g^{-1} ever reported for birnessite MnO_2 systems (the specific capacities of typical birnessite MnO_2 systems reported are between 250 – 280 mAh g^{-1}). The battery was also able to demonstrate excellent long-term stability of 99% over 100 cycles at low current density of 0.2

A g^{-1}, and even with high current density of 5 A g^{-1}, a respectable stability of 84% was achieved over 2000 cycles. This excellent electrochemical performance may be due to the following two factors: (1) Low Gibbs free energy of Zn^{2+} adsorption at the oxygen vacancy vicinity which results in highly accessible electrochemical active surface area; and (2) after the formation of Zn-O, more electrons are available for delocalizing into the electrode which aids in enhancing the attainable capacity. Thus, based on our collective results, generating oxygen vacancies into MnO_2 would be a feasible approach for the future development of high performance ZIB for efficient energy storage (Fig. 1).

Keywords: Zn ion battery; oxygen vacancies; MnO_2; high capacity

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[2] M. Song, H. Tan, D. Chao and H. J. Fan, Recent Advances in Zn–Ion Batteries. *Adv. Funct. Mater.* **28**, 1802564 (2018).

Short-biography

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Xiong Ting graduated from Chongqing Technology and Business University with a Master Degree in environment engineering, and her research project was to develop new photocatalysts for air purification. She is currently pursuing her Ph.D. degree in the department of Materials Science & Engineering at National University of Singapore under A/P Junmin Xue. Her research interest focuses on the design of materials for energy storage and conversion.

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Junmin Xue is a professor in Department of Materials Science and Engineering, National University of Singapore. He received his PhD degree from Shanghai Institute of Ceramics, Chinese Academy of Sciences. His current research is focused mainly on catalysis and energy storage materials.

Research and Development of Next-Generation Battery Systems: Lithium-Sulfur Batteries and All-Solid-State Batteries

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Abstract

Research and development of lithium-ion batteries (LIBs) have focused on the efficient use of energy. Application fields of LIBs are spreading from portable commercial use (mobile phone and laptop PC) to large-scale energy systems (electric vehicle and accumulator for household-use). Recently, the usages (utilities, needs, requirements and demands) of industrial-scaled electricity storage systems using LIBs are increasing for applications alongside renewable energy systems (photovoltaic and/or wind energy) and frequency regulation demands. At the same time, solutions such as safety and capacity (energy density) are beginning to be strongly anticipated. In recent years, we are conducting research on 'lithium-sulfur battery' which is a high-capacity type battery and 'all-solid-state battery' which is a high-safety type battery. In this presentation, two next-generation battery systems will be introduced including developed innovative analysis techniques.

1. Lithium-sulfur (Li-S) batteries

Li-S batteries have been investigated. Because S forms compounds with Li, and is abundant, inexpensive, and non-toxic, S is suitable as a positive active material for the Li secondary battery. The total reaction between S and Li^+ is,

$$S_8 + 16Li^+ + 16e^- \rightarrow 8Li_2S \tag{1}$$

The theoretical capacity of S is estimated to be 1,672 mAhg^{-1}, which is almost 10-fold greater than that of other transition metal compounds, such as conventional Li_xCoO_2 ($0.5 < x < 1$; 137 mAhg^{-1}), $Li_xMn_2O_4$ ($0 < x < 1$; 148 mAhg^{-1}). However, the S positive electrode (S-PE) has the following intrinsic drawbacks: volumetric expansion during Li insertion, low conductivities of S and Li_2S_x ($2 < x < 8$, intermediate), slow electrode kinetics between S and Li_2S_x, and dissolution of Li_2S_x from the S-PE into an electrolyte. The dissolved Li_2S_x diffuses to the negative electrode side and is oxidized by the redox shuttle mechanism, which leads to rapid capacity degradation and low Coulombic efficiency of the cell (Fig. 1). Mixtures of Li salts and glyme behave like ionic liquids (ILs) and are classed as 'solvate ionic liquids' (SILs). SILs show higher thermal and electrochemical stabilities in comparison with pure glyme, because the glyme molecule is strongly coordinated to Li^+ and forms the stable $[Li(glyme)]^+$ complex cation. Long-cycle-life charge-discharge of 800
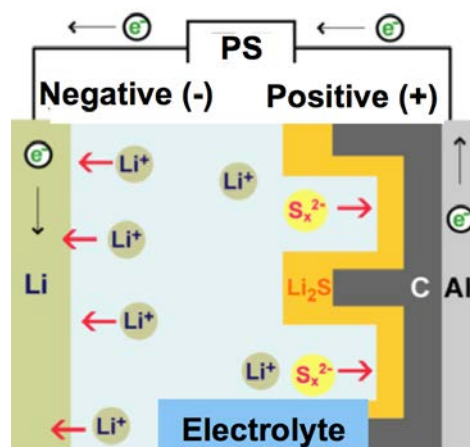

Fig. 1 Reaction mechanism of lithium-sulfur batteries.

cycles have been achieved in triglyme (CH_3-O-(C_2H_4O)$_3$-CH_3)-based SIL systems [1].

2. All-solid-state batteries

Various electrolytes (solid polymers and inorganic electrolytes) have been considered as possible safe materials for safe battery systems. The solid inorganic and polymer electrolytes mainly used in all-solid-state lithium batteries are oxide- or sulfide-based inorganic materials and poly(ethylene)oxide (PEO). In particular, the practical application of batteries under development is of top priority, and not only improved battery performance (cycle life and rate capability) but also reduced cost and a simplified fabrication process are important. Therefore, we developed 'solvent-free' 4V-class lithium-ion polymer secondary batteries with $LiNi_{1/3}Mn_{1/3}Co_{1/3}O_2$ positive electrodes (i.e. using a reduced amount of scarce Co) and graphite negative electrodes (whose handling is very easy in the manufacturing process), as shown in Figure 2 [2]. And, recently, good compatibility between inorganic / polymer hybrid electrolytes were found. In this presentation, our attempts for sufficient solid electrolyte systems will be discussed.
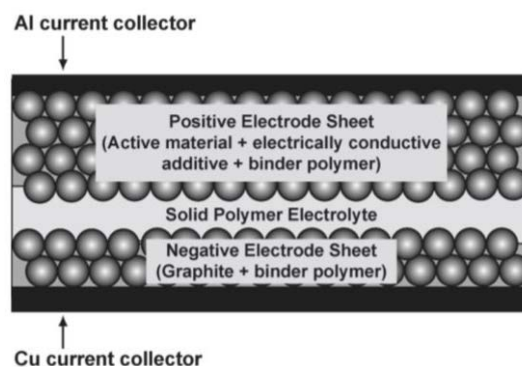
Fig. 2 Cross-sectional image of solvent-free all solid-state lithium-ion polymer secondary battery.

