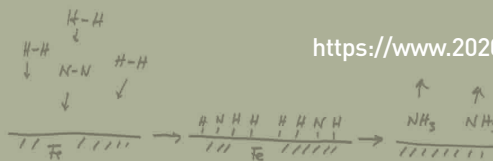


International

<https://www.2020ertlsymp.com/>



6th Ertl Symposium on Electrochemistry and Catalysis

24-27 November 2020 in Gwangju, South Korea

co-supported by GIST Ertl Center

KECS Environmental & Industrial Electrochemistry Division

Energy and
environmental
Transition in
Chemistry (ETC)

On-site and
On-line Event



Prof. Dr. Gerhard Ertl
Nobel Laureate 2007

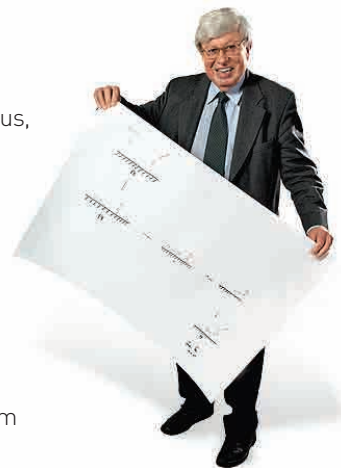
Fritz-Haber-Institut der Max-Planck-Gesellschaft Berlin, Germany
"for his studies of chemical processes on solid surfaces"

THE KOREAN
ELECTROCHEMICAL
SOCIETY



Gerhard Ertl

Born in 1936 in Bad Cannstadt, Germany. PhD in Physical Chemistry in 1965 from Technische Universität München, Germany. Prof. Emeritus, Fritz-Haber-Institut der Max-Planck-Gesellschaft, Berlin, Germany. Ertl has laid the foundation of a scientific discipline through his enormously systematic and thorough studies. He has often returned to the same problem in surface chemistry decade after decade in order to use new experimental methods to obtain answers to questions posed earlier. His ability to describe in detail how an experiment is to be designed and interpreted has helped him to provide the methodological platform for an entirely new area of research.



Agenda of the Ertl Center

The first period (2008-2010)

- Foundation of the center

The second period (2011-2014)

- Center of excellence (COE) in electrochemistry and catalysis research

The third period (2015-beyond)

- Continuous research

Role of the Ertl Center

- Bridge between basic research and industrial applications
- Encouragement of continuous research in Electrochemistry and Catalysis (Surface Science)
- Focused on international collaboration
- Promotion of "practical Learning" movement (DASAN)
- Organization of Ertl symposium



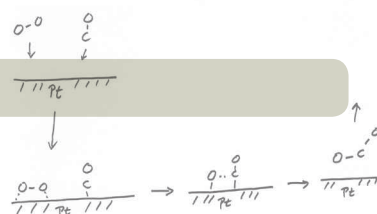
Introduction

At the beginning of the 21st century our world is facing serious problems with regards to environment, climate, energy conversion, raw materials, water and food. All these global problems are seeking scientific solutions, especially from physical chemistry and electrochemistry, and in this connection analysis and dynamics are of tremendous importance. It is expected that the 6th Ertl symposium will provide a good opportunity in these attempts, and we wish great success to all the people involved in this enterprise.

Honorary Chair

Gerhard Ertl

FHI der MPG & GIST Ertl Center



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Key Topics

- Complex Kinetics
- Computational Electrochemistry
- Effluent Treatment
- Self-Organization
- Surface and Interface Analysis
- Water Electrolysis and *vice versa*

Award Lectures (2020 Ertl Prize Winner)

Sang Hoon Kim	KIST
Olaf Magnussen	Christian-Albrechts-Universität zu Kiel

Keynote and Contributed Speakers

Malte Behrens	Christian-Albrechts-Universität zu Kiel
Andreas Friedrich	German Aerospace Center (DLR)
Zhifeng Ding	University of Western Ontario
Hiroki Habazaki	Hokkaido University
Hyung Chul Ham	Inha University
Beomgyun Jeong	KBSI
HyungKuk Ju	CSIRO & KIER
Jongsik Kim	KIST
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Jongwoo Lim	Seoul National University
Daniel Mandler	The Hebrew University of Jerusalem
Antonina L. Nazarova	University of Southern California
Naoya Nishi	Kyoto University
Joey D Ocon	UP Diliman
Jin-Soo Park	Sangmyung University
Satpal Singh Sekhon	Sangmyung University
Hyun Ook Seo	Sangmyung University
Joongpyo Shim	Kunsan National University
Yunpei Si	Kyungpook National University
Yan-Yan Song	Northeastern University
Yujin Tong	University of Duisburg-Essen & FHI der MPG
Trinh Ngoc Tuan	Electric Power University
Hamilton Varela	University of São Paulo
Min Yang	Harbin Institute of Technology
Boon Siang Jason Yeo	National University of Singapore

Abstract Submission by 15 September 2020

150-300 words with only ONE image (figure or photo or table) in WORD file

E-mail submission: ertl@gist.ac.kr

Special Issue

The symposium proceedings will be published in a special issue of **Journal of Energy Chemistry** (IF = 7.216) on Energy Transition in Chemistry. Articles will be subject to the standard peer review for an Elsevier journal. The Journal of Energy Chemistry website is active for this special issue (VSI: ETC) and contributions can be uploaded starting **15 August 2020**. The deadline for submission of manuscripts is **15 December 2020**.

Guest Editor: Jaeyoung Lee (GIST)

Conference Fee & On-line Registration

- ▶ Regular participants: 230 Euro (300,000 KRW) /
- Student participants: 150 Euro (200,000 KRW) /
- Overseas on-line participants: 0 Euro

The registration fee includes a pdf file of the book of abstracts and Tutorial Course.

Payment: in CASH or Credit Card


Conference Venue

The 6th Ertl Symposium will be held at the Ertl Center for Electrochemistry and Catalysis, GIST. The hall has state-of-the-art conference facilities and is an ideal meeting location.

GIST can be reached by bus, train, or airplane from Incheon International Airport and is well connected by plane (40 min. from Gimpo (Seoul) Airport), high-speed KTX train (90 min. from Gwangmyeong Station) and express bus (3 hrs 30 min. from Seoul, Busan and Pohang).



Program

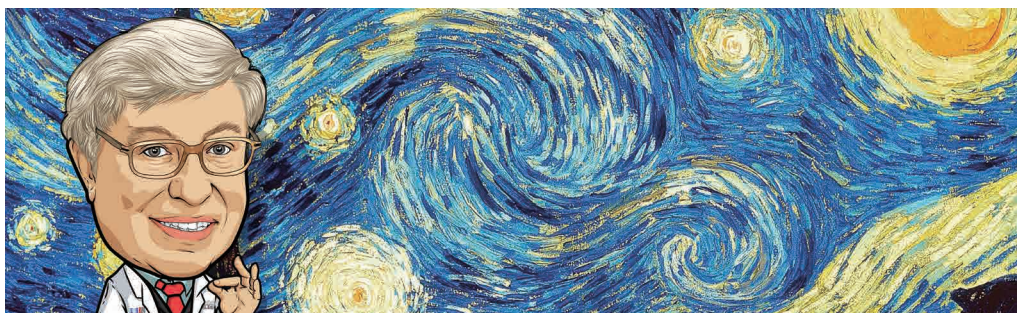
 recorded speech

Time	25 November (Wednesday)	26 November (Thursday)	27 November (Friday)
08:30 - 09:00	Registration		Planning Discussion 2022 7 th Ertl Symposium (Main Theme & Place)
09:00 - 09:15	Opening address (Jaeyoung Lee)	Award Ceremony (Hye Jin Lee)	
09:15 - 09:45	Tutorial Course Beomgyun Jeong	Keynote Speech 5 Zhifeng Ding (PM 07:15)	
09:45 - 10:15		Keynote Speech 6 Naoya Nishi (AM 09:45)	
10:15 - 10:45	Keynote (Opening) Speech 1 (24 November) Hamilton Varela (PM 10:15)	Keynote Speech 7 Hiroki Habazaki (AM 10:15)	
10:45 - 11:05	Contributed Speech 1 Youngkook Kwon	Contributed Speech 10 Antonina L. Nazarova (PM 05:45)	
11:05 - 12:00	Lunch		
12:00 - 14:45	Poster Session	Excursion	  THE Ertl Center
15:00 - 15:20	Contributed Speech 2 Joey D. Ocon (PM 02:00)	Contributed Speech 11 Min Yang (PM 02:00)	
15:20 - 15:40	Contributed Speech 3 Jin-Soo Park	Contributed Speech 12 Joongpyo Shim	
15:40 - 16:10	Keynote Speech 2 Yujin Tong (AM 07:40)	Keynote Speech 8 Yan-Yan Song (PM 02:40)	
16:10 - 16:40	Keynote Speech 3 Malte Behrens (AM 08:10)	Keynote Speech 9 Boon Siang Jason Yeo (PM 03:10)	
16:40 - 17:00	Coffee Break		
17:00 - 17:40	Award Lecture 1 Sang Hoon Kim	Award Lecture 2 Olaf Magnussen (AM 09:00)	
17:40 - 18:00	Contributed Speech 4 Jongsik Kim	Contributed Speech 13 Young Dok Kim	
18:00 - 18:20	Contributed Speech 5 Wooyul Kim	Contributed Speech 14 HyungKuk Ju	
18:20 - 18:40	Contributed Speech 6 Trinh Ngoc Tuan (PM 04:20)	Contributed Speech 15 Shrine Maria Nithya Jeghan	
18:40 - 19:30	Dinner		
19:30 - 20:00	Keynote Speech 4 Andreas Friedrich (AM 11:30)	Keynote Speech 10 Daniel Mandler (PM 12:30)	
20:00 - 20:20	Contributed Speech 7 Hyung Chul Ham	Contributed Speech 16 Jongwoo Lim	
20:20 - 20:40	Contributed Speech 8 Satpal Singh Sekhon	Contributed Speech 17 Hyun Ook Seo	
20:40 - 21:00	Contributed Speech 9 Hyung-Kyu Lim	Contributed Speech 18 Yunpei Si	
21:15 - 24:00	Poster Session (re-air)	Closing remarks	

25 November (Wednesday)

Award Lecture 40 min, Keynote Lecture 30 min, Invited Lecture 25 min, Contributed Oral 20min		
Program		Time
8:30 - 9:00	Registration	30
9:00 - 9:15	Opening address : Jaeyoung Lee	15
9:15 - 11:05	OP-01 Tutorial Course: Beomgyun Jeong (Korea Basic Science Institute, Republic of Korea) ► Ambient Pressure X-ray Photoelectron Spectroscopy for Electrode/Electrolyte Interface Characterization in Electrochemistry	60
	OP-02 Keynote: Hamilton Varela (University of São Paulo PO Box, Brazil) ► The Electrocatalytic Efficiency of the Oxidation of Small Organic Molecules under Oscillatory Regime	30
	OP-03 Contributed Oral: Youngkook Kwon (Ulsan National Institute of Science and Technology, Republic of Korea) ► Electrochemical Interface for Electrocatalytic Carbon Dioxide Conversion	20
11:05 - 12:15	Lunch	70
12:15 - 15:00	Poster Session	165
15:00 - 16:40	OP-04 Contributed Oral: Joey D. Ocon (University of the Philippines, Philippines) ► Arsenic Removal by Advanced Electrocoagulation Processes: The Role of Oxidants and Kinetic Modelling	20
	OP-05 Contributed Oral: Jin-Soo Park (Sangmyung University, Republic of Korea) ► Effect of the Type of Ionomer in Catalyst Ink on the Performance of Energy Conversion Devices	20
	OP-06 Keynote: Yujin Tong (Fritz Haber Institute of the Max Planck Society, Germany) ► Solvated Electron at the Electrochemical Interface	30
	OP-07 Keynote: Malte Behrens (University of Duisburg-Essen, Germany) ► Cryptomelane Powders Applied as OER Catalyst: The Role of Synthesis Conditions and Microstructure for the Activity	30
16:40 - 17:00	Coffee Break	20

17:00 - 18:40	<p>OP-08 Award Lecture: Sang Hoon Kim (Korea Institute of Science and Technology, Republic of Korea) ► Nanoporous Gold as a Versatile Material for Catalysis and Electrodes</p>	40
	<p>OP-09 Contributed Oral: Jongsik Kim (Korea Institute of Science and Technology, Republic of Korea) ► Investigating Catalytic Feature of Period IV Metal Sulfide Surfaces Active to Yield •OH Via Catalytic H₂O₂ Scission</p>	20
	<p>OP-10 Contributed Oral: Wooyul Kim (Sookmyung Women's University, Republic of Korea) ► Real Time Observation of Artificial Photosynthesis using Time-Resolved Infrared Spectroscopy</p>	20
	<p>OP-11 Contributed Oral: Trinh Ngoc Tuan (Electric Power University, Vietnam) ► Evaluating Status of Using, Environmental Risks of Solar Cell and Proposing Management and Recycle Methods Suitable for Vietnam</p>	20
18:40 - 19:30	Dinner	50
19:30 - 21:00	<p>OP-12 Keynote: K. Andreas Friedrich (Institute of Engineering Thermodynamics, Germany) ► Hydrogen Generation by Different Electrolysis Technologies: Status and Future Development</p>	30
	<p>OP-13 Contributed Oral: Hyung Chul Ham (Inha University, Republic of Korea) ► Electrochemical Ammonia Synthesis on the Hetero Ru-Based Atom Catalysts: A DFT Study</p>	20
	<p>OP-14 Contributed Oral: Satpal Singh Sekhon (Sangmyung University, Republic of Korea) ► Biomass-Derived Bifunctional Oxygen Electrocatalysts for ORR and OER</p>	20
	<p>OP-15 Contributed Oral: Hyung-Kyu Lim (Kangwon National University, Republic of Korea) ► Understanding Catalytic Activity in the Carbon-Based Fuel-Cell Catalysts</p>	20



26 November (Thursday)

Program		Time
8:30 - 9:00	Registration	30
9:00 - 9:15	Award Ceremony : Hye Jin Lee	15
9:15 - 11:05	OP-16 Keynote: Zhifeng Ding (The University of Western Ontario, Canada) ► Graphene Quantum Dots for Efficient and Low-Cost Light-Emitting Electrochemical Cells	30
	OP-17 Keynote: Naoya Nishi (Kyoto University, Japan) ► Base Metal Nanostructure Formation via Reductive Deposition at the Non-Aqueous Liquid/Liquid Interface between Ionic Liquid and Oil	30
	OP-18 Keynote: Hiroki Habazaki (Hokkaido University, Japan) ► Nanostructured Anodic Films on Iron: Formation Mechanism and Electrocatalytic Applications	30
	OP-19 Contributed Oral: Antonina L. Nazarova (University of Southern California, United States) ► Electrochemical Behavior and Cycloaddition Activity of Bismuth(III)-acetylides Towards Organic Azides Under Copper(I)-Catalyzed Conditions	20
11:05 - 12:15	Lunch	70
12:15 - 15:00	Excursion	165
15:00 - 16:40	OP-20 Contributed Oral: Min Yang (Harbin Institute of Technology, China) ► High Efficient Supercapacitors Electrodes Based on One Dimensional Self-ordered Molybdenum based Compound Nanotube Arrays	20
	OP-21 Contributed Oral: Joongpyo Shim (Kunsan National University, Republic of Korea) ► High Energy and Long Cycle Life Rechargeable Zn-Air Batteries using Aqueous Acidic Electrolyte	20
	OP-22 Keynote: Yan-Yan Song (Northeastern University, China) ► Incorporating Electrochromic Effect with Photothermal Conversion for the Enhancement of Pseudocapacitance via Spurring Li-ions Intercalation	30
	OP-23 Keynote: Boon Siang Jason Yeo (National University of Singapore, Singapore) ► Enhancing CO ₂ Electroreduction to Ethanol on Copper-Silver Composites by Opening an Alternative Catalytic Pathway	30
16:40 - 17:00	Coffee break	20

17:00 – 18:40	OP-24 Award Lecture: Olaf Magnussen (Kiel University, Germany) ► Atomic-scale Insights into Structural Changes at Pt Electrodes	40
	OP-25 Contributed Oral: Young Dok Kim (Sungkyunkwan University, Republic of Korea) ► Ultra-Low Loading of Iron Oxide on Bare and Pt-Loaded Al ₂ O ₃ for Enhanced Catalytic Activity	20
	OP-26 Contributed Oral: Hyung Kuk Ju (KIER, Republic of Korea) ► Green Ammonia Synthesis via Alkaline Electrolytic Process using Metal Oxide Based Nanolayers on 3-D Vertical Graphene Electrode	20
	OP-27 Contributed Oral: Shrine Maria Nithya Jeghan (Yeungnam University, Republic of Korea) ► Hierarchical Nanosheets of Cobalt Iron Layered Double Hydroxide-Nickel Selenide as an Efficient Electrocatalyst for Water Splitting	20
18:40 – 19:30	Dinner	
19:30 – 21:00	OP-28 Keynote: Daniel Mandler (The Hebrew University of Jerusalem, Israel) ► Energy Storage Systems Assembled by Electrochemical Deposition	30
	OP-29 Contributed Oral: Jongwoo Lim (Seoul National University, Republic of Korea) ► Modulating Dynamic Surface Restructuring of a Layered Transition Metal Oxide Catalyst for Water Oxidation Reaction	20
	OP-30 Contributed Oral: Hyun Ook Seo (Sangmyung University, Republic of Korea) ► Fe-Loaded Rutile TiO ₂ Particles as a Visible Light-Responsive Photocatalysts: Annealing Temperature Dependency	20
	OP-31 Contributed Oral: Yunpei Si (Kyungpook National University, Republic of Korea) ► Electrochemical Sensor for Small Metabolites Analyses in Human Biofluids	20
	Closing remarks	

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List of Oral Presentations (25 Nov.)

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OP-02 (Keynote)	Hamilton Varela	The Electrocatalytic Efficiency of the Oxidation of Small Organic Molecules under Oscillatory Regime	2
OP-03 (Contributed)	Youngkook Kwon	Electrochemical Interface for Electrocatalytic Carbon Dioxide Conversion	3
OP-04 (Contributed)	Joey D. Ocon	Arsenic Removal by Advanced Electrocoagulation Processes: The Role of Oxidants and Kinetic Modelling	4
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OP-07 (Keynote)	Malte Behrens	Cryptomelane Powders Applied as OER Catalyst: The Role of Synthesis Conditions and Microstructure for the Activity	7
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OP-23 (Keynote)	Boon Siang Yeo	Enhancing CO ₂ Electroreduction to Ethanol on Copper-Silver Composites by Opening an Alternative Catalytic Pathway	23
OP-24 (Award)	O.M. Magnussen	Atomic-scale Insights into Structural Changes at Pt Electrodes	24
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OP-30 (Contributed)	Hyun Ook Seo	Fe-Loaded Rutile TiO ₂ Particles as a Visible Light-Responsive Photocatalysts: Annealing Temperature Dependency	30
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6th Ertl Symposium on
Electrochemistry and Catalysis

Oral Session



Ambient Pressure X-ray Photoelectron Spectroscopy for Electrode/Electrolyte Interface Characterization in Electrochemistry

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In electrochemistry, the electrode surface undergoes various chemical transitions that are represented in a characteristic hysteresis pattern in cyclic voltammetry (Figure 1). Thermodynamics and ex situ spectroscopic analyses have explained the change of surface state before and after an electrochemical reaction. However, this approach cannot answer questions on the identity of catalytic sites in the electrochemical reaction. Direct spectroscopic observation in reaction (in situ) or in simultaneous performance evaluation (operando) is required for more exact information on surface oxidation state in reaction.

XPS is a very useful tool for identifying the oxidation state of the surface, but it could not be operated with an aqueous solution due to the requirement of an ultrahigh vacuum environment. Recently, a near ambient pressure XPS (APXPS) that is operated at pressures over 25 mbar has been developed where water can exist in the liquid phase at room temperature. Combining ingenious methods of sample configuration, it becomes possible to probe the electrode/electrolyte interface in an electrochemical reaction. It is expected that APXPS will be a way for identifying catalytic sites for electrochemical reaction and actual surface chemistry corresponding to a peak in voltammetry.

In this tutorial, the following topics will be covered: working principle and basic capabilities of APXPS, experiment platforms for probing electrode/electrolyte interface with APXPS, recent studies with electrochemical APXPS instruments, the prospect of APXPS for electrochemistry, and anticipated scientific achievements.

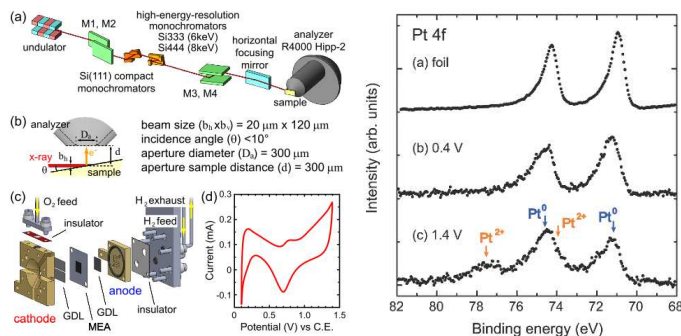


Figure (Left) Synchrotron-based AP-HAXPES setup for studying the membrane/electrode assembly in a fuel cell^[1]. (Right) AP-HAXPES results of platinum electrocatalyst at different potentials^[2].

References

- [1] Y. Takagi, H. Wang, Y. Uemura, E. Ikenaga, O. Sekizawa, T. Uruga, H. Ohashi, Y. Senba, H. Yumoto, H. Yamazaki, S. Goto, M. Tada, Y. Iwasawa, T. Yokoyama, *Applied Physics Letters* **2014**, *105*, 131602
- [2] Y. Takagi, H. Wang, Y. Uemura, T. Nakamura, L. Yu, O. Sekizawa, T. Uruga, M. Tada, G. Samjeské, Y. Iwasawa, T. Yokoyama, *Phys. Chem. Chem. Phys.* **2017**, *19*, 6013

The Electrocatalytic Efficiency of the Oxidation of Small Organic Molecules under Oscillatory Regime

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Many hydrogen-carriers (viz. ammonia, borohydride, formaldehyde, formic acid, methanol, ethanol, and glycerol) have been considered for the direct use in fuel cells and also in the electrochemical reform, where they are oxidized instead of water at lower potentials. We have investigated the electro-oxidation of formaldehyde, formic acid, methanol, and ethanol^[1], and of ethylene glycol, glycerol, and glucose^[2] on polycrystalline platinum in acidic media, and compare the activity under conventional and oscillatory regimes. The comparison is carried out by different means and generalized by the use of simple identical experimental conditions in all cases. In these curves, the activity, as inferred by the peak current, decreases in the following sequence: formaldehyde ~ formic acid > methanol > ethanol ~ ethylene glycol > glucose > glycerol. The ubiquitous occurrence of potential oscillations is associated with excursions of the electrode potentials to lower values, which noticeably decreases the overpotential of the anodic reaction, when compared to that in the absence of oscillations. The figure below illustrates typical results. Considerable enhancement in the power density was observed in an idealized fuel cell operated with those fuels when operated under oscillatory regime. Furthermore, the spontaneous self-cleaning processes, present important advantages to the use of autonomous oscillations to reach both higher and long-term activities. Results are discussed in connection with those obtained in direct liquid fuel cells^[3].

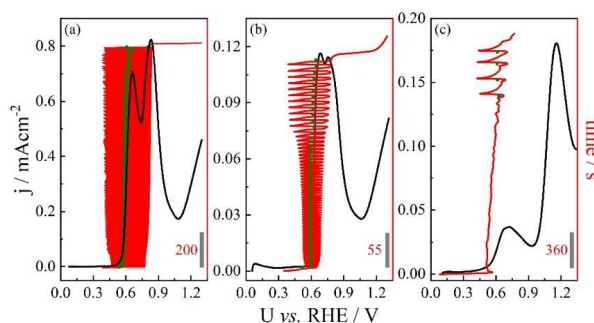


Figure Slow potentiodynamic sweeps (black lines, 0.002 V s⁻¹) for the platinum electrode in 0.5 mol L⁻¹ of (a) ethylene glycol, (b) glycerol, and (c) glucose, in 0.5 mol L⁻¹ H₂SO₄ aqueous solution. Galvanostatic curves (red lines) obtained at (a) 0.70, (b) 0.10, and (c) 0.01 mA cm⁻². The mean potential at each cycle is given in green. T = 25 °C.

References

- [1] M. V. F. Delmonde, L. F. Sallum, N. Perini, E. R. Gonzalez, R. Schlögl, H. Varela, *J. Phys. Chem. C* **2016**, *120*, 22365
- [2] G. B. Melle, T. Altair, R. Romano, H. Varela, **2020**, *in preparation*
- [3] J.A. Nogueira, H. Varela, *submitted 2020*

Electrochemical Interface for Electrocatalytic Carbon Dioxide Conversion

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The efficient electrochemical conversion of CO₂ to fuels or stock chemicals with high-energy density would be a major step forward in the introduction of a carbon neutral energy cycle. Especially, understanding the role of electrocatalysts, supports, and electrolytes that can efficiently reduce CO₂ to fuels with high selectivity is a subject of significant interest.

One of the achievements in electrochemical CO₂ reduction is the clarification of the catalysts toward two-electron involved products such as CO and formate. For instance, CO is selectively generated on Au, Ag, and single-atom catalysts and formate has been selective on Hg, Pb, Sn or alloy catalysts. Interestingly, from our recent work, CO/formate ratio can be selectively controlled on formate selective catalyst by tuning the interfacial electric field.^[1] On copper catalyst, the selection of alkali cations has direct influence on activity and product selectivity; increasing the size of mono-valent cations can increase the activity and selectivity toward C-C coupled products by modulating the interaction energy between adsorbates and electric fields at the interface.^[2] In addition, copper catalyst with a specific atomic-scale gap accelerates the reaction kinetics and selectivity to C₂₊ products as illustrated in Figure 1.^[3] Therefore, understanding the roles of catalyst, support and electrolyte offers the design of efficient, yet cheap electrochemical CO₂ reduction systems.

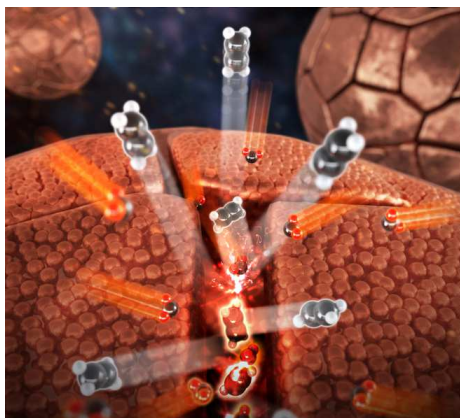


Figure Electrochemical CO₂ reduction in atomic-scale gap controlled copper catalyst.

References

- [1] Y. Kwon et al., *ACS Sustain. Chem. Eng.* **2020**, 8, 2117.
- [2] Y. Kwon et al., *J. Am. Chem. Soc.* **2016**, 138, 13006.
- [3] Y. Kwon et al., *Adv. Energy Mater.* **2020**, 1903423.

Arsenic Removal by Advanced Electrocoagulation Processes: The Role of Oxidants and Kinetic Modelling^[2]

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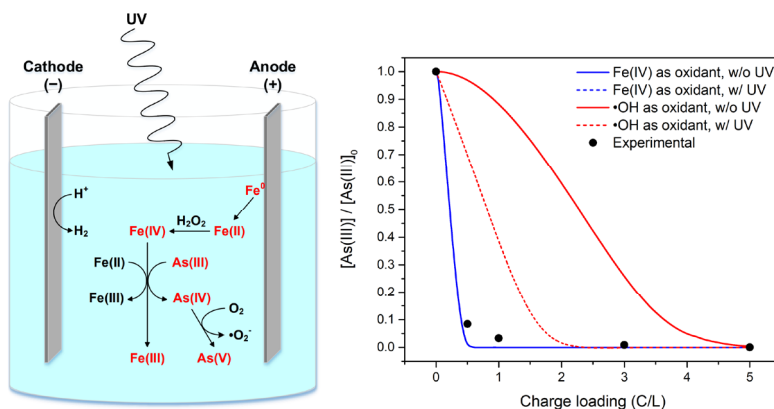
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Arsenic (As) is a naturally occurring element in the environment that poses significant risks to human health^[1]. Several treatment technologies have been successfully used in the treatment of As-contaminated waters. However, limited literature has explored advanced electrocoagulation (EC) processes for As removal. The present study evaluates the As removal performance of electrocoagulation, electrochemical peroxidation (ECP), and photo-assisted electrochemical peroxidation (PECP) technologies at circumneutral pH using electroactive iron electrodes^[2]. The influence of As speciation and the role of oxidants in As removal were investigated. We have identified the ECP process to be a promising alternative for the conventional EC with around 4-fold increase in arsenic removal capacity at a competitive cost of 0.0060 \$/m³. Results also indicated that the rate of As(III) oxidation at the outset of electrochemical treatment dictates the extent of As removal. Both ECP and PECP processes reached greater than 96% As(III) conversion at 1 C/L and achieved 86% and 96% As removal at 5 C/L, respectively. Finally, the mechanism of As(III) oxidation was evaluated, and results showed that Fe(IV) is the intermediate oxidant generated in advanced EC processes, and the contribution of •OH brought by UV irradiation is insignificant.



References

- [1] K. L. B. Solis, R. Q. Macasieb, R. C. Parangat Jr., A. C. Resurreccion, J. D. Ocon, *Water* **2020**, *In press*.
- [2] M. F. Montefalcon, M. Chiong, A. C. Resurreccion, S. Garcia-Segura, J. D. Ocon, *Catalysts* **2020**, *In press*.

Effect of the Type of Ionomer in Catalyst Ink on the Performance of Energy Conversion Devices

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Hydrogen is considered the best meaning of the store energy coming from renewable and intermittent power sources. Water electrolysis provides a sustainable solution for the production of hydrogen, and it is well suited to couple with energy sources such as renewable energy likes solar, wind and so on. In the past, little research has been done on the water electrolysis because to low demand. However, increasing desire for new and renewable energy has rekindled the interest on water electrolysis. Water electrolysis is promising electrochemical energy conversion devices. The membrane-electrode assembly (MEA), which is a component of the water electrolysis, is one of the most important factors as an electrochemical reaction site. Component of MEA is electrolyte membrane and two electrodes. Among them, cathode electrode is important to performance of hydrogen production in high current density. Main components of cathode electrode inks are Pt/C, ionomer dispersions and organic solvents. Ionomer binder dispersion is important factor of forming electrode structure. In this study, the effects of ionomer solutions on the electrode and the performance of electrochemical reactions were investigated. This was done through characterization of the ionomer film and electrochemical evaluation of the membrane-electrode assembly.

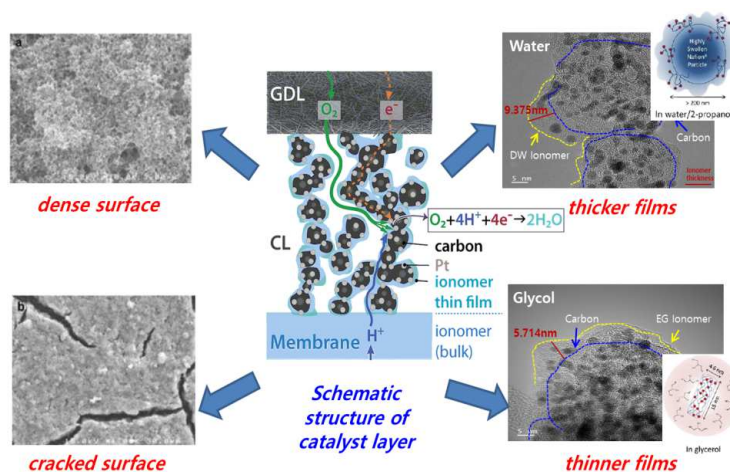


Figure Schematic diagram of showing the surfaces (left top and bottom) and micro-structures (right top and bottom) of catalyst layers with respect to ionomer binders.

Acknowledgements

This research work was supported in part by the Hydrogen Energy Innovation Technology Development Program of the National Research Foundation of Korea (NRF) funded by the Ministry of Science, ICT, & Future Planning (2019M3E6A1063677) and in part by the Technology Development Program to Solve Climate Changes of the National Research Foundation (NRF) funded by the Ministry of Science, ICT & Future Planning (NRF-2018M1A2A2063866).

Solvated Electron at the Electrochemical Interface^[1]

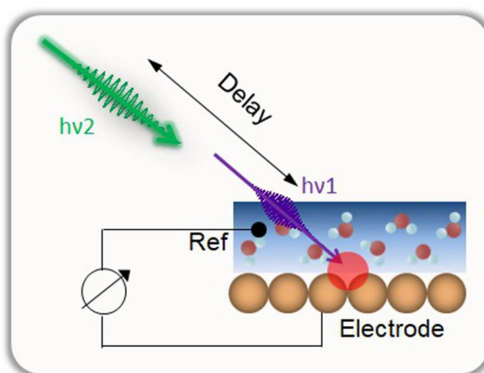
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The hydrated electron has fundamental and practical significance in radiation and radical chemistry, catalysis and radiobiology. While its bulk properties have been extensively studied, its behavior at electrochemical interfaces is still unclear due to the lack of effective tools to characterize this short-lived species at the condensed matter interfaces. To solve this problem, our group developed a new technology based on ultrashort laser and electrochemical detection (two-photon pump electrochemical probe technique). As shown in the scheme, here we introduce ultra-short pulse lasers in the traditional electrochemical detection system. One of the lasers is used to excite charge transfer or dipole inversion, and the other laser is used to track the relaxation of the excited state that was triggered by the first laser, while detecting photocurrent or photovoltage in both processes. By adjusting the photon energy of two pulsed lasers and their time difference, we can both obtain the spectral information of the surface species and track ultrafast dynamic processes. In this report, I will use the example of the solvation process of hot electrons at the gold/water interface to show you how this new technique works. This technology will play an important role in the tracking and analysis of various processes in electrochemistry.



References

- [1] F. Lapointe, M. Wolf, R. K. Campen, Y. Tong, *ChemRxiv. Preprint*, <https://doi.org/10.26434/chemrxiv.11739819.v1>

Cryptomelane Powders Applied as OER Catalyst: The Role of Synthesis Conditions and Microstructure for the Activity

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Cryptomelane ($(\text{K})\text{MnO}_2$) powders were synthesized by different methods with the same bulk crystal structure (Figure 1a) and chemical composition, but different microstructure (surface area, crystallite size, particle morphology etc.)^[1]. Their performance in the oxygen evolution reaction (OER) covered a wide range and with different trends for electrocatalysis in alkaline electrolyte and chemical water oxidation using Ce^{4+} .

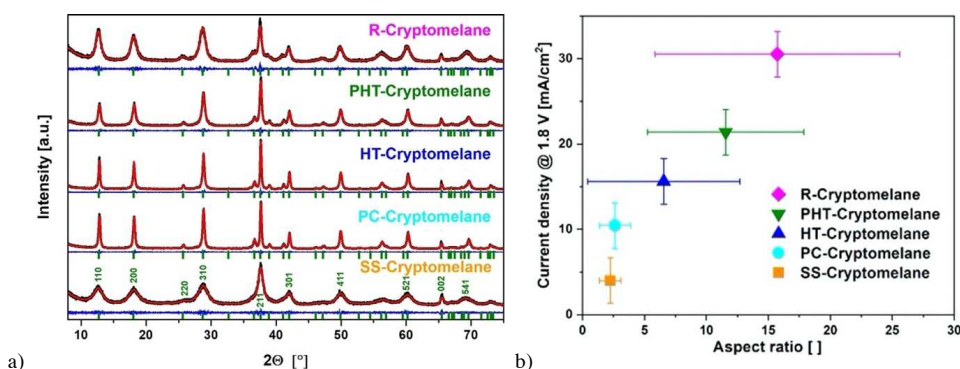


Figure a) Rietveld refinements of the PXRD patterns of the different cryptomelane catalysts, and **b)** correlation between the OER activity and the aspect ratio of the particles.

The decisive factors that explain this difference were identified in the catalysts' microstructure. Chemical water oxidation activity is substantially governed by the exposed surface area, while the electrocatalytic activity is determined largely by the electric conductivity, which was found to correlate with the particle morphology in terms of needle length and aspect ratio in this sample series (Figure 1b). Structure-sensitivity is discussed as an alternative explanation for the observed behavior and the transfer of these results to other transition metal oxide catalysts will be discussed in our contribution.

References

- [1] J. Heese-Gärtlein, D. M. Morales, A. Rabe, T. Bredow, W. Schuhmann, M. Behrens, *Chem. Eur. J.* **2020**, *26*, 12256.

Nanoporous Gold as a Versatile Material for Catalysis and Electrodes

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Nanoporous gold (NPG) is gold based sponge-like reticulate structures with nanometer sized pores in the entire body. For the last two decades, there have been extensive research interests for NPG due to their high surface area, high number of active sites, high conductivity, easy modification, tuneable porosity, and good bio-compatibility. Application fields of NPG are mainly electrochemistry based and they are from catalysis, sensor, energy materials to bio-related applications. In this presentation, our research activities on NPG for catalysis, sensors and energy applications will be discussed such as detection of organic molecules in water, catalyst for hydrogen oxidation, and energy applications for supercapacitors and fuel cells.

In the latter part of the presentation, I will discuss not only the applications, but also the advance on the preparation methods of NPG realized in our lab on rigid substrates such as silicon wafers and glasses and our recent realization of NPG films on flexible substrates.

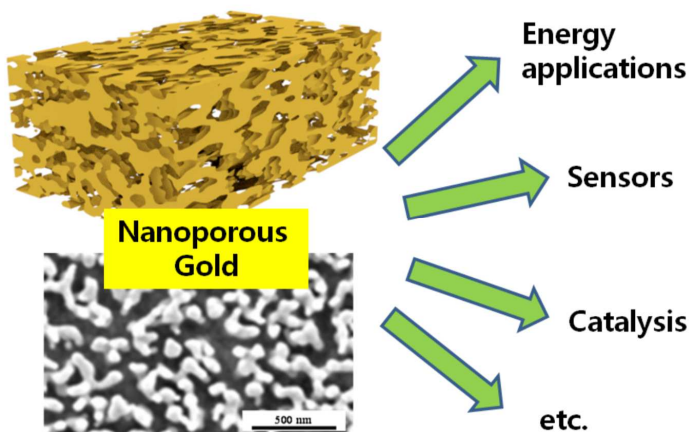


Figure Schematic and various application field for nanoporous gold.

Keywords: Nanoporous Gold, Supercapacitors, Fuel Cells



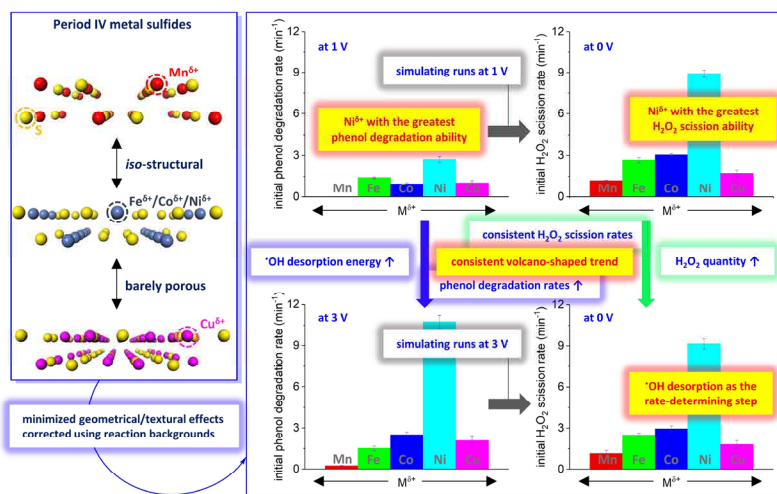
Investigating Catalytic Feature of Period IV Metal Sulfide Surfaces Active to Yield $\cdot\text{OH}$ Via Catalytic H_2O_2 Scission

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S-modified surface $\text{Fe}^{\delta+}$ ($\delta \leq 2$) species found in S-doped Fe_2O_3 and FeS_2 are recently sought after due to their outstanding catalytic nature to cleave H_2O_2 , leading to the production of $\cdot\text{OH}$ utilized to oxidatively decompose refractory contaminants. We pioneered the use of complimentary phases such as Fe_3S_4 and Fe_7S_8 to outperform FeS_2 because of their incorporation of $\text{Fe}^{\delta+}$ vacancies open to H_2O_2 , yet, found their limitation in recycling H_2O_2 cleavage due to the substantial leaching of $\text{Fe}^{\delta+}$ species^[1]. Our goal, therefore, is to locate S-modified metal ($\text{M}^{\delta+}$) species 1) to better catalyze H_2O_2 fragmentation and 2) to be of greater tolerance against the leaching of $\text{M}^{\delta+}$ species than $\text{Fe}^{\delta+}$ counterparts.^[2] We envision to synthesize metal sulfides (MS) using cheap, ubiquitous metals belonging to the same period in the periodic table (Mn, Fe, Co, Ni, and Cu) and to understand the catalytic nature of $\text{M}^{\delta+}$ species in terms of their Lewis acidic strengths and their surface H_2O_2 scission dynamics.^[2] Noteworthy, this type of fundamental kinetic study has been rarely attempted in the (electro-) Fenton or environmental catalysis community, to the best of our knowledge. In this presentation, we highlight or showcase ‘periodic trend’ and ‘rate-determining step’ for S-modified metals of metal sulfides in cleaving H_2O_2 , both of which are elucidated by a series of characterization and control experiments^[2].



References

- [1] Y. J. Choe, J. Y. Byun, S. H. Kim, J. Kim, *Applied Catalysis B* **2018**, 233, 272-280.
- [2] J. Kim, Y. J. Choe, S. H. Kim, S.-C. Lee, S. Bhattacharjee, *Applied Catalysis B* **2019**, 253, 60-68.

Real Time Observation of Artificial Photosynthesis using Time-Resolved Infrared Spectroscopy

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Direct observation of key intermediates on the catalyst surface is one of the biggest challenges in various photo/electro-catalysis including CO₂ reduction reaction O₂ reduction reaction, etc. For a rational understanding of the reaction mechanism, combined studies encompassing complementary tools such as electrochemical characterization, computational calculations and operando spectroscopies should be conducted. Among various operando spectroscopies, the time-resolved attenuated total reflection-surface enhanced infrared absorption spectroscopy (ATR-SEIRAS) is particularly suitable for the investigation of electrochemical CO₂RR as it allows observation of interfacial processes in real-time owing to its high surface sensitivity. Additionally, time-resolved analysis would reveal the kinetic relevancy of intermediates and their relationship with the reactants and the products based on their dynamic behavior during the reaction. Lastly, a combination of the operando spectroscopic studies with material characterization would enable a correlation of the behavior of the intermediates and the catalyst conditions. Herein, I will introduce in situ time-resolved FT-IR (or ATR mode) spectroscopic techniques to acquire the isotopically labeled products and key intermediates from the photoreduction of carbon dioxide.

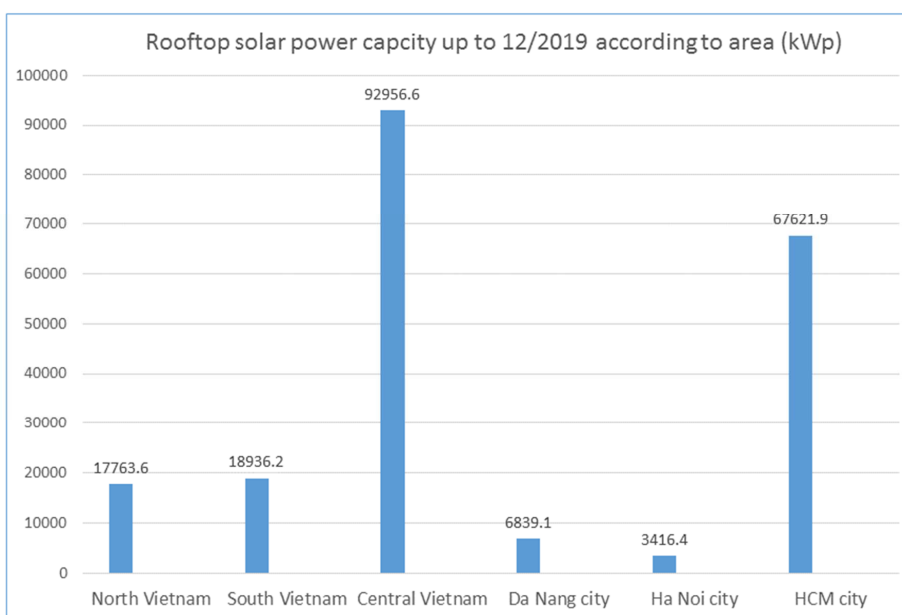
Evaluating Status of Using, Environmental Risks of Solar Cell and Proposing Management and Recycle Methods Suitable for Vietnam

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In recent years, solar energy in Vietnam has developed greatly due to electric power demand and investment attracting policy of government. Up to December, 2019, there are 85 solar energy companies and with power capacity of 5384.6 MWp and 377,943 MWp of rooftop solar power which were installed and operated. However, fast increase of those energy projects without orientation and environmental impact assessment will cause serious environmental risks in next 20 years (expiry date of solar panel is over). In this report, we provide updating information about the status of producing, using, and releasing waste of solar cell in Vietnam. Besides, solar panel recycling methods also are presented in order to propose suitable managing policies for Vietnam condition.



Hydrogen Generation by Different Electrolysis Technologies: Status and Future Development

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Hydrogen generation by electrolysis is expected to play an important role as a crosslinking technology between power generation on one hand and transport and industry on the other hand. When produced by water electrolysis from renewable energies - such as solar or wind - hydrogen can directly replace fossil fuels in transport and industry, thereby helping in the integration of renewable energies in other energy sectors. The relevant technologies are either the mature alkaline water electrolysis (AEL), the newer proton exchange membrane (PEMEL) water electrolysis, or the less-mature high-temperature solid oxide electrolysis (SOEL). The AEL has the benefit of using inexpensive materials and a superb durability record, whereas the PEMEL can excel with small footprint, high current densities and simplified system design. SOEL has the potential of highest electrical efficiencies when high-temperature heat is available but still requires scale-up efforts for reaching MW power levels.

The electrolysis research activities at DLR date back to the late 80s of the last century when the first technical “power-to-gas” projects was demonstrated in Saudi Arabia with the name of HySolar. This was the beginning of the electrochemical research activities which later-on focused on fuel cell development. With the increasing share of renewables in the German electricity sector, the need for hydrogen energy as a sector coupling technology became evident restarting the activities at DLR which presently have the following priority areas:

- Polymer electrolyte membrane electrolysis
- High temperature co-electrolysis of steam and CO₂
- Alkaline membrane electrolysis

Some examples from this research will be presented. In PEMEL gas diffusion layers (GDL), such as felts, foams, meshes and sintered plates, are key stack components, but these are either inefficient or expensive. Therefore a new type of GDL produced via vacuum plasma spraying (VPS) is presented, which offers a large potential for cost reduction. With this technology, it is possible to introduce a gradient in the pore-size distribution along the thickness of the GDL by varying the plasma parameters and titanium powder particle sizes. The results presented herein demonstrate a promising solution to reduce the cost of one of the most expensive components of the stack.

For SOEL degradation effect for co-electrolysis of steam and CO₂ will be shown and the possible mitigation strategies discussed. Furthermore, the successful integration of solar heat into a solid oxide electrolyzer will be presented. The experimental setup of the prototype system consisting of a solar simulator, a solar steam generator, a steam accumulator and a solid oxide electrolyzer as well as first results with regard to solar steam generation and electrochemical performance of the electrolyzer are shown. Lastly, the recent progress in achieving similar performance levels of alkaline membrane electrolysis (AEMEL) compared to PEMEL will be discussed.

The three electrolysis technologies are expected to find applications due to highly diversified applications and markets. All three technologies have a significant potential for further technology development and cost reduction.

Acknowledgements

The research leading to these results has received funding from the European Union for the Fuel Cells and Hydrogen Joint Technology Initiative under grant n° 621237, “INSIDE”, under grant agreement No 735485 “QualyGrid” and from national projects “LastEISys” and “WESpe” by Federal Ministry for Economic Affairs and Energy. Additional financial support was received from DLR’s basic funding for the project “Future Fuels”.

Electrochemical Ammonia Synthesis on the Hetero Ru-Based Atom Catalysts: A DFT Study

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The electrochemical ammonia synthesis through nitrogen reduction is one of the most attractive and emerging chemical process in hydrogen storage and transportation. We studied electrochemical nitrogen reduction reaction (N₂RR) on the hetero-double atomic Ru catalysts embedded in modified defective graphene (RuM/C, Ru: ruthenium, M: 3d transition metal, C: carbon support) using density functional theory computation. We systematically investigated the energetically optimized geometries of RuM/C. Also the free energies of nitrogen dissociation reaction on each catalyst were calculated to determine which mechanism to follow for NRR on RuM/C. In addition, we calculated the adsorption energy of possible reaction intermediates to identify the limiting potential and detailed reaction mechanism for NRR on each catalyst. We found that RuM/C showed obviously enhanced NRR activity compared to Ru single and homo-double atomic catalyst. This is because the adsorption energy of reaction intermediates, including NH_2^* , has been adjusted to an appropriate level by strain, ligand, and support effect. We also found that the most promising candidate is RuFe/C.

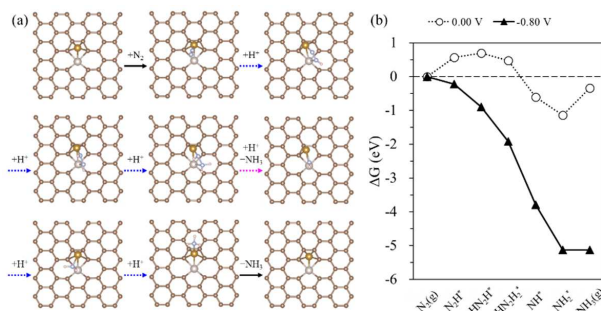


Figure N2RR performance in RuFe/C.

References

- [1] H.-J. Neef, *Energy* **2009**, *34*, 327
- [2] C.H. Christensen, T. Johannessen, R.Z. Sørensen, J.K. Nørskov, *Catal. Today* **2006**, *111*, 140
- [3] J. Kong, A. Lim, C. Yoon, J.H. Jang, H.C. Ham, J. Han, S. Nam, D. Kim, Y.-E. Sung, J. Choi, H.S. Park, *ACS Sustainable Chem. Eng.* **2017**, *5*, 10986
- [4] Y. Yao, H. Wang, X. Yuan, H. Li, M. Shao, *ACS Energy Lett.* **2019**, *4*, 136
- [5] V. Kordali, G. Kyriacou, C. Lambrou, *Chem. Commun.* **2000**, *17*, 1673
- [6] Y. Abghoui, E. Skúlason, *J. Phys. Chem. C* **2017**, *121*, 6141

Biomass-Derived Bifunctional Oxygen Electrocatalysts for ORR and OER

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Oxygen electrode catalysts are important as inter-conversion of O_2 and H_2O is crucial for energy technologies. However, the sluggish kinetics of oxygen-reactions (ORR and OER) are a hindrance to their scalable production, whereas scarce and costly Pt and Ir/Ru-based catalysts with high electrocatalytic activity are commercially unviable. Since good ORR catalysts are not always efficient for OER and vice versa, bifunctional catalysts that unify the efficient catalytic activities of both ORR and OER are crucial. The lower electrocatalytic activity of alternative catalysts based on carbon nanomaterials could be enhanced by heteroatom-doping, porous structure and tuning morphology. Heteroatom-doped porous carbons derived from biomass have recently emerged as low-cost, earth-abundant, renewable and sustainable environment-friendly materials as bifunctional oxygen catalysts. The tunable morphology, mesoporous structure and high concentration of catalytic active sites of these materials can be improved by heteroatom-doping, and N-doping enhances ORR activity and also improves OER activity, along with tolerance to methanol crossover and good durability. Biomass-derived porous carbons with abundant micropores, rich edge defects, ultrathin nanosheet architecture and ultrahigh surface area are thus suitable as efficient bifunctional oxygen catalysts. In the present study, bifunctional oxygen electrocatalysts derived from low-cost, renewable and sustainable biomass via a facile and green synthesis route will be discussed. The N self-doping of these materials avoids the use of toxic chemicals, and has emerged as a green approach. The facile and green synthesis could be further optimized to develop biomass-derived N self-doped porous carbon materials as metal-free high performance bifunctional oxygen catalysts.



Scheme Schematic view of the synthesis of bifunctional oxygen catalysts from biomass.

Acknowledgements

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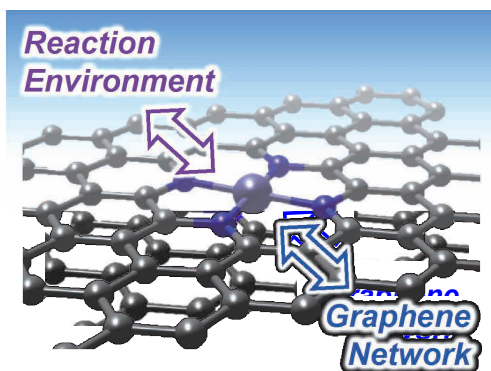
Understanding Catalytic Activity in the Carbon-Based Fuel-Cell Catalysts

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Polymer electrolyte membrane fuel cells (PEMFCs) have advanced substantially over the past few decades, both in fundamental and in engineering aspects. However, significant breakthroughs are still required to lower their cost and enhance their durability in order to replace fossil fuels with clean hydrogen fuels eventually. The most serious problem of current PEMFC technology is its expensive cost per unit of power output; this high cost is the result of the electrodes containing a large amount of expensive Pt and having limited long-term stability. To resolve these problems, carbon-based materials can be considered promising alternatives to Pt due to their cost-effectiveness and high stability. Among various carbon-based catalyst materials, metal-free N-doped graphene or metal-Nitrogen-Carbon materials (Me-N-C; Me = Fe, Co, etc.) have been considered as promising next-generation catalysts. For a rational design that will maximize the oxygen reduction reaction (ORR) performance and its stability, it is critical to understand the underlying ORR and deactivation mechanism within these graphene-based catalyst materials. In this presentation, by using density functional theory (DFT) and molecular dynamics (MD) simulation methods, we have focused on the explication of atomic-scale behaviors of carbon-based catalyst materials in the PEMFC system.



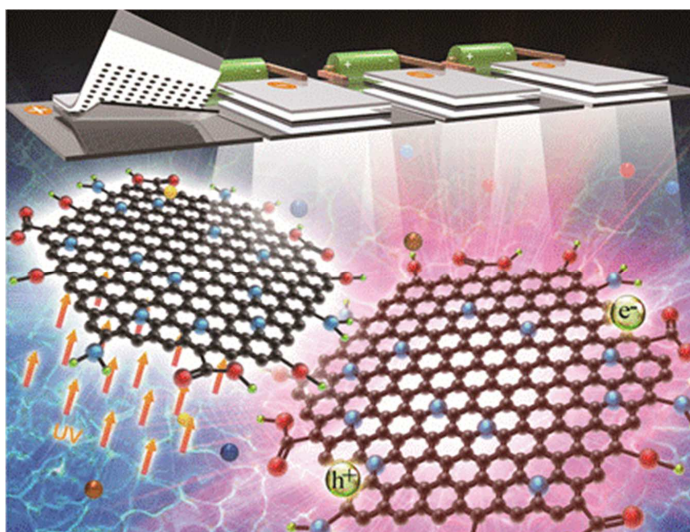
Graphene Quantum Dots for Efficient and Low-Cost Light-Emitting Electrochemical Cells^[1]

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Energy costs associated with artificial lighting account for more than 20% of total electricity consumption for the average Canadian household. Finding alternative and more efficient solutions is key to saving energy and reducing our carbon footprint. Quantum dot-based LEDs (QLEDs) have recently been gaining popularity in consumer-grade televisions and displays. However, these semiconductor quantum dots typically contain cadmium, a toxic earth metal, which decreases its long-term environmental viability. Graphene quantum dots (GQDs) show promise as an alternative emissive material due to their low cost, high stability, and tunable emission wavelength. Doping the graphene lattice with various heteroatoms significantly changes the structure and surface states, allowing additional control over the emissive properties and performance. We demonstrate here a top-down electrochemical exfoliation method for producing high quality GQDs that is both low-cost and scalable. Next, photoluminescence (PL) and electrochemiluminescence (ECL) of these graphene quantum dots were studied to determine the effects of doping. Optimization of preparation conditions and doping levels has shown to increase quantum efficiencies. Finally, the electroluminescent performance of our GQDs was explored in a full device of lighting-emitting electrochemical cells.



References

- [1] K. Chu, J.R. Adsetts, S. He, Z. Zhan, L. Yang, J. M. Wong, D. A. Love, Z. Ding, *Chem. Eur. J.* **2020**, DOI: 10.1002/chem.202003395.

Base Metal Nanostructure Formation via Reductive Deposition at the Non-Aqueous Liquid/Liquid Interface between Ionic Liquid and Oil

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Two years ago in the 5th Ertl symposium, I presented a method to form metal nanostructures at the liquid/liquid interface in the ionic liquid-water (IL-W) two-phase system. This IL/W method utilizes the spatial selectivity of the reaction site only at the liquid/liquid interface, which is achieved by the separation of metal precursor ions dissolved in the water phase and reducing agent in the IL phase. The metal reduction reaction is regarded as the electron transfer across the liquid/liquid interface, which enables us to analyze the reaction process with liquid-liquid electrochemistry^[1]. Moreover, the usage of ILs (not molecular oils) leads to the formation of 1-dimensional (1D) nanostructures despite the 2D geometry of the liquid/liquid interface, as a result of the structure-forming ability of ILs at the air^[2-4], liquid^[4,5], and solid^[6,7] interfaces. By using this IL/W method, we have successfully prepared 1D nanostructures of noble metals such as Au^[8,9], Ag^[10], Pt^[11], and Pd^[9,12], and also their composites with polymer^[13] and reduced graphene^[14].

In this presentation, I would like to introduce our very recent efforts to develop a sister method that uses another liquid/liquid interface between IL and oil (O). Wet chemical techniques for the metal nanostructure formation in general, including our IL/W method, use water and therefore cannot escape from the limitation of the metal element to noble ones. In contrast, the IL/O method^[15] is free from water and can be used even for base metals, expanding the applicability and versatility of wet chemistry for the metal nanostructure formation. In the presentation I will introduce the IL-O two-phase system explored where the liquid/liquid interface can be electrochemically polarizable, the measurement results of the electron and ion transfers across the IL/O interface, and nanostructures of some base metals prepared.

References

- [1] T. Kakiuchi and N. Nishi, *Electrochemistry* **2006**, *74*, 942.
- [2] N. Nishi, Y. Yasui, T. Uruga, H. Tanida, T. Yamada, S. Nakayama, H. Matsuoka, T. Kakiuchi, *J. Chem. Phys.* **2010**, *132*, 164705.
- [3] N. Nishi, T. Uruga, H. Tanida, T. Kakiuchi, *Langmuir* **2011**, *27*, 7531.
- [4] N. Nishi, T. Uruga, H. Tanida, *J. Electroanal. Chem.* **2015**, *759*, 129.
- [5] S. Katakura, K. Amano, T. Sakka, W. Bu, B. Lin, M. Schlossman, N. Nishi, *J. Phys. Chem. B* **2020**, *124*, 6412.
- [6] N. Nishi, J. Uchiyashiki, Y. Ikeda, S. Katakura, T. Oda, M. Hino, N. Yamada, *J. Phys. Chem. C* **2019**, *123*, 9223.
- [7] N. Nishi, T. Yamazawa, T. Sakka, H. Hotta, K. Hanaoka, H. Takahashi, *Langmuir* **2020**, *36*, 10397.
- [8] N. Nishi, T. Kakinami, T. Sakka, *Chem. Commun.* **2015**, *51*, 13638.
- [9] Y. Zhang, N. Nishi, T. Sakka, *Electrochim. Acta*, **2019**, *325*, 134919.
- [10] Y. Zhang, N. Nishi, T. Sakka, *Colloids Surf. A*, **2020**, *597*, 124747.
- [11] Y. Zhang, N. Nishi, K. Amano, T. Sakka, *Electrochim. Acta*, **2018**, *282*, 886.
- [12] Y. Zhang, N. Nishi, T. Sakka, *ACS Appl. Mater. Interfaces* **2019**, *11*, 23731.
- [13] N. Nishi, I. Yajima, K. Amano, T. Sakka, *Langmuir* **2018**, *34*, 2441.
- [14] Y. Zhang, N. Nishi, I. Koya, T. Sakka, *Chem. Mater.* **2020**, *32*, 6374.
- [15] Y. Kuroyama, N. Nishi, Y. Zhang, T. Sakka, *to be submitted*.

Nanostructured Anodic Films on Iron: Formation Mechanism and Electrocatalytic Applications

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Anodizing of metals has received increased attention as a simple electrochemical process to form self-ordered nanostructured films. The most well-known example is the highly ordered nanoporous anodic alumina films formed by two-step anodizing of high purity aluminum. Self-ordered titania nanotubes are formed by anodizing of titanium, exploring various applications including photocatalysis of organic pollutants, self-cleaning surface, solar cells and biocompatible surfaces. In the last decades, anodizing process to form nanostructured anodic films have expanded to a range of metals. Here, our recent studies on formation of nanoporous and nanotubular anodic films on iron and electrocatalytic applications of anodic films on iron and its alloys are introduced.

Anodizing of iron in ethylene glycol electrolytes containing ammonium fluoride and water forms nanoporous or nanotubular self-ordered anodic films. The water concentration is one of the key parameters to control whether nanoporous or nanotubular anodic films are formed. STEM/EDS analysis disclosed clearly the enrichment of fluoride species at the cell boundaries in addition to the metal/film interface for the film with nanotubular morphology. Preferential chemical dissolution of the fluoride-rich cell boundary induced the development of the nanotubular morphology.

Anodizing of iron-containing alloys, such as Fe-Ni-Co and Ni-Fe alloys, formed porous films consisting of fluoride-rich metal oxyfluoride. We recently found that such porous films are excellent precursor of the highly active oxygen evolution reaction (OER) electrocatalysts in alkaline media. The fluoride-rich porous films were converted readily to highly active hydroxide films under the OER condition and showed high stability.

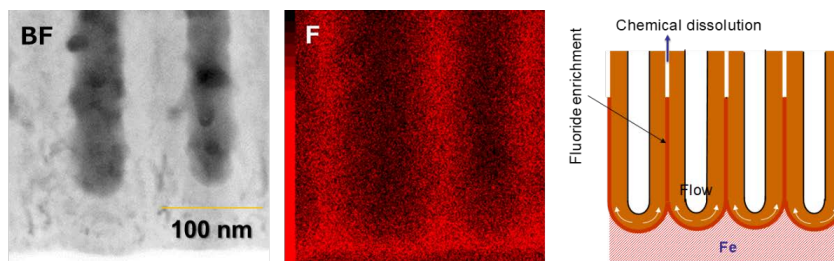


Figure Distribution of fluoride in the nanotubular anodic film on iron.

References

- [1] L. Fadillah, D. Kowalski, Y. Aoki, H. Habazaki, *Electrochim. Acta* **2020**, 364, 137316.
- [2] K. Shahzad, D. Kowalski, C. Zhu, Y. Aoki, H. Habazaki, *ChemElectroChem* **2018**, 5, 610-618.
- [3] K. Shahzad, E. Tsuji, Y. Aoki, S. Nagata, H. Habazaki, *Electrochim. Acta* **2015**, 151, 363-369.

Electrochemical Behavior and Cycloaddition Activity of Bismuth(III)-acetylides Towards Organic Azides Under Copper(I)-Catalyzed Conditions

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With the increased interest in the area of novel, nontoxic and biocompatible nanomaterials, Bi-doped systems have become a hot topic in industry and electrochemical engineering.¹⁻² In this work we performed cyclic voltammetry studies of the activity of bismuth(III)-acetylides in the presence of copper(I) catalyst ([Cu]).³⁻⁴ In addition, an in-depth kinetic analysis of bismuth(III) substrate (A[X]) reactivity towards organic azides ([Z]) was studied *in situ* using cyclic voltammetry, as well as proton magnetic resonance spectroscopy. To study the electronic and steric factors influencing the observed reactivity trends, a wide scope of novel organobismuth(III) compounds carrying a diphenyl sulfone heterocyclic scaffold was probed.

Our study revealed a restricted binding ability to the copper(I)-species for some para-derivatized bismuth (III) acetylides whereas others exhibited enhanced reactivity towards azide addition. Apparent rate constants and parameters of the corresponding π -intermediate and triazolidine formation reaction were obtained by step-wise kinetic cyclovoltammetry studies, that enabled the formulation of a quantitative kinetic model for the mechanism of the copper-mediated 5-bismuth(III)-1,2,3-triazole formation.

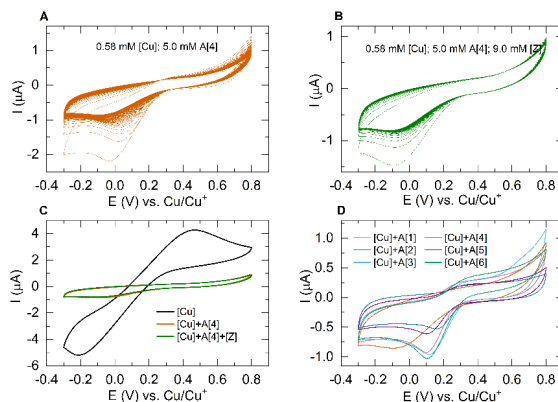


Figure Cyclic voltammogram of kinetic studies of the cycloaddition reaction of bismuth(III)-acetylides to organic azides in the presence of the copper(I)-triflate toluene complex at 25 °C in dry DMSO at 100 mV/sec. Conditions: 3-electrode cell with glassy carbon as the working electrode, copper foils as counter and reference electrodes. (A) Kinetic studies of catalyst-bismuth(III) acetylide coordination; (B) Kinetic studies of azide insertion; (C) Voltammograms in the presence of the indicated reagents, added in the order specified; (D) Average of onset oxidation and reduction potential values for variable complexes of bismuth(III)-acetylides with copper(I).

References

- [1] R. Mohan, *Nat. Chem.* **2010**, 2 (4), 336-336.
- [2] M. Wu, B. Xu, Y. Zhang, S. Qi, W. Ni, J. Hu, J. Ma, *Chem. Eng. J.* **2020**, 381.
- [3] B. T. Worrell, S. P. Ellery, V. V. Fokin, *Angew. Chem. Int. Ed.* **2013**, 52 (49), 13037-13041.
- [4] V. Hong, A. K. Udit, R. A. Evans, M. G. Finn, *ChemBioChem* **2008**, 9 (9), 1481-1486.

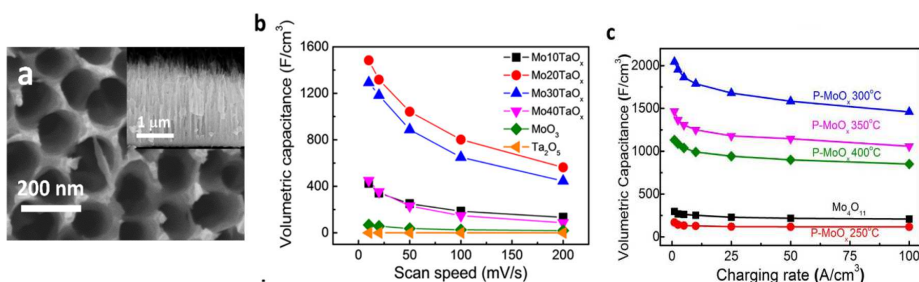
High Efficient Supercapacitors Electrodes Based on One Dimensional Self-ordered Molybdenum based Compound Nanotube Arrays

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Recently, molybdenum oxide have received attention owing to their unique chemical and physical properties and the resulting high potential in energy conversion and storage (such as battery and supercapacitor)^[1]. However, the poor conductivity, low catalytic activity and poor stability of pure Mo oxide limits the practical application. The formation of one dimensional nanoporous materials, especially heterostructure nanotubes have been proved effective way to overcome these shortage^[2]. Here, one dimensional self-ordered MoTaOx, and MoOx/MoP nanotube arrays were synthesized by electrochemical anodization and used as negative electrodes for supercapacitors. Both of these nanotubular compounds show high volumetric capacitances and high cycling stabilities in the acidic solution^[3-5].



References

- [1] X. Hu, W. Zhang, X. Liu, Y. Mei, Y. Huang, *Chem. Soc. Rev.* **2015**, *44*, 2376.
- [2] Q. Wei, F. Xiong, S. Tan, L. Huang, E. H. Lan, B. Dunn, L. Mai, *Adv. Mater.* **2017**, *29*, 1602300.
- [3] B. Jin, X. Zhou, L. Huang, M. Lickleder, M. Yang, P. Schmuki, *Angew. Chem. Int. Ed.*, **2016**, *55*, 12252–12256.
- [4] B. Jin, S. Hajazi, H. Chu, S. Mohajernia, N. T. Nguyen, M. Yang, M. Altomare, P. Schmuki, *Appl. Mater. Today*, **2019**, *17*, 227–235.
- [5] B. Jin, S. Hejazi, F. Pyczak, M. Oehring, S. Mohajernia, O. Tomanec, S. Kment, R. Zbořil, N. Nguyen, M. Yang, P. Schmuki, *ACS Appl. Mater. Inter.*, **2019**, *11*, 45665–45673.

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High Energy and Long Cycle Life Rechargeable Zn-Air Batteries using Aqueous Acidic Electrolyte

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As one of the proposed post lithium-ion technologies, rechargeable zinc-air batteries have received considerable attention due to its desirable properties, such as high energy density, high stability, non-explosive risk and environmental benignity. But zinc-air batteries mostly operate in alkaline solution, such as KOH and NaOH, for the purpose of higher activity of both the zinc electrode and air electrode. Though the electrochemistry of zinc in alkaline electrolytes is easily reversible, the alkaline solution which is not only react with atmosphere CO₂ to form K₂CO₃ or KHCO₃, but also makes the zinc non-uniform dissolution and deposition, and finally results in dendritic growth during charge-discharge cycling. This is detrimental to zinc-air battery performance and cycle life.

ZnSO₄ solution which has strong interaction among Zn²⁺ ions and oxygen of the water molecule imposes a strong energy barrier for Zn²⁺ to solvate/desolvate, theoretically inhibits the formation of dendritic growth when used as electrolyte. Hence, in our work, we use nontoxicity, low cost ZnSO₄ solution as the electrolyte. Co or Fe-based catalysts were chose as air electrode catalyst for oxygen reduction and evolution reactions, because of low price and abundant oxygen vacancies. These materials were then assembled in rechargeable zinc-air batteries and test, maybe we can get the desirable electrocatalytic activities.

References

- [1] V. Mathew, B. Sambandam, S. Kim, S. Kim, S. Park, S. Lee, M.H. Alfuruqi, V. Soundharrajan, S. Islam, D.Y. Putro, J.-Y. Hwang, Y.-K. Sun, J. Kim, *ACS Energy Lett* **2020**, 5, 2376–2400.
- [2] B.W. Olbasa, F.W. Fenta, S.-F. Chiu, M.-C. Tsai, C.-J. Huang, B.A. Jote, T.T. Beyene, Y.-F. Liao, C.-H. Wang, W.-N. Su, H. Dai, B.J. Hwang, *ACS Appl. Energy Mater.* **2020**, 3, 4499–4508.

Incorporating Electrochromic Effect with Photothermal Conversion for the Enhancement of Pseudocapacitance via Spurring Li-ions Intercalation

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Supercapacitors usually suffer from a poor performance at lower temperatures. Employing the solar thermal energy is a potential approach for improving the local temperature for improving energy storage device on site. In this work, the electrochromic effect of supercapacitor electrode materials is applied to accelerate photothermal conversion by boosting the Li^+ ion intercalation performance in energy storage. For this purpose, we prepared a thin nickel hexacyanoferrate (NiHCF) layer on the surface of nickel oxide (NiO) nanotubes via an ionic exchange reaction. The bilayered nanotubes provided a specific capacity of 153.7 F g^{-1} at 0.2 A g^{-1} in a neutral electrolyte, which was closed to the capacity of commercial carbon electrode. More importantly, the specific pseudocapacitance was remarkably boosted by the NIR light irradiation (114.6 % under the power density of 0.640 W cm^{-2}). This enhancement can be ascribed to the high photothermal conversion at the colored state, thus largely raising surface temperature of electrode. At a higher temperature, the improvement of pseudocapacitance is thus achieved via spurring Li-ions intercalation, as the ions diffusion rate in electrode materials is largely dependent on the local temperature

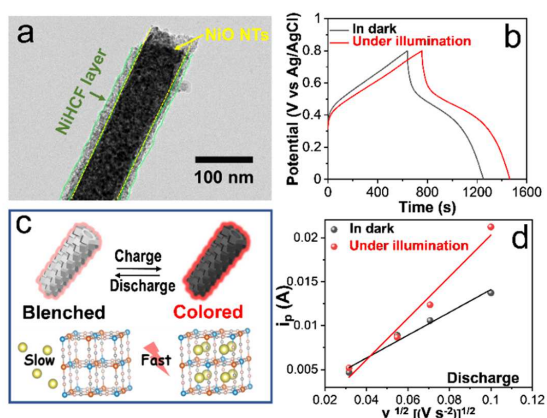


Figure a) Transmission electronic microscope image of the nanotubes; b) comparison of GCD curves of sample in dark and under 0.640 W cm^{-2} 808 nm laser irradiation; c) illustration of electrochromic-photothermal synergistic effect for triggering Li^+ intercalation; d) ion diffusion rate from CV data, the bigger slope of curves demonstrates the faster ion diffusion rate.

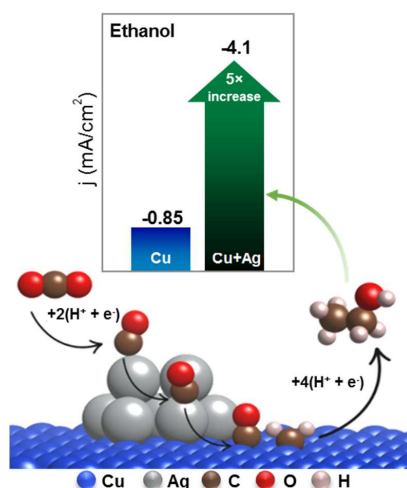
Enhancing CO₂ Electroreduction to Ethanol on Copper-Silver Composites by Opening an Alternative Catalytic Pathway

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A fundamental question in the electrochemical CO₂ reduction reaction (CO₂RR) is how to rationally control the catalytic selectivity. For instance, adding a carbon monoxide-producing metal like silver to copper shifts the latter's CO₂RR selectivity towards C₂ products, but the underlying cause of the change is unclear. Herein, we show that CuAg boundaries facilitate the coupling of carbon-containing species to give ethanol, through an otherwise closed pathway. Oxide-derived Cu nanowires mixed with 20 nm Ag particles (Cu:Ag mole ratio of 1:20) reduce CO₂ to ethanol with a current density of -4.1 mA/cm² at -1.1 V vs. RHE and ethanol/ethylene Faradaic efficiency ratio of 1.1. These figures of merit are respectively 5 and 3 times higher than those for pure oxide-derived Cu nanowires. CO₂RR using different Ag:Cu ratios and Ag particle sizes reveals that ethanol production scales with CO production on the Ag sites and the abundance of CuAg boundaries, and, very interestingly, without significant modifications to ethylene formation. Computational modelling shows selective ethanol evolution via Langmuir-Hinshelwood *CO + *CH_x (x = 1, 2) coupling at CuAg boundaries, and that the formation of energy-intensive CO dimers is circumvented.



References

- [1] L.R.L. Ting, O. Piqué, S.Y. Lim, M. Tanhaei, F. Calle-Vallejo, B.S. Yeo, *ACS Catalysis*. In Press.

Atomic-scale Insights into Structural Changes at Pt Electrodes

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Platinum dissolution and restructuring are primary degradation mechanisms that limit the lifetime of Pt-based electrocatalysts for electrochemical energy conversion. This is a major factor in slowing global-scale commercialization of fuel cell vehicles and spurred extensive research efforts, which mainly focussed on polycrystalline and supported nanoparticle catalysts. Single-crystal studies offer the prospect of a more detailed understanding of these processes at the atomic level. In this talk, studies of well-defined Pt(100) and Pt(111) electrode surfaces by in situ and operando surface-sensitive methods and ab initio theory are discussed.

In the first part, studies of Pt dissolution and restructuring due to surface oxidation are presented^[1]. Using high-energy surface X-ray diffraction, on-line inductively coupled plasma mass spectrometry, and density functional theory calculations an atomic-scale picture is obtained, which explains the dependence of the dissolution rate on the atomic structure of the exposed facets. It is shown that the locations of the extracted Pt atoms after Pt(100) oxidation reveal surprising differences from the Pt(111) case, resulting in different surface stability. The evolution of a specific stripe oxide structure on Pt(100) produces unstable surface atoms which are prone to dissolution and restructuring, leading to order of magnitude higher dissolution rates.

As a second case, in situ Video-rate STM studies of CO-covered Pt(111) electrodes are discussed. These reveal that removal of a small fraction of CO adsorbates in the pre-oxidation regime leads to drastic increases in the surface mobility within the adlayer^[2]. As shown by density functional theory calculations, the CO lattice can then locally relax into patches with a (1 × 1) arrangement, which can rapidly propagate across the surface. In addition, the STM observations indicate the formation and slow diffusion of vacancies in the Pt surface layer^[3].

References

- [1] T. Fuchs, J. Drnec, F. Calle-Vallejo, N. Stubb, D.J.S. Sandbeck, M. Ruge, S. Cherevko, D.A. Harrington, O.M. Magnussen, *Nat. Catal.* **2020**, accepted for publication.
- [2] J. Wei, R. Amirbeigi, Y.X. Chen, S. Sakong, A. Gross, O.M. Magnussen, *Angew. Chem. Int. Ed.* **2020**, 59, 6182–6186; doi: 10.1002/anie.201913412
- [3] J. Wei, Y.-X. Chen, O.M. Magnussen, *Chem. Comm.* **2020**; doi: 10.1039/D0CC04046K



Ultra-Low Loading of Iron Oxide on Bare and Pt-Loaded Al_2O_3 for Enhanced Catalytic Activity

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In the first part of this talk, recent progress in catalytic activity of Fe-oxide nanoparticles deposited using temperature-regulated chemical vapor deposition will be reviewed. Using this method, Fe-oxide can be impregnated in mesoporous substrate in a highly dispersed manner. Fe-oxide-deposited mesoporous Al_2O_3 turned out to be reactive for catalytic reactions such as room temperature CO oxidation, oxidation of volatile organic compounds and reduction of NO by CO. More recently, we found that the catalytic activity of Pt/ Al_2O_3 toward CO oxidation at room temperature can be enhanced by deposition of Fe-oxide on Pt/ Al_2O_3 , and its activity is much higher than Fe-oxide/ Al_2O_3 without Pt as well, i.e., there is a synergy effect of Pt and Fe-oxide. Particularly, as Fe-loading decreased from ~10 to 0.34 wt%, catalytic activity toward CO oxidation gradually increased. Results of various analyses of catalysts attributed this Fe-oxide-induced enhancement effect to the boundary sites of Pt-Fe on Fe-Pt/ Al_2O_3 . It is worth noting that the enhanced catalytic activity of Pt/ Al_2O_3 upon Fe-oxide loading was observed even in the presence of water vapor (40% of the relative humidity). In addition, Fe-oxide-loaded Pt/ Al_2O_3 showed high thermal stability, and the catalytic activity at room temperature was retained after repeated exposure to high temperatures. Our results show the potential of Fe-oxide-loaded Pt/ Al_2O_3 prepared by tr-CVD as a catalyst for low-temperature CO oxidation in practical applications.

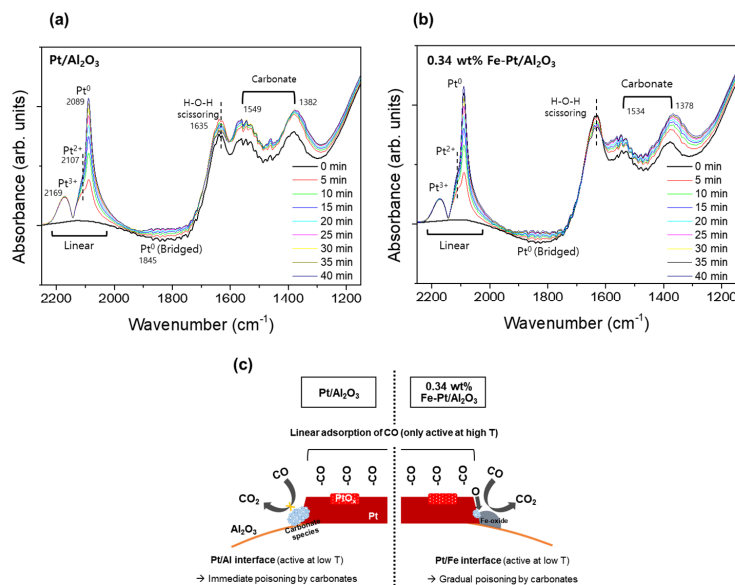


Figure DRIFT spectra obtained during 40 minutes of CO flow (1% of CO balanced with dry air) over the surface of (a) Pt/ Al_2O_3 and (b) 0.34 wt% Fe-Pt/ Al_2O_3 at room temperature. (c) Proposed mechanism of CO oxidation over 0.34 wt% Fe-Pt/ Al_2O_3 .

References

- [1] B.J. Cha, S. Y. Kim, C. M. Choi, J. Y. Sung, M. C. Choi, H. O. Seo, Y. D. Kim, *Chemical Engineering Journal*, **2021**, in press.

Green Ammonia Synthesis via Alkaline Electrolytic Process using Metal Oxide Based Nanolayers on 3-D Vertical Graphene Electrode

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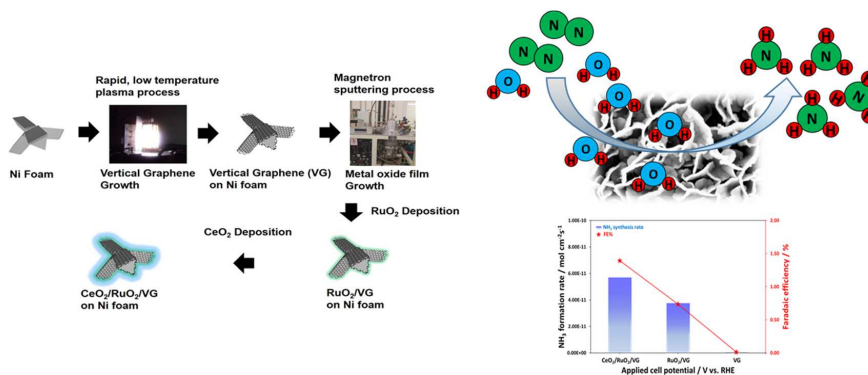
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Hydrogen is considered as a next generation source of energy which has potential to replace fossil fuels and ammonia is considered as the best carrier of hydrogen for energy storage and transport. Recently, the low temperature, ambient pressure, electrochemical synthesis of ammonia has attracted significant attention as a low energy and renewable alternative to synthesize ammonia compared to energy intensive, high temperature & pressure, conventional process of producing ammonia by the “Haber Bosch” process. Electrochemical synthesis at low temperature and ambient pressure (<100°C and < 1 bar) offers significant advantages over Haber-Bosch process which involve high temperatures of ~500°C and high pressure of ~200. However, electrochemical synthesis route’s wide adoption has hindered due to the poor yield arising from the ineffective catalysts and their long-term stability. Therefore, there is strong need to discover new catalysts and new material which can offer stable and high yield of ammonia production. In this work we report, to the best of our knowledge, the first time demonstration of utilizing novel metal oxide based catalyst material for electrochemical ammonia production, Ruthenium oxide (RuO₂) and Cerium oxide (CeO₂) which in combination with a unique 3-D graphene structure produced by a single step, low-temperature plasma process, and acts as an excellent and stable catalyst material. Finally, the long-term capability of this composite material have been successfully demonstrated using the CeO₂/RuO₂ on VG electrocatalyst where we achieved average ammonia synthesis yield of 50.56 $\mu\text{g h}^{-1} \text{mg}_{\text{total cat.}}^{-1}$ ($1.11 \times 10^{-10} \text{ mol s}^{-1} \text{cm}^{-2}$) with faradaic efficiency of 2.96% for 36 hr.



Hierarchical Nanosheets of Cobalt Iron Layered Double Hydroxide-Nickel Selenide as an Efficient Electrocatalyst for Water Splitting

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Designing non-precious active and stable bifunctional electrocatalysts for water splitting still remains a challenging issue. Although significant process has been developed by various scientific groups, but industrially the large-scale hydrogen production is not yet achieved. Therefore, the catalyst with cost effective and simple synthesis process to achieve overall water splitting is essential to promote the lab scale process. In this work, nickel foam supported CoFe-LDH decorated on NiSe sheets (CoFe-LDH@NiSe/NF) prepared through hydrothermal and electrodeposition process. Remarkably, the hierarchical nanosheets of CoFe-LDH @NiSe with the unique structure feature exhibit excellent performance for oxygen evolution reaction (OER) and hydrogen evolution reaction (HER) in alkaline medium. The intrinsic catalytic activity might be due to raise in conductivity of NiSe and CoFe-LDH facilitates the exposure of active sites their by increases the overall performance towards water splitting. Specifically, the nanosheets of NiSe and CoFe-LDH might also have strong synergic effect enhancing the catalytic activity. This type of hierarchical structures can be used for metal-air batteries in energy storage technologies.

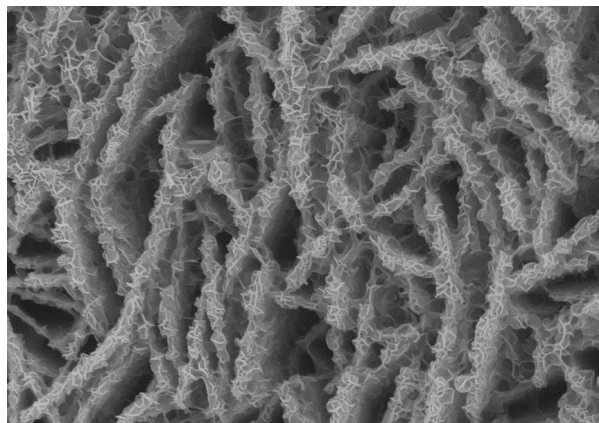


Figure CoFe-LDH@NiSe nanosheets supported on nickel foam.

Energy Storage Systems Assembled by Electrochemical Deposition

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Can batteries and supercapacitors be prepared by electrochemical deposition? What is the advantage of electrochemical deposition as compared with the classical methods?

In the proposed lecture, we will present a few approaches based on either electrochemical deposition or electrophoretic deposition for assembling energy storage systems. We will show that our “nano to nano” approach, whereby electrochemistry can be used for driving the deposition of nanomaterials from their dispersion, can be used for assembling supercapacitors and hybrid systems. For example, reduced graphene oxide with high porosity was driven by high-voltage electrochemical deposition to form a binder-free capacitor electrode for lithium-ion capacitors^[1]. The high voltage was used to drive the continuous and constant reduction of graphene oxide as well as for generation hydrogen, which was responsible for the porous structure. Electrophoretic deposition has also its advantages and can be used for the co-deposition of a few materials simultaneously. For example, Ketjenblack used as the physical storage material and NiCo_2O_4 as the chemical storage compound were dispersed in the presence of Ni^{2+} ^[2]. The latter assisted in positively charging the surface of both materials and thus resulted in similar deposition rates by electrophoretic deposition on nickel foam. This enabled us to nicely control the NiCo_2O_4 to KB ratio in the hybrid electrode and optimize its performance. Finally, we have shown that a capacitor-battery hybrid system can be formed by electrochemically exfoliation graphene and intercalating nickel(II) ions inside^[3].

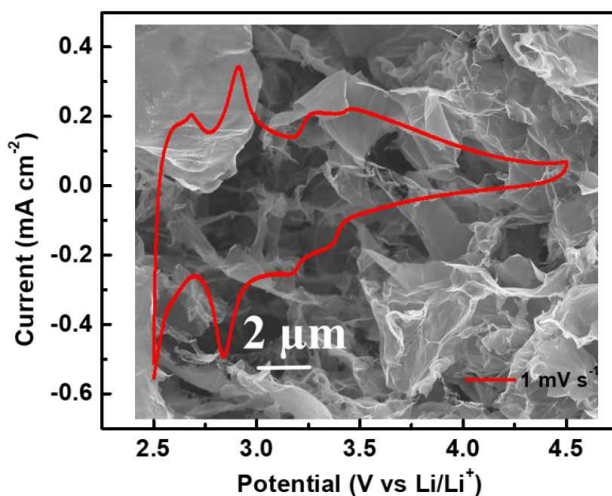


Figure Electrochemical deposition of highly porous reduced graphene oxide.

References

- [1] Y. Zhan, E. Edison, W. Manalastas, M. R. J. Tan, R. Satish, A. Buffa, S. Madhavi, D. Mandler, *Electrochim. Acta* **2020**, 337, 135861.
- [2] Y. Ouyang, O. Geuli, Q. Hao, D. Mandler, *ACS Appl. Energy Mater.*, **2020**, 3, 1784-1793.
- [3] D. Mukherjee, T. Schoetz, O. Geuli, H-J. Yen, Q. Hao, D. Mandler, submitted.

Modulating Dynamic Surface Restructuring of a Layered Transition Metal Oxide Catalyst for Water Oxidation Reaction

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Rationally manipulating the *in situ* formed catalytically-active surface of catalysts remains a tremendous challenge for highly-efficient water electrolysis. Here we present a cationic redox-tuning method to redirect dynamic surface restructuring from the same parent structure, for electrochemical oxygen evolution reaction (OER). Partially doping the layered transition metal oxides domified modified redox transitions during the OER, which was monitored by *operando* X-ray absorption spectroscopy. Surface-restructured transition metal oxides showed an OER activity approximately two orders of magnitude higher than that of benchmark RuO₂ and sustained this high activity for 500 h without degradation, making it among the best OER electrocatalysts ever reported. This work makes a stride in modulating surface restructuring and opens up new opportunities to design superior OER electrocatalysts via tuning cationic redox.

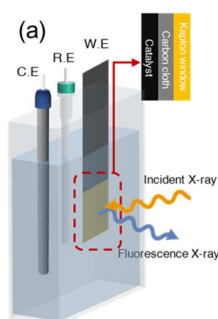


Figure monitoring surface reconstruction during OER.

Fe-Loaded Rutile TiO₂ Particles as a Visible Light-Responsive Photocatalysts: Annealing Temperature Dependency

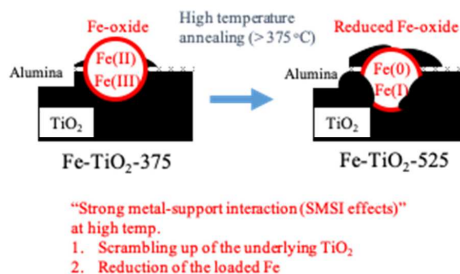
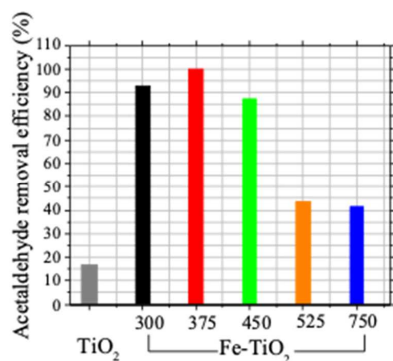
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We modified a commercial rutile TiO₂ particles (200 ~ 300 nm) via temperature regulated chemical vapor deposition (tr-CVD) of Fe-oxide and subsequent thermal annealing at various temperatures. The photocatalytic activity of the rutile TiO₂ particles towards acetaldehyde oxidation under the visible light irradiation can be enhanced by the small loading of Fe-oxide, but the enhancements effects of Fe-loading were depended on the annealing temperature in the range of 300 ~ 750 °C. The enhancement effect of the Fe-loading was most significant when Fe-loaded TiO₂ particles were annealed at 375 °C, on the other hands, higher temperature annealing (525, 750 °C) resulted in the reduction of the enhancement effects of Fe-loading. Careful examinations on the property changes of the Fe-loaded TiO₂ particles upon the annealing temperature with various analysis techniques including XPS and TOF-SIMS revealed that the annealing temperature dependent enhancement effects were largely attributed to the stronger metal support interaction between the loaded Fe oxide and TiO₂ at high temperature.



Electrochemical Sensor for Small Metabolites Analyses in Human Biofluids

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As a straightforward and cost-effective tool, the electrochemical sensor has been widely used to determine small metabolites (e.g., glucose, dopamine, uric acid and ascorbic acid) in human body and evaluate biological homeostasis^[1]. To enhance the sensing performance, carbon nanomaterials, polymers, metal and metal oxides nanoparticles have been used because of good electrical conductivity, catalytic activity, large surface area, and synergistic effect of their composite. In this work, we demonstrate a carbon complex, polymer, and metal nanoparticles composite modified screen printed carbon electrode (SPCE) for the determination of small metabolite concentrations in buffer and human biofluids^[2]. The electrode surfaces were characterized by field emission scanning electron microscopy and X-ray photoelectron spectroscopy, while the electrochemical sensing performance was studied by electrochemical impedance spectroscopy and different voltammetric techniques. In addition, a commercial assay kit and liquid chromatography techniques were used to validate the electrochemical sensing results.

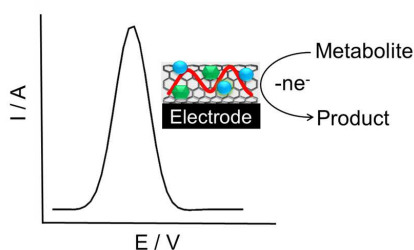


Figure A demonstration of an electrochemical sensor for determining the small metabolite using a polymer, carbon complex, and metal nanoparticles modified SPCE.

References

- [1] Y. Si, H.J. Lee, *Curr Opin Electrochem* **2020**, 22, 234
- [2] Y. Si, Y.E. Park, J.E. Lee, H.J. Lee, *Analyst* **2020**, 145, 3656

6th Ertl Symposium on
Electrochemistry and Catalysis

Poster Session



Ni-Mn Oxide/Hydroxide Coated Activated Carbon for Capacitive Deionization

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Capacitive deionization (CDI) is a low cost and environmental-friendly technology that has the potential to surpass current popular desalination techniques. CDI involves the polarization of two porous electrodes gaining a positive and a negative surface charge. The applied electric field allows salt ions to adsorