P-25 Enhanced Fuel Generation for Carbon-neutral Circulation and Oxygen Vacancy Formation Discovered from Electrochemical Reduction of Oxalic Acid Yu Sun¹, Sho Kitano¹, Kenichi Kato, Miho Yamauchi^{1,2}

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 AVC corresponding to the electrical potential distribution in the SE images was able to be observed when the applied voltage is less than or equal to 1 V.

Secondary electron image of the cross-sectional surface of PVK solar cell

NiO

ITO

Glass

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CoNi Nanosheets As Support for Pt electrocatalyst With Low loading For ORR



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First Principles Studies on the Activity and Stability of Catalysts for Energy Transformation

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potentials. Highly dehydrated M-complexes are the most stable ones.

intermediate species for dissolution during OER

All-Solid-State thin film battery with (104)-oriented LiCoO₂ cathode Key Words: Lithium-Ion Battery, Cathode Thin Films, Pulsed Laser Deposition All-Solid-State lithium-ion battery (LIB) is highly in-demand because of the fascinating advantages, such as, the combustible material-free constitution and better handling of Introduction stacked-cell structure which realizes high power output. Toward practical application, improvement of Li-ion conduction in a solid-state battery remains as an issue to be addressed. In order to establish All-Solid-State LIB, a better understanding of ion conduction in solid Theme materials, especially at an interface, is necessary. In this work, (104)-oriented single crystalunder like LiCoO₂ cathode film, as well as a thin film battery, are fabricated as an ideal system for Discussion investigation of Li conduction and an influence of interface in a solid-state battery. (104)-oriented LiCoO₂ film on Battery performance of a thin film battery an off-cut Nb:SrTiO₃ (001) substrate with (104)-oriented LiCoO₂ cathode Layered compound LiCoO₂ was grown by PLD on Nb:SrTiO₃ (001) Structure of All-Solid-State thin film battery substrate with a 5° off-cut toward Nb:SrTiO₃ [110] direction. with an oriented LiCoO₂ cathode layer 5° off-cut LiCoO₂ 000000 😑 Li Li metal structure Nb:SrTiO₃ (001) substrate Co Amorphous Li₃PO₄ 0 0 STO (001) [001] An orientation of LiCoO₂ is Single oriented [110] 0 determined by an orientation of LiCoO₂ 0 0 the Nb:SrTiO₃ substrate. 000000 Cathode STO [110] (a) Out-of-plane 2θ scan LiCoO₂ (104) // Nb:SrTiO₃ (001) Nb:SrTiO₃ substrate LiCoO₂ (001) // Nb:SrTiO₃ (111) ਲ<mark>ੂੰ</mark> 10⁶ 10⁴ 10⁴ Comparison of battery performance between (104)- and (001)-oriented $LiCoO_2$ cathodes 20 40 Ō 60 80 100 120 20 / degree For charge process, an identical CC-CV sequence was used, that is, (b) Pole figure of LiCoO₂ 003 (c) Cross-sectional STEM-HAADF 1 C charge to 4.2 V followed by CV charge at 4.2 V for 2 hours. image of the LiCoO₂ film For discharge curve measurement, discharge rate was changed from 0.1 C to 100 C. (104)-oriented LiCoO₂ cathode (001)-oriented LiCoO₂ cathode Charge with 1C
 Discharge 4.5 Charge with 1C
 Discharge 0.1 C 4.5 0 1 C 4.0 4.0

(104)-oriented LiCoO₂ grows on a Nb:SrTiO₃ (001) substrate [Fig. (a)]. Introducing a vicinal off-cut to the substrate surface facilitates growth of *c*-axis in the same azimuth as SrTiO₃ [110], resulting in a single crystal-like (104)-oriented LiCoO₂ film [Fig. (b) and (c)].

2 nm

Nb:SrTiO₃ [110]

Conclusion

P-29

- (104)-oriented single crystal-like LiCoO₂ film was grown by introduction of an off-cut Nb:SrTiO₃ substrate and optimization of deposition conditions.
- An All-Solid-State battery incorporating a (104)oriented LiCoO₂ cathode layer kept high capacity even at high discharge rate.
- going to be discussed.
 Using the single oriented LiCoO₂ cathode, lithium-ion conduction in solid materials and at interfaces, as well as grain boundaries, will be investigated more precisely.

• An origin of the kinks appearing in discharge curves of

a thin film battery with (104)-oriented LiCoO₂ cathode is

≥ 3.5 щ

3.0

2.5

0 20

100 C

40 60 80 100 120

Capacity / mAhg⁻¹

All Solid State Battery Specially Promoted Research Group, GREEN K. Kawashima, Y. Matsuki, Y. Tanaka, S. Miyoshi, N. Ohta, K. Mitsuishi, T. Ohnishi, T. Ohno, K. Takada E-mail:KAWASHIMA.Kazuhiro@nims.go.jp

≥ 3.5 ш

3.0

2.5

100 C

Future Plan

20

40 60

Capacity / mAhg

80

100 120

ò



Modelling of Grain Boundary Resistances Influence on the Performance of Solid State Batteries Technology Integration Unit (TIU), GREEN, National Institute for Materials Science (NIMS), Tsukuba, Ibaraki 305-0044, Japan P-31 Baber JAVED Email: JAVED.Baber@nims.go.jp





Length (µm)

Funding supported by





Acknowledgement

Thermodynamic Stability of Ternary Alloy Nanoparticles

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Cross-sectional Nanoscale Mapping of Mechanical Properties of Composite Films



Keywords : bimodal AFM, Young's modulus, composite electrode for LIB

Purpose

The packing density and porosity of the composite film and mechanical strength of each material are important parameters that influence on the cycling performance of LIBs because the volume expansion and mechanical stress may destroy the electrical connections between binders, current collectors.

Abstract

We apply bimodal AFM to $LiCoO_2$ positive and graphite negative composite electrode films before and after charge-discharge cycles in a coin cell, and demonstrate the nanoscale Young's modulus mapping of their cross-sections.

Cross-sectional SEM and EDS



(a,c) Pristine and (b,d) 100% State-of-Charge (a,b) $LiCoO_2$ and (c,d) Carbon Composite Electrode Films.

Red : Active Materials (LiCoO₂/Carbon) Yellow : Electrolyte, Binder, Conductive Additive Blue: Current Collector (Al foil/Cu foil)

Conclusions and Future Perspectives

- Cross-sectional nanoscale mapping of mechanical properties of composite electrode films for lithium ion batteries were successfully demonstrated by bimodal AFM.
- Applications of this technique for a wide variety of materials are now on-going.

Bimodal AFM in the Same Area



(a,c,e,g) Pristine and (b,d,f,h) 100% SOC (a,b,e,f) $LiCoO_2$ and (c,d,g,h) Carbon Composite Electrode Films.





R:接触面積、 k_1/Q_1 :定数、 $A_{1,free}$:振幅、 $A_{1,set}$:設定振幅 ϕ_1 :位相変化、 k_2 :定数、 Δf_2 :周波数変化、 f_2 :共振周波数 E_{tip} 、 v_{tip} :Tipのヤング率、ポアソン比 E_{sam} 、 v_{sam} :試料のヤング率、ポアソン比



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Applications of in situ x-ray techniques to various electron transfer reactions at solid/liquid interfaces

KEK PF & PF-AR

SPring-8



Key Words: in situ, solid/liquid interfaces, synchrotron radiation light sources



In order to design highly efficient and durable materials for the energy conversion devices such as fuel cells, rechargeable batteries, and photocatalysts, it is important to understand the mechanism of multielectron transfer reactions taking place at the solid/liquid interfaces.

This work is a collaboration with the Nanostructured Electrocatalyst Group.

Theme under Discussion Our research interest is the development of in situ characterization techniques for the electrochemical processes at the solid/liquid interfaces and their applications to the actual energy conversion materials. Here, we performed in situ XAFS analysis of various electrocatalysts and demonstrated in situ XPS measurements.

Theory and Experimental Set-ups

X-ray Absorption Fine Structure; XAFS



X-ray Photoelectron Spectroscopy; XPS

E_b= hv-E_{kin}- ϕ Incident X-ray: hv Conduction Band Valevce Band 2p 2s 1s

Experimental Set-ups for in situ XAFS & XPS



Conclusion

- Pt complexes act as molecular catalysts for HER without being converted into Pt metal clusters.
- The primary factor for the enhancement of the ORR rate is inhibition of Pt oxide formation by Ce³⁺ species.
- In situ XPS was successfully demonstrated.

Results

Molecular Catalysts for HER

Pt-CeO_x Nanocomposites for ORR



T. Masuda, K. Uosaki, et al., Appl. Phys. Lett. 2013, 103, 111605. Future Plan

400 800 Bias / mV 1200

- Applications of the in situ XPS for the actual energy conversion materials.
- Identification of the intermediate species of the ORR.
- In situ real time monitoring of electrochemical processes at solid/liquid interfaces.

Solid/liquid Interface Analysis Group, GREEN Takuya Masuda E-mail: MASUDA.Takuya@nims.go.jp

Development of in-house Angle-resolved Hard X-ray Photoelectron Spectroscopy



Key Words: Hard X-ray Photoelectron Spectroscopy



X-ray photoelectron spectroscopy (XPS) is a powerful tool to investigate surface compositions, oxidation states and electronic structures of materials with very high surface sensitivity. However, most battery materials are covered with various thin films such as passivation films and deposits of electrolyte, solvent residue and their decomposition products.

Theme under Discussion

XPS is combined with ion-sputtering techniques to perform depth-resolved chemical analyses of such buried interfaces. However, ion-sputtering often causes a severe damage to the surface composition and structure. Here, we developed a "non-destructive" depth analysis technique based on the laboratory-based hard x-ray photoelectron spectroscopy, socalled angle-resolved hard x-ray photoelectron spectroscopy (AR-HAXPES).

Introduction



Non-destructive depth analysis (~20 nm) can be performed by HAXPES.



MULTIPROBE, 5-axes stage (Omicron Nanotechnology) EW-4000 (VG Scienta) X-ray Source: Focused Cr Ka @5414.9 eV) (ULVAC-PHI) Scienta Omicron **Non atmospheric exposure analysis NIMS 蓄電池基盤プラットフォーム

NIMS Battery Research F



Conclusion

http://www.nims.go.jp/brp/nims/

- An angle-resolved HAXPES apparatus which allows to control the detection depth in the range of 1-50 nm was constructed.
- Its non-destructive depth analysis capability was successfully demonstrated.



Future Plan

- Applications of the in-house AR-HAXPES to a wide range of battery materials.
- Analyses of solid electrolyte interfaces on lithium negative electrodes for Li-ion batteries and oxide films on magnesium negative electrodes for Mg-ion batteries.

Solid/liquid Interface Analysis Group, GREEN Takuya Masuda E-mail: MASUDA.Takuya@nims.go.jp



In Situ Observations of Electrochemical Processes in Polymer Electrolyte Membrane Fuel Cells



Takuya Masuda and Kohei Uosaki

Research Center for Advanced Measurement and Characterization, National Institute for Materials Science (NIMS) Global Research Center for Environment and Energy based on Nanomaterials Science (GREEN), National Institute for Materials Science (NIMS) International Center for Materials Nanoarchitectonics (WPI-MANA), National Institute for Materials Science (NIMS)



T. Masuda, K. Ikeda, K. Uosaki, Langmuir, 2013, 29, 2420-2426.

Conclusions

- PFSI adsorbed on both the gold and platinum surfaces in the double layer region.
- The adsorbed amount of PFSI increased at the gold surface as the potential was made more positive in the double layer region.

T. Masuda, S. Faridah, P. Singh, H. Naohara, K. Uosaki, J. Phys. Chem. C, 2013, 117, 15704-15709.

- Not much potential dependence was observed at the platinum surface in the double layer region.
- PFSI desorbed from the both surfaces when the potential was made more positive to form the surface oxides.
- Once the oxides were reduced, PFSI re-adsorbed on the surfaces.
- The desorption of PFSI upon formation of the oxide was confirmed by surface X-ray scattering (SXS) in an MEA-like configuration.



- Although excess Li₂O remained, garnet phase was obtained a single phase.
- Impedance plots and Arrhenius plots of the pellet (1) will probably show electron conductivity.
- Blackening of pellet could be prevented by sandwiching the powder with Li₂O.
- Improvement of ion conductivity.
- Synthesis of garnet-type solid electrolyte using Li₂O less than this work.
- Fabrication of composite positive electrode using LiCoO₂ and garnet-type electrolyte by UHP.

All Solid State Battery Specially Promoted Research Team, GREEN

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P-38

In-situ TEM specimen holders for environment and energy materials Key Words: Transmission electron microscopy, in-situ observation, specimen holder Transmission electron microscopy (TEM) is one of most indispensable tools to characterize nanomaterials with atomic scale. Furthermore, recently control techniques of TEM observation environments have been highly required to understand material structures and Introduction phenomena during materials' actual uses. We can observe materials under various environments such as at high/low temperature, in gas/phases, biasing and so on. In this research, we used TEM specimen holders to control observation environments, Theme because specimen holders are independent from a microscope leading to easier development under and modification of the holders. We developed a light irradiation specimen holder system for Discussion solar cells and photocatalysts, and gas environment heating holder for catalytic materials to observe their structures and phenomena under working conditions. Light irradiation Gas environment & heating Light irradiation specimen holder system Gas environment & heating specimen holder system TEM TEM Specimen holder Control Gas tank Specimen holde Pressure gauge JEM-ARM200 F (JEOL L r control PC Controller Specin **Bi-prism** gauge P.S Mirror Connector Heater 🌡 Light selection Gas Nozzle Power CCD camera Light CCD camera supply Analysis devices source Gas Analysis devices Sample: Pt nanoparticles on multilayer graphene layers Electron holography Hologram : interference pattern between Graphene layers: Transferred CVD graphene object and reference waves Pt nanoparticles: Sputtered nanoparticles energy Ex. Nonmagnetic materials Observation conditions <code>TEM:JEM-2100</code> (LaB $_6$ gun) <code>Accel. voltage: 200 kV</code> <code>Environment: vacuum</code> (2X10 $^{-5}$ Pa) and O $_2$ (0.3 Pa) Wavefront Wavefront Temperature: 500, 700 °C Phase shift ⇔ Charge Charge Electrostatic potential HAN e etching of graphene layers Charge distribution Phase shift: $\theta(x) = C_E V_o t(x)$ C_F: constant V_o: inner potential t: thickness Sample: CaFe₂O₄/ ZnFe₂O ₄ multi-layer film Faceting nanoparticles contacted Alternately deposited by PLD technique Pt nanoparticle to graphene layer step J. Xing et al, Appl. Phys. Lett. 104 (2014) 163105. ~ 15 layers for CaFe₂O₄ and ZnFe₂O₄ Keeping crystalline nanoparticle structure Reconstructed TEM Hologram phase image Line profile of phase image Following graphene structure (rad) Specific angles arising from Phase shift of graphene crystalline structure 120°, 240° and 300° $(n, 0) \rightarrow (n, 0)$ $(n, n) \rightarrow (n, n)$ Crystallographically equivalent direction Armchair \rightarrow Armchair Zigzag \rightarrow Zigzag Position Conclusion Future Plan We developed a light irradiation specimen holder • We plan to do in-situ EELS (electron energy loss spectroscopy) analysis for characterization as well as

- system for in-situ TEM holography of solar cells and photocatalytic materials.
- We developed a gas environment heating specimen holder system for in-situ TEM observation of catalytic materials.
- We plan to apply the developed specimen holder systems to various materials.

holography and observation.

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P-40 Self-Healing Micellar Ion Gels Based on Multiple Hydrogen Bonding

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National Institute for Materials Science, Center for Green Research on Energy and Environmental Materials



Conclusion

-Room temperature self-healable ion gel electrolytes with high mechanical integrity was fabricated by exploiting multiple intermicellar hydrogen bonding and jammed micelle structure in ionic liquids.

-Unique features such as i) excellent mechanical and electrochemical properties, ii) good self-standing ability, iii) fast self-healing at room temperature, and iv) solution processability, make the ion gel a promising solid electrolyte for future applications in the field of flexible electronics.



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Relationship between incident wavelength of DR-SFG intensity and electrode potentia

OR-SFG: Information about both molecules and electronic state



0 100 200 300 400 500 Potential/ mV vs. Ag/AgCI (sat. NaCI)

DR-SFG of CO adsorbed on the Pt electrode in 0.1 M H₂SO.

Resonance to the 50, level of CO adsorbed on Pl

Conclusion

- We developed a spectroscopic method to measure and analyze the information on the electronic state of the interface, which is thought to greatly affect the activity of the electrode catalyst.
- We developed a measurement technology capable of detecting reactive intermediate species which is important for understanding electrocatalytic reaction.

Investigate the electrode surface reaction

Monitoring fuel cell reaction intermediate species by surface enhanced infrared spectroscopy (SEIRAS) +4e E9= 1.229 V

Oxygen Reduction Reaction (ORR)



In-situ spectroscopic studies of the electrode interface structure using light

Key Words: Electrocatalysis, Oxygen reduction reaction, Non-linear spectroscopy

For the purpose of constructing environment and energy materials, we created an environmental field, where the function of materials appears during the

measurements. We develop "in situ" measurement technologies to analyze in atomic and molecular level aim to elucidate the surface/interface phenomena.

Many important energy transfer processes are taking place at the solid/liquid

interface. In order to understand the interfacial phenomenon in detail by applying

interfacial spectroscopy, not only the interface structure of the adsorbed

molecules but also the electronic structure of the interface during the chemical

Introduction

Theme

under

Discussion

DR-SFG

freque

ncv tunable

Investigate the interfacial

P-42

electronic state of electrocatalysis Monitoring electronic state of electrocatalysis by using double resonance sum frequency generation spectroscopy (DR-SFG)

reaction are detected with high time resolution.

solid / liquid interface is important to understand the mechanism of electrocatalytic activity

Estimated electronic structure



The resonant potential will change with incident wavelength

Future Plan

- Established the techniques that can be measured "in situ" where electrode reactions proceed will be expected to further advance the detailed understanding of academic reaction mechanisms.
- It is now possible to provide guidelines for developing innovative catalysts for storage batteries and fuel cells.

Nanointerface laser spectroscopy group **GREEN** leader Hidenori Noguchi E-mail: NOGUCHI.Hidenori@nims.go.jp

Enhancing Catalytic Performance of Metal Honeycomb Catalysts for Hydrogen Production by Surface Alloying



Key Words: Honeycomb catalysts, Methane steam reforming, Surface allying



Developing high-performance and low-cost catalysts for hydrogen production is important for automobile and household fuel cells. Metallic honeycomb catalysts have several advantages compared with pelleted catalysts, such as, low pressure drop, fast heat and mass transport. We aim to develop Ni-based alloy honeycomb catalysts for on-site and small-scale hydrogen production system, in order to realize high-efficient and low-cost hydrogen production.

Theme under Discussion We have developed Pure Ni honeycomb catalysts for methane steam reforming (MSR) without using noble metals and porous oxide supports. In order to pursue higher performance of Ni honeycomb catalyst at low temperatures, we assemble Ni honeycomb catalysts with further higher cell density, and improve their catalytic properties for MSR by surface alloying.

Assembling & surface alloying

> High cell density honeycomb was assembled using thin Ni foil. Surface alloying was performed using impregnation method.



(a) Calcination Surface alloying by impregnation method with Ni and Re nitrates (b) Reduction H₂

• Parameters of assembled Ni				
honeycomb				
Number of turns:	6			
Surface area:	43.8 cm 1			
Volume:	0.5 cm			
Cell height:	0.4 mm			
Cell spacing:	1 mm			
Cell density:	2300 cpsi			
BET surface area:	0.02 m²/g			



Re oxides

Ni(Re)+Re

NiO

Conclusion

- Ni honeycomb catalysts with a high cell density of 2300 cpsi were assembled.
- Surface Ni-Re alloying significantly enhanced catalytic activity of the honeycomb catalysts for methane steam reforming.

Activity enhancement by surface alloying

Methane conversion of Ni honeycomb after hydrogen reduction at various temperatures





The activity significantly increased with Ni-Re surface alloying.

- The CH₄ conversion was close to the chemical reaction equilibrium even at a high space velocity of 6500 h⁻¹.
- > In situ XAFS analysis of NiRe surface alloy during hydrogen reduction



- NiRe alloy phase is formed on the surface of honeycomb after calcination and hydrogen reduction.
- Re significantly promoted the reduction of NiO to metallic Ni, enhancing the activity of honeycomb catalysts for MSR.

Future Plan

- Examine the stability of catalytic activity of the surface alloyed Ni honeycomb.
- Application of the develped honeycomb catalysts to small-scale hydrogen production system.

Hydrogen Production Materials Group, GREEN Ya Xu E-mail: XU.Ya@nims.go.jp

Hydrogen Production Materials Group



Key Words: Hydrogen, Purification, Reforming, Catalysts, Electrolysis membrane



Ya Xu

Development of Ni-based alloy and intermetallic catalysts for hydrogen production from steam reforming of methane and methanol.



Hideki Abe

R&D of phase-separated alloy catalysts for the high-throughput production of hydrogen fuels from CH_4 and CO_2 .



Chikashi Nishimura

Development of membranes based on vanadium alloys to produce highly pure hydrogen for PEFC. We try to apply our membranes for extraction of hydrogen gas from ammonia decomposed gas at 300-350°C.





Hydrogen extraction device equipped with quadruple-layered vanadium alloy membranes with the area of 64 cm³. Permeation flow of 0.56m3/hr. is achieved.

Scheme of vanadium alloy membrane to extract pure hydrogen from gas mixture.

Hybrid Membranes for Electrolysis Jedeok Kim

R&D of temperature tolerant hybrid membrane with controlled high proton conducting path for water electrolysis and fuel cells.



Water electrolysis, fuel cell works, and



Design of controlled high H⁺ conducting path

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application.

P-45 Topologically Immobilized Catalysis Centre for Lowtemperature H₂ Production from Natural Gas

阿部 英樹 研究担当 環境・エネルギー拠点水素製造材料グループ 図 Abe.hideki@nims.go.jp 技術移転 外部連携部門 連携企画室 technology-transfer@nims.go.jp



Keywords Hydrogen, Catalyst, Topology Development of high-performance, long-lifetime catalysts is highly desired to produce 研究の狙い value-added chemicals such as H₂ and CO from natural gas to meet the demands of Purpose expanding markets of unconventional natural-gas resources. A topology-tailored catalyst, *i.e.*, "rooted catalyst: Ni#Y2O3", has been successfully 研究の要点 developed to realize the desired long-term stable, highly efficient conversions of natural Points gas below the operation temperature of conventional supported catalysts.

Catalytic performance of the rooted catalyst: Ni#Y₂O₂



The current (left) and future (right) managements of the natural gas resource toward the efficient and environment-friendly production of valuable chemicals.



^{12.5} 9.3 550 °C; CH4:CO2:N2 = 10:10:5 mLmin-

16.5

0.8

The catalytic performance of the developed, rooted catalyst in comparison to the conventional supported catalysts toward the CO₂ reforming of CH₄ to produce H₂ and CO from natural gas.

7.2

26.5 34.2

Application and Future Development

- Efficient production of synthesis gas (H₂ + CO) from natural gas
- Production of valuable chemicals such as ethene and/or ethane from natural gas

Catalytic performance emerging from the nanotopology of Ni#Y₂O₂



The nano-scale topology of the rooted catalyst. a) the outlook, b,c) the cross-section and d) high-resolution images of one of the Ni#Y2O3 catalyst particles.



a) transmission electron microscope (TEM) image, b,c) in-situ TEM snapshots of supported Ni/Al2O3 catalyst after use. d) A model showing how the nano-topology can inhibit the unwanted accumulation of byproducts, CNT (carbon nanotubes).

Issues of Technology Transfer

- Needs to scale up the catalyst production (current: ~ 10 g/day)
- Needs to get incorporated in pilot plants
- > Wants to collaborate with industries toward commercialization





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Interface Computational Science Group Image: Computational Science Group Image: Science Group

Electrolyte, electrode and their interfaces play essential roles for the performance of the (electro)catalysts, the energy storage and conversion devices such as batteries & solar cells. Understanding of the microscopic properties and behaviors is a key for design of new materials systems. We have addressed these issues by using large(multi)-scale first-principles simulations as well as machine learning techniques with high-throughput computations.

Theme under Discussion

Introduction

We have developed density functional theory based molecular dynamics (DFT-MD) code for efficient sampling of the phase space and machine learning techniques for high throughput search. With these machineries, we have examined a variety of systems and issues relevant to batteries, catalysts and solar cells, and proposed meaningful insights.

DFT-MD study on battery interfaces



Conclusion

- Efficient DFT-MD code for the K computer was developed.
- Microscopic mechanisms of battery interfaces & electrolytes were revealed.

from TFSA anion

- Interfaces of solar cells & catalysts were elucidated.
- Proposed descriptors are predictive for various properties.

Development of codes and methods

Development of parallel DFT-MD sampling code "stat-CPMD"

+ Hybrid parallelization (MPI+OM	(P)
+ Parallel thermodynamic integrati	on
+ Efficient parallel sampling	
+ Efficient use of the K computer	State State

	r erformance on the re computer				
	Code name	Efficiency: MFLOPS/P EAK(%)	# nodes for the efficiency	SIMD ratio (%)	
	stat-CPMD	28.2	1536	71	
	RSDFT (Gordon-bell prize)	29.2	1024		
	Target	20%		60%	

DFT study on perovskite solar cells

Perovskite solar cells (PSC)

stable vacant

(MAPbI₃),

PbI₂-rich flat (PbI₂)_a(MAPbI₃)₇ ← + First comprehensiv

+ First comprehensive DFT study on PSC surfaces Two stable states: Stable Vacant & Pbl₂-rich flat

+ First DFT study of suggesting cation migration: Crucial for degradation



+ predictive power confirmed

a thousand scale dataset.

Materials informatics for batteries

Development of descriptors for crystalline solids



Future Plan

- Establishment of DFT electrochemistry theory for interface
- Design of new systems for batteries, solar cells, and catalysts
- Deployment of proposed descriptors towards large-scale battery material screening with multiple property criteria.

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