Keywords: Lithium-sulfur battery; All-solid-state battery; Electrolytes; Electrochemistry

References

[1] *J. Am. Chem. Soc.*, **133**, 13121 (2011). *J. Electrochem. Soc.*, **160**, A1304 (2013). *Electrochemistry*, **85**, 680 (2017).

[2] *Chem. Select*, **2**, 3848 (2017).

Short-biography

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Biography; Shiro Seki is an Associate Professor of Kogakuin University. He received Ph.D. from Yokohama National University in 2006 under the supervision of Prof. Masayoshi Watanabe. He joined Central Research Institute of Electric Power Industry as Research Scientist in 2003, and moved to Kogakuin University in 2017. His research interests include innovative batteries and their materials and analysis.

Advanced hybrid lithium-air batteries achieved by atomically iron sites anchored on N-doped carbon

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[2]National University of Singapore (Suzhou) Research Institute, Suzhou 215123, P. R. China

Abstract

Lithium-air (Li-air) batteries have attracted worldwide attention owing to the high energy densities (2-3 Wh kg^{-1}). However, conventional aprotic Li-air battery with nonaqueous organic electrolyte suffers from the decomposition of the organic electrolyte, corrosion of the lithium metal anode and serious degradation of the air cathode caused by clogs of insoluble discharge products (Li_2O_2). On the contrary, hybrid Li-air configuration as shown in Fig.1(b) consists of a lithium metal anode protected from air by a Li^+- based solid state electrolyte and an air electrode in aqueous solution can effectively avoid these problems. For the Li-O_2-H_2O system, four electrons are transferred per oxygen molecule, leading to the highest energy density of 3804 Wh kg^{-1}.[1] It is well known that one of the most challenges for hybrid Li-air battery is the poor efficiency and stability of the catalyst in cathode. Previously, noble metals, such as Pt or its alloys, had been regarded as the best efficient catalysts for oxygen reduction reaction, but it simultaneously limits the further application of Li-air batteries because of high cost and scarcity. Inspired by these issues, the key point of promoting the development of hybrid Li-air batteries is preparation of highly effective and efficient catalysts. Recently, many researches have demonstrated that single isolated atoms with maximum atom utilization efficiency, high activity and selectivity show prominent catalytic performance as ORR catalyst.[2] Based on this concept, we prepared atomic iron sites coordinated by N-doped carbon derived from covalent organic framework according to Fig. 1(a). The as-obtained catalyst further exhibited satisfied electrocatalytic performance, like lower onset potential and longer stability compared to others, as ORR catalyst (Fig. 2). The Li-air cell prepared demonstrated excellent electrochemical performance as well (Fig. 3).

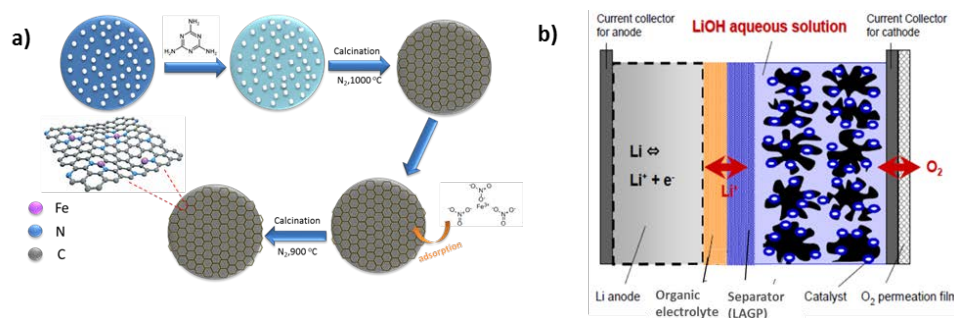**Keywords: single iron sites; oxygen reduction reaction; hybrid Li-air batteries.**

Figure 1. (a) Synthesis procedure of SAs-Fe N-doped carbon; (b) Illustration of hybrid Li-air battery.
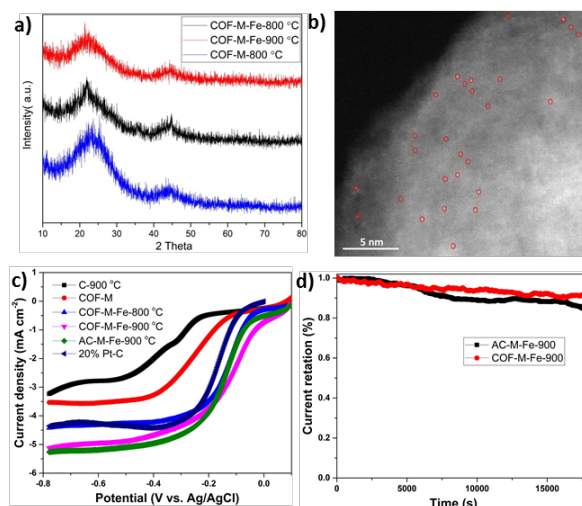
Figure 2. (a) XRD patterns of SAs-Fe N-doped carbon; (b) HAADF-STEM of SAs-Fe N-doped carbon; (c) ORR catalytic performance of as-prepared materials; (d) Stability of as-prepared materials.
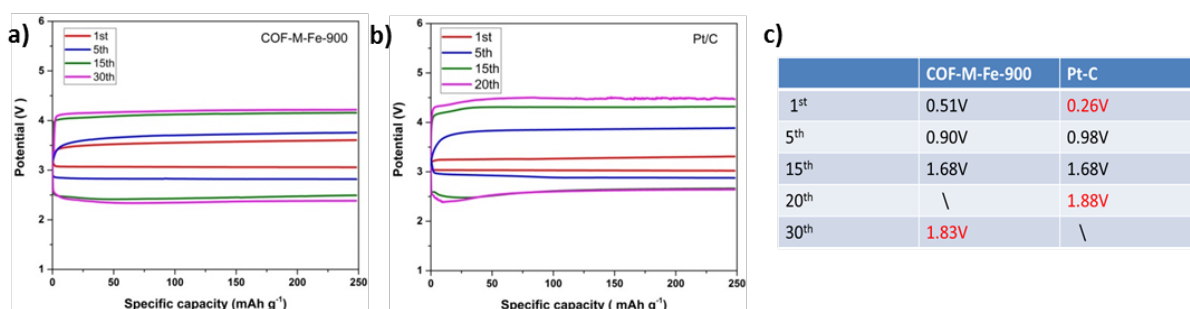

Figure 3. Hybrid Li-air batteries electrochemical performance of (a) SAs-Fe N-doped carbon; (b) 20% commercial Pt/C; (c) overpotential comparison.

Acknowledgements

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[2] Yuanjun Chen, Shufang Ji, Qing Peng, Dingsheng Wang, Yadong Li, Single-Atom Catalysts: Synthetic Strategies and Electrochemical Applications, *Joule*, **2**, 1242-1264 (2018).

Short-biography

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Biography; The second year PhD candidate, the research focus on preparation of catalysts for hybrid Li-air batteries

Dual-band Electrochromic Windows/Electrochromic Batteries

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Cambridge Centre for Advanced Research and Education in Singapore,

Abstract

About 30 to 40% of the primary energy consumption in the world are used by buildings for heating, ventilation, and air conditioning (HVAC); and lighting. It is therefore desirable to develop technologies which can reduce the building energy consumption without changing the building aesthetics. Electrochromic smart windows can contribute substantially in this regard. Electrochromism is the phenomenon of solar transmittance regulation through the windows by an externally applied electric potential. Dual-band electrochromic smart windows is the latest technology with independent control of the near-infrared (NIR) and visible (VIS) light transmittance through the windows.

Most of the dual-band electrochromic materials developed to date are nanocomposites formed by the deliberate and delicate integration of NIR-selective and VIS-modulating components which operate in different potential windows. High cost, complex synthesis of the nanocomposites, and inadequate application performance (low optical modulation, long switching time and short cycle life) are the current technical challenges in the development of dual-band electrochromic smart windows.

We discovered that WO_3 and transition metal doped-TiO_2 can be nano-engineered to serve as single-component electrochromic materials to deliver a very satisfying dual-band performance at a low cost. We will present our discovery process in this seminar and the technological developments we have introduced along the way to increase the utility of electrochromism in smart windows development.

Keywords: Smart Windows; Dual-band electrochromism; Electrochromic battery

Acknowledgements

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Energy Environ. Sci., 2018, 11, 2884

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5. Cao, S., Zhang, S., Zhang, T., Yao, Q., Lee, J. Y.*, Joule. 2018, Accepted.

Short-biography

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Biography;

Jim-Yang is Professor of the Department of Chemical and Biomolecular Engineering at the National University of Singapore (NUS); director of the Center for Energy Research & Technology (CERT), and the co-director of the Singapore Energy Center (SgEC). He is also a Senior Principal Fellow appointment at the Energy Studies Institute (ESI). He graduated from the University of Singapore with first class honors, received his Master and Ph.D degrees from the University of Michigan at Ann Arbor; and was a Postdoctoral Fellow at the University of Texas at Austin before joining NUS. He is an Associate Editor of Industrial & Engineering Chemistry Research, an Editorial Advisory Board member of Energy Technology (Wiley), and a series advisor for the Cambridge Series in Chemical Engineering. He is a Professional Engineer (Chemical) and an elected Fellow of Academy of Engineering Singapore. His research interests are materials for energy storage and conversion; membranes for water reuse; and the size and morphology controlled synthesis of nanomaterials and their self-assembly. He has been a Highly Cited Researcher since 2014.

Toward fabrication of GaInN-based devices: Epitaxial growth and characterization of GaInN by RF-MBE

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Takeyoshi Onuma[1], and Tohru Honda[1]

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Abstract

GaInN is an alloy semiconductor of InN and GaN with band gaps of about 0.7 eV and 3.4 eV, respectively. GaInN alloys have been attracting considerable attention for light emitters and light receivers covering the entire visible range. Using the light emitters and light receivers, the applications such as micro light-emitting diodes (μ-LEDs), laser lighting and optical wireless power transmission can be expected.

The growth of high-quality GaInN-based device structures including GaInN film and GaInN/GaInN quantum wells on the film have still been challenging topics, owning to the heteroepitaxial growth with a large lattice mismatch system of about 11 % between GaN and InN. The deeper understanding of the growth kinetics and mechanism of GaInN has still been required.

In this presentation, the epitaxial growth and characterization of GaInN by radio-frequency plasma-assisted molecular beam epitaxy (RF-MBE) toward the fabrication of GaInN-based devices were reported.

GaInN films were typically grown on the commercially available GaN/Al$_2$O$_3$ templates by RF-MBE. X-ray diffraction (XRD) reciprocal space mapping (RSM) measurements were used for determining the In composition x of Ga$_{1-x}$In$_x$N and relaxation ratio of Ga$_{1-x}$In$_x$N from GaN. In some cases, *in-situ* XRD RSM measurements during the growth of Ga$_{1-x}$In$_x$N were carried out at beamline 11XU of the synchrotron radiation facility Spring-8. Photoluminescence (PL) measurements were also carried out for obtaining optical properties of Ga$_{1-x}$In$_x$N films.

Figure 1 show RSMs taken after the growth for 98, 301 and 602 sec in *in-situ* RSM measurements. Figure 2 shows the evolution of relaxation ratio and In composition of GaInN, calculated from the GaInN peak position observed at RSMs. From the evolution of relaxation ratio, GaInN was found to be gradually relaxed. Now we focus on the evolution of In composition. The In composition at initial stage was lower than the value of about 55 %, which is expected from the supplied flux ratio during growth. As GaInN grew, the composition increased. Finally, the composition was reached to 55 % of In composition. This means that the In composition of GaInN at the interface region of GaInN/GaN is lower than that of the bulk GaInN region. This can be explained by compositional pulling effect under compressive strain state. Thus, *in-situ* XRD RSM measurements are the powerful technique to know the growth kinetics and mechanism of GaInN.

The correlation between XRD results and optical properties of the grown films will be also reported.
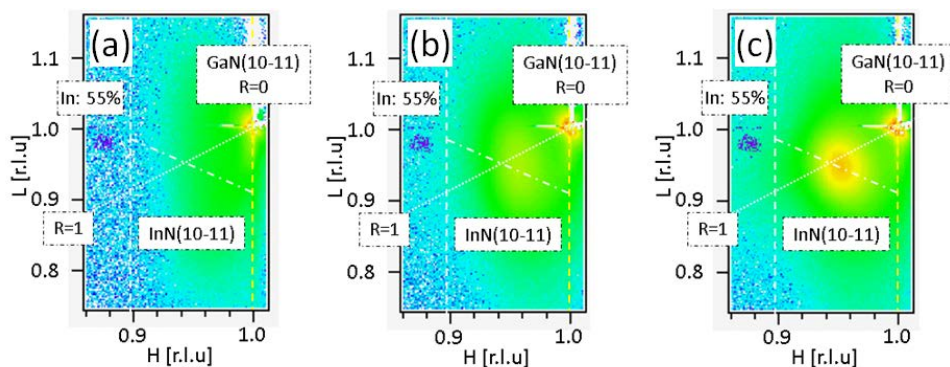
Fig. 1 RSMs taken after the growth of GaInN for (a) 98 sec., (b) 301 sec. and (c) 602 sec.
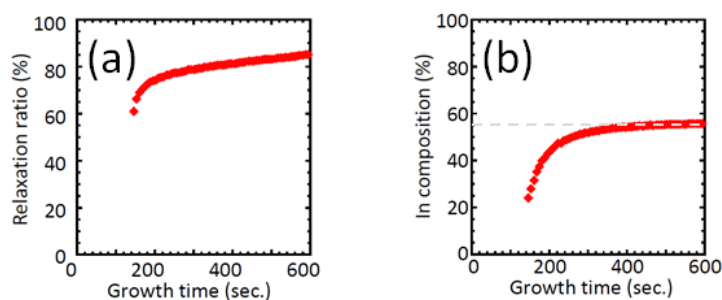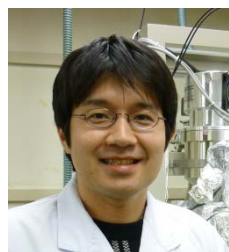

Fig. 2 Evolution of (a) relaxation ratio and (b) In composition of GaInN calculated from GaInN peak position observed at RSMs.

Keywords: GaInN; molecular beam epitaxy (MBE); epitaxial growth

Short-biography

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Biography; Tomohiro Yamaguchi received doctoral degree from Ritsumeikan University in 2003. He worked at Prof. Hommel's group in Bremen University (Germany) and at Prof. Nanishi's group in Ritsumeikan University (Japan) in 2004-2007 and 2007-2011 as a post doctor, respectively. Since 2011, he has been an associate professor at Kogakuin University in Japan. His research interests focuses on the development of crystal growth of group-III nitrides, especially InN and related alloys, by RF-MBE and group-III oxides by mist CVD. He published over 100 scientific papers and had over 10 invited talks.

Study of 2D Materials for Energy and Device Applications Using High Resolution Transmission Electron Microscopy

Ashutosh Rath, Haiwen Dai, Jiaxin Yan, Zhen Quan Cavin Ng, Daniel H.C. Chua* and Steven Pennycook

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Abstract

Two-dimensional (2D) materials have witnessed popular attention from the scientific academia as well as industry for their major potential in electrochemical and device applications. The applications of 2D materials do not only rely on their intrinsic properties but also highly depends on the tunability. Thus, fabricating these materials at their stoichiometric state and understanding their structure-property correlation is important.

In this work, we study the spectrum of highly crystalline molybdenum sulphide/oxide-based materials such as MoS_2 (2-H), MoO_2, hybrid MoS_2/MoO_2 nanostructures, reduced molybdenum oxide flakes and polycrystalline 2D finned CuS nanostructures. The samples were prepared using chemical vapour deposition (CVD) and RF Magnetron Sputtering. The as-fabricated samples were scrutinized with a repertoire of materials characterization techniques such as Raman spectroscopy, X-ray diffraction (XRD), scanning electron microscopy (SEM) and transmission electron microscopy (TEM) and X-ray Photoelectron Spectroscopy (XPS). Our results reveal that, by tuning growth parameters, different samples demonstrate unique morphologies, which can be unequivocally tied to their chemical composition. We also explore their potential application as electrochemical catalysts (in particular, hydrogen evolution reaction (HER)) and resistive RAM. Three examples will be shown.

In the case of MoS_2/MoO_2 nanostructures (Figure 1), HER testing of the samples demonstrates that crystalline MoS_2 is, in fact, negligible compared to the samples with the slight inclusion of MoO_2 impurity. The hybrid MoS_2/MoO_2 exhibited a much higher activity as compared to the MoS_2 samples. We further demonstrate that in addition to the large specific surface area exposing more active sites and using the conductive substrate to improve interlayer conductivity, chemical heterogeneity is essential to attain any substantial HER catalytic activity. The inclusion of MoO_2/MoS_2 heterogeneity works much more favorably for its promotion of the active apical S^{2-} ions and its better transport efficiency, resulting in an overall improvement of HER activity.

In the case of reduced molybdenum oxide flakes (Figure 2), we report a facile temperature-controlled synthesis of triangular MoO_2 and square Mo_4O_{11}. The triangular and square flakes showed metallic behavior with conductivity as high as ~940 S/cm and ~28 S/cm in DC measurement. The decrease in oxygen level from Mo_4O_{11} to MoO_2 affected the density of states mapped in Mo $4d$ orbitals, leading to higher conductivity for triangular MoO_2. Further Mott-Schottky analysis on MoO_{3-x} regrown on a carbon fiber paper (CFP) revealed hole mobility of $10^5 - 10^8$ cm^2 V^{-1} s^{-1}. The hole carriers at high frequencies are attributed to potential oxygen acceptors and molybdenum vacancies resulted from limited reduction power of hydrogen. [1].

In the case of 2D finned covellite (CuS) nanostructures, it exhibits ReRAM behaviour with resistances having two orders of magnitude differences between 0 to -0.5V. This unique morphology gives rise to the very low voltage of -3 V and 1 V for writing and reset respectively, with a writing time of 20ms. This memory is volatile and returns to a default state of lower resistance within 10ms. The difference in resistance is hypothesised to be caused by a phase transition between CuS (low resistance) and Cu_2S (high resistance), a result of the polycrystalline finned structure of the CuS [2].
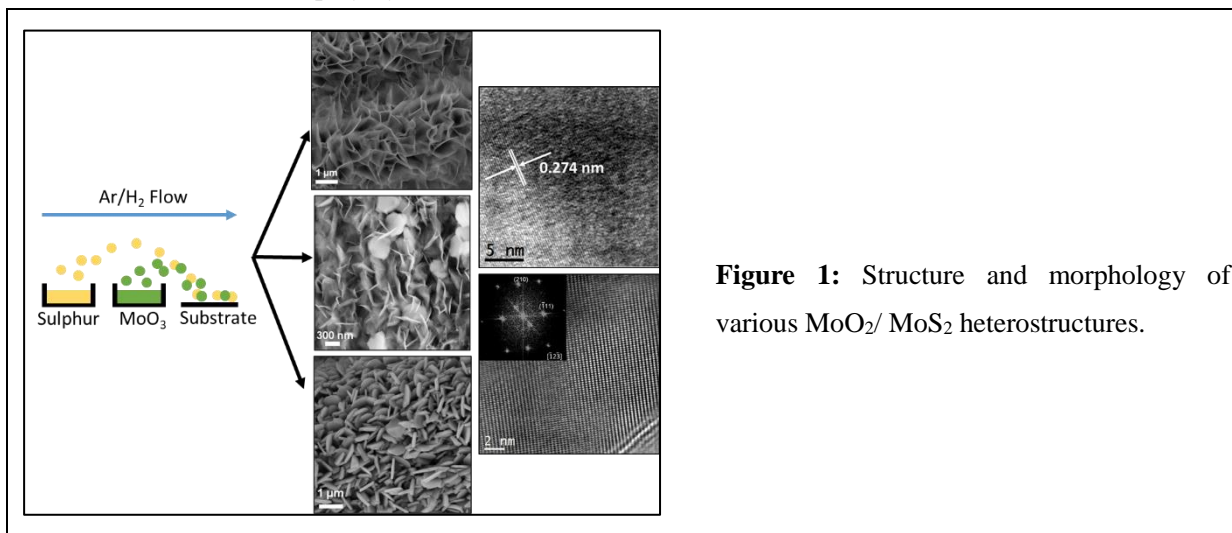

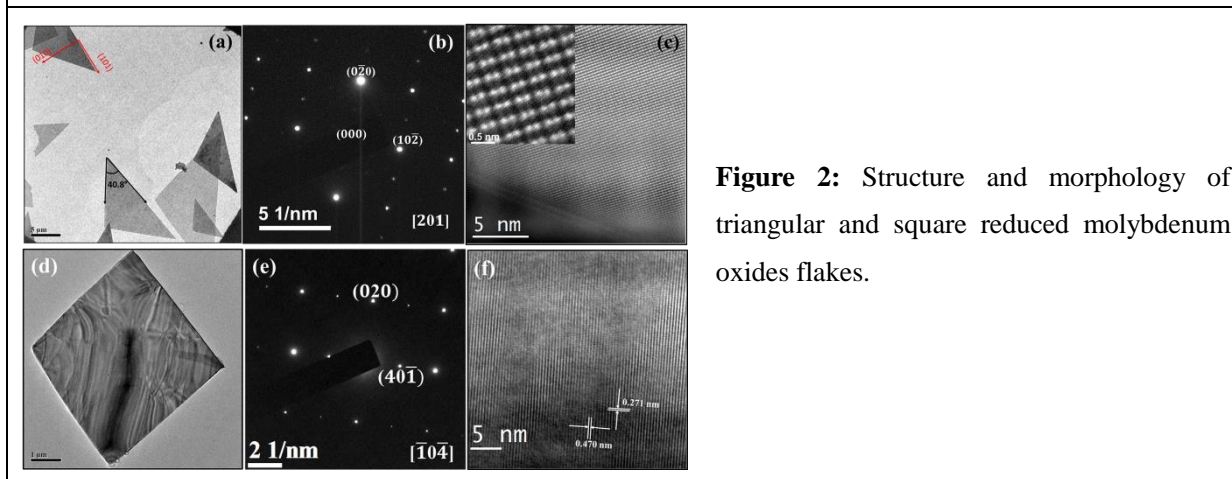**Figure 1:** Structure and morphology of various MoO_2/ MoS_2 heterostructures.

Figure 2: Structure and morphology of triangular and square reduced molybdenum oxides flakes.

Keywords: 2D Materials; HRTEM; Clean Energy

Reference

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Applications of a High Resolution Mass Imaging Microscope (FIB-TOF-SIMS)

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Abstract

Secondary ion mass spectrometry (SIMS) is one of the surface analysis techniques for visualizing the elemental distribution in microscopic view with very high sensitivity. Some species (electron, ion, neutral and so on) are emitted from a sample surface by ion beam bombardment. In the principle of SIMS, the secondary ions which are generated from micro region by scanning the primary ion beam, are detected by a mass spectrometer with pixel-by-pixel. In particular, focused ion beam time-of-flight SIMS (FIB-TOF-SIMS) was developed by Prof. Sakamoto, is a unique apparatus compared with the others[1]. Figure 1 shows the photograph and schematic image of FIB-TOF-SIMS. The Ga-FIB which was newly designed in order to obtain a very fine beam spot size, was employed as the primary ion beam. This apparatus has some features. The primary feature is very high lateral resolution about 40 nm, which is the world record. Other features are *in situ* FIB micro machining for internal structure analysis, and a sample cooling system for volatile component in biological sample and electrolyte in vacuum. In this paper, we introduce some applications (biological science, material science, environmental science) of the FIB-TOF-SIMS.

Aerosol is very fine particles suspended in atmosphere and it has a fear about the influence on both human health and climate change. It is required to identify causal substances and to understand and suppress the actual condition of emission. Aerosol has various structures depending on its origin and transport process in air. So the three dimensional imaging technique with individual particle is needed. By using other SIMS apparatus and the other surface analysis techniques, the individual particle analysis has been challenged so far, but the structure of individual particle could not be observed, because the sensitivity and/or lateral resolution of these techniques were not enough[2]. Figure 2 shows the secondary electron image of aerosol particles before and after FIB micro machining, and the secondary ion images in cross-section. This particle has a beautiful spherical shape, and magnesium and calcium existed in the interior of the particles with phase separation. This particle is called fly ash emitted from the combustion of fossil fuel, since the mineral component becomes liquid at high temperature and it is rather rapidly cooled at a rate at which both phase separation occurs and keeping spherical shape is maintained.

Keywords: SIMS; surface analysis; aerosol; biological sample; battery.

Acknowledgements

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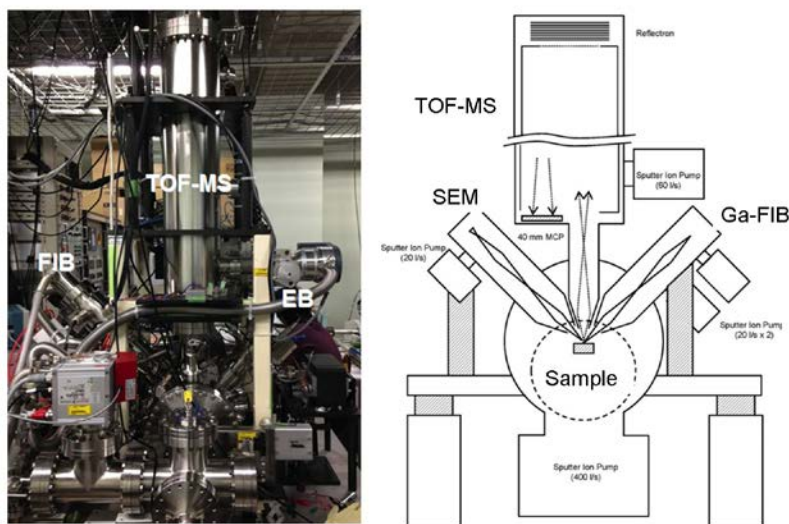
Figure 1　The photograph and schematic image of FIB-TOF-SIMS apparatus.
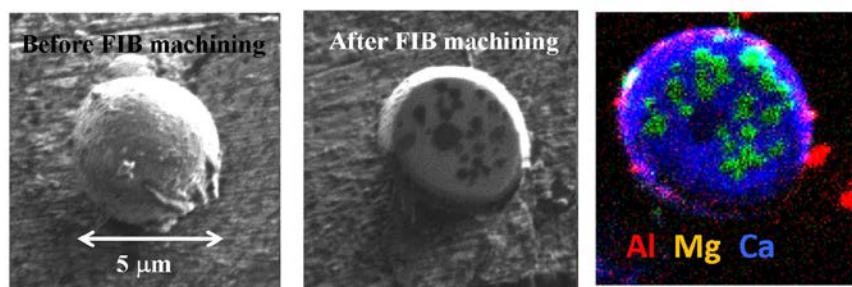

Figure 2　The secondary electron image of aerosol particles before and after FIB micro machining, and the secondary ion image in cross-section.

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Biography; I studied applied chemistry and analytical science at the University of Tokyo, and earned my Ph.D. Now I study the development and improvement of the SIMS and Atom Probe at Kogakuin University.

Embedment of Cu co-catalyst into TiO$_2$ for exceptionally active and stable photocatalysts

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Abstract

Solar to chemical energy conversion through the use of photocatalysts has been an appealing approach as one sustainable route to reduce our dependency on non-renewable fossil fuels. However, the photocatalyst performance is limited by its poor electron–hole pair separation due to fast recombination rate. Therefore, addition of co-catalyst should aid in an efficient charge separation and this can be realized via addition of a co-catalyst. These conventional techniques include deposition–precipitation, photoreduction [1], hydrothermal and vapour phase deposition [2] which typically result in surface loading effects. Moreover, the loading amount is purposely kept minimal (below 10 wt%) as excessive loading causes both aggregation and light blocking issues which constrain the performance and stability of the photocatalyst. This work demonstrates a high concentration (Cu : TiO$_2$ weight ratio > 1) of a Cu NP co-catalyst embedded into TiO$_2$ nanosheets towards interdispersion and inclusion of the Cu co-catalyst without compromising its critical dispersivity and light absorption properties. The exceptional photocatalytic H$_2$ performance of 16.1 ± 0.35 mmol g^{-1} h^{-1} stems from the embedment and confinement of the small Cu NPs within the TiO$_2$ matrix which facilitates a shorter diffusion distance, thereby increasing the number of electrons available for catalytic reactions. Thus, this work highlights a facile approach towards optimal interfacing of the hybrid catalyst constituents to mitigate the limited interfacial contact and charge transfer challenges usually faced in the design of photocatalyst.

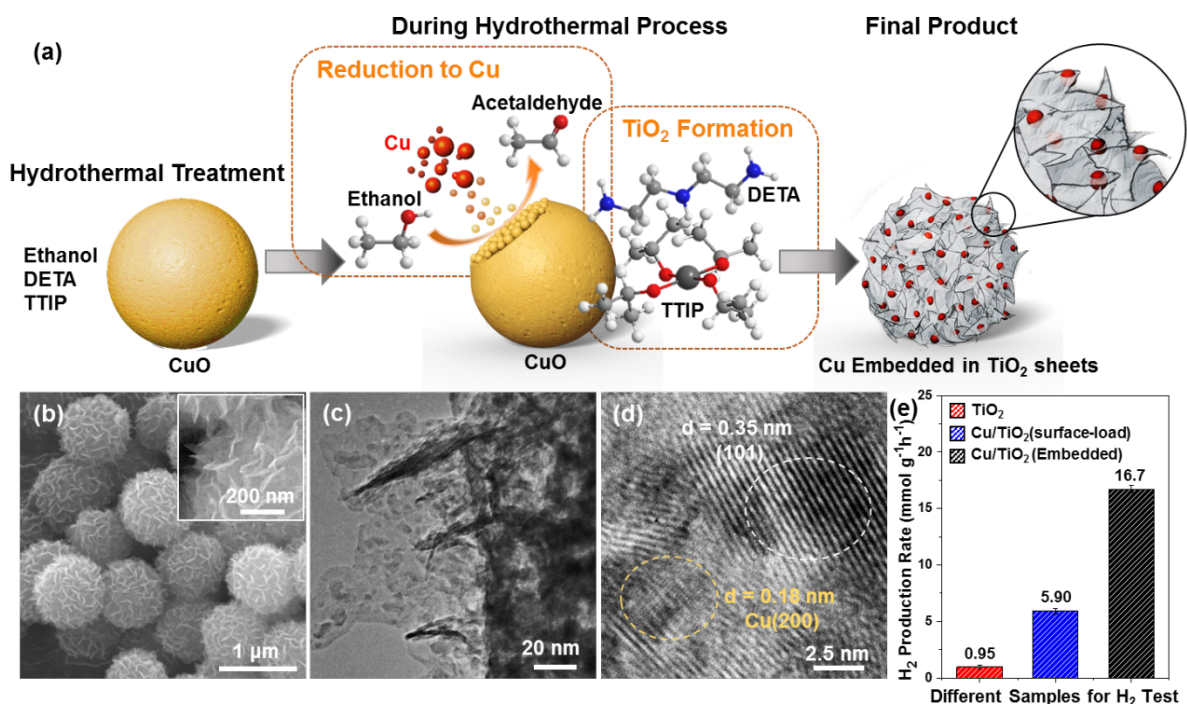**Keywords: Cu embedment; high hydrogen production rate;**

Fig. (a) Schematic diagram of the synthesis of Cu embedded TiO_2 sheets. (b, c, d) SEM images, TEM image and HRTEM image of Cu/TiO_2 (embedded) (e) H_2 production rate of TiO_2, Cu/TiO_2 (surface load) and Cu/TiO_2 (embedded).

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Short-biography

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Biography; I have received my BEng (Hons) degree in Engineering Science from National University of Singapore (NUS) in 2015. Currently studying a Ph.D in Electrical & Computer Engineering in National University of Singapore, under the supervision of A/Prof Ho Ghim Wei. My research interest focuses on the area of renewable energy resources, particularly the design of nanomaterials for photocatalytic VOCs degradation and hydrogen generation.

Fabrication and Characterization of a Layered LiCoO₂ Thin Film on a Quartz Glass Spray-coated with an Aqueous Ammonia Solution Involving Metal Acetates

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Abstract

Layered LiCoO₂ (LCO) has been extensively studied and successfully applied as a Li intercalation compound in the lithium-ion batteries (LIBs), owing to its high specific energy and structural stability that promotes extended battery cycle-ability [1]. For a successful application in thin-film LIBs, high-quality thin films of LCO have been fabricated by physical deposition techniques such as magnetron sputtering and pulsed laser deposition (PLD). However, they are associated with expensive and complicated experimental setups, requiring ultrahigh vacuum systems. Wet chemical processes such as the sol-gel method have been established as cost-effective alternatives to the abovementioned physical deposition techniques. However, the information on the deposition of layered LCO thin films on amorphous substrates, by wet chemical processes is no reports.

In the present study, we attained to fabricate and characterize a layered LCO thin film on an amorphous quartz glass substrate by heat-treating a spray-coated precursor film by using an aqueous precursor solution. The spray-coating method has recently emerged as a coating technique of choice benefiting from its relatively simple and inexpensive instrumentation set-up, reduced material losses and ability to be scaled up for mass production.

An aqueous ammonia solution S_{aq} and an ethanol-based solution S_{EtOH}, both containing LiCH₃COO and Co(CH₃COO)₂, were prepared at room temperature. The spray-coating onto a quartz glass substrate of 20×20 mm² size, which was preheated to 180°C, was separately performed using 3.00 g of newly prepared S_{aq}, with the identical spray-coating parameters used in our previous work [2]. The obtained precursor film was then heat-treated at 500°C for 0.5 h in air to obtain the film F_{spray}. Another precursor film was formed by spin-coating 100 μL of S_{EtOH} onto the F_{spray} film. The spin-coating was done at ambient temperature and pressure *via* a double-step process as follows: the first step was carried out at 500 rpm for 5 s, and the second step at 2000 rpm for 30 s. The precursor film formed on top of the F_{spray} film was then heat-treated at 500°C for 0.5 h in air to obtain the final film F_{ss}.

The X-ray diffraction patterns of the resultant films (fig. 1(a)) showed peaks assignable to the layered-structure of LiCoO₂. Raman spectroscopy measurements revealed the vibrational modes assignable to layered LiCoO₂, with minor content less than 5 mol% of spinel-type Co₃O₄ (fig. 1(b)). The Hall-effect measurements indicated that the resultant thin film of 0.21 μm thickness is a *p*-type semiconductor with

an electrical resistivity of 30(20) Ω cm, and a carrier concentration and carrier mobility of $6(4) \times 10^{16}$ cm^{-3} and $2(1)$ cm^{-2} V^{-1} s^{-1}, respectively. Thus, this is the first report to fabrication of LCO thin films on an amorphous substrate by wet chemical process.
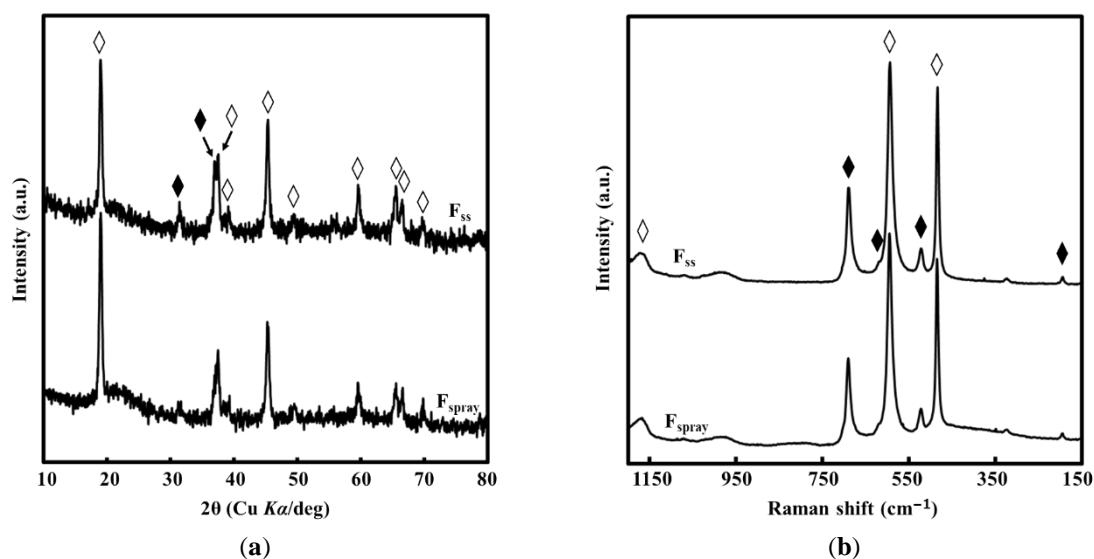

(a)   (b)

Figure 1. (a) XRD patterns of **F$_{spray}$** and **F$_{ss}$**. (b) Raman spectra of **F$_{spray}$** and **F$_{ss}$**. In both figures, the peaks assignable to the vibration modes for layered LCO and the Co_3O_4 are represented by using ◊ and ♦, respectively.

Keywords: Layered-structure LiCoO$_2$; Aqueous solution; Spray-coating.

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Short-biography

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Biography; Dr. Nagai is associate professor at the Department of Applied Physics, School of Advanced Engineering, Kogakuin University of Technology & Engineering (KUTE-Tokyo) from 2018. He has been engaged in research in the fields of materials science and nanotechnology.

Mesoporous Mo$_2$C Microflower Supported Pt Single Atoms for Efficient Oxygen Reduction

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Abstract

Oxygen reduction reaction (ORR) is an important half reaction that limits the efficiency of many energy storage devices, such as fuel cells and metal-air batteries. Platinum is by far the most efficient catalyst material for ORR, as well as for many other electrochemical reactions. However, the scarcity and high cost of Pt hinders its practical use on an industrial scale. Therefore, tremendous research efforts nowadays are devoted to boosting the mass-specific activity of Pt-based catalysts. [1, 2]

Single atom catalysts (SACs) are explored as a promising route to maximizing the specific catalytic activity and reducing the usage of precious metals. In doing so, a suitable support material is paramount in effectively anchoring and stabilizing the single atoms. [3] Molybdenum carbide Mo$_2$C is a promising support material for Pt atoms, as Mo can interact with Pt and thus has an anchoring effect for Pt. However, commercial Mo$_2$C often suffers from low surface area and dense structure, which limits its use as a host material for single atoms. [4]

Herein, a mesoporous Mo$_2$C microflower supported Pt SAC material is synthesized and demonstrated to have high mass-specific catalytic efficiency for oxygen reduction reactions (ORR). The single atomic Pt structure is confirmed by high-angle annular dark field imaging (HADDF-STEM). Catalysts with various Pt loadings are also investigated and the catalyst with an intermediate Pt loading of 2.36 wt% achieved the best ORR performance. The Mo$_2$C support material used in this work has a novel structure that enhances dispersion of the Pt atoms and contributes to the high catalytic activity.
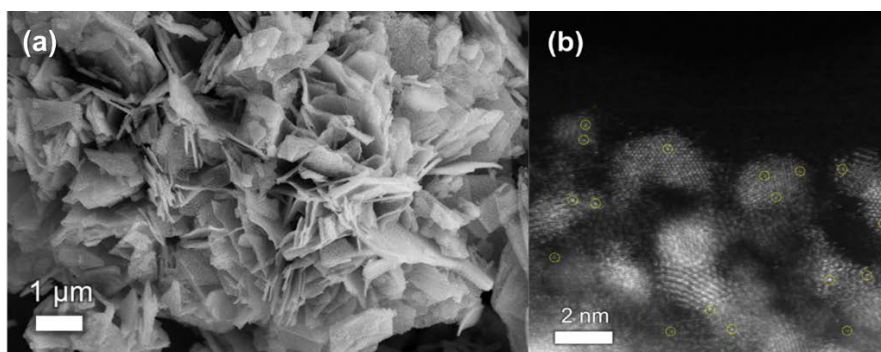
Figure 1. SEM (a) and STEM (b) of the Mo$_2$C/Pt SAC. Pt single atoms are indicated with yellow circles

Keywords: Single atom catalyst; Platinum; Molybdenum carbide; Oxygen reduction; Electrocatalysis.

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Short-biography

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Zhang Lei graduated from National University of Singapore (NUS) in 2016 with a B.Eng. (Hons.) in Materials Science and Engineering. She is currently working as a research engineer and pursuing a Ph.D. in the department of Materials Science & Engineering, NUS. Her research area includes designing and synthesizing nanomaterials for electrochemical applications and water treatment.;

2D Layered, 2D Non-layered and 2D Non-layered Holey Materials for Energy Storage and Conversion

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Abstract:

We have been exploring a large group of 2D materials for both energy storage and conversion, for the next generation technologies, such as electrical vehicles and green energy. The large group of 2D materials can be made into 2D layered, 2D non-layered and 2D non-layered holey morphologies. Their compositions can be tuned into carbon-based, metal sulfides, phosphides, nitrides, carbonitrides and nanocomposites. Both the types and population of active sites responsible for charge transfer, storage and electrocatalysis can be maximized by the approaches such as site-engineering/doping, control in the type and number of vacancies, facet manipulation, and control in pore size, pore size distribution and surface area. These 2D materials can be derived from different precursors. We have been exploring those 2D materials derived from Metal Organic Frameworks (MOFs), which can be grown into various 3D, 2D, 1D and 0D morphologies. There is great flexibility in control over varying length scales from atomic scale up to bulk structure that allows access to an almost endless variety of MOF-based and MOF-derived active materials. 2D active materials are shown to be exceptionally high performing as electrodes in supercapacitors and rechargeable batteries, where the MOF-derived nanohybrids are among the best performing materials for both electrocatalysts and electrodes. The 2D layered, 2D non-layered and 2D non-layered holey active materials can be fabricated into either free-standing forms, nano- or micro-powders, grown on conducting substrates, or assembled together with other types of active materials. In this talk, we present the latest development of these different types of 2D active materials conducted in our lab and the key understandings that have been made so far.

Biography
Professor John Wang is Professor and Head of Department of Materials Science and Engineering, National University of Singapore. He has more than 30 years of experience in education and research of functional materials and materials chemistry. His current research focuses include: energy materials and devices, 2D materials chemistry, and nanostructured materials for sustainable energy. Professor John Wang has published >400 papers in prestigious, top international refereed journals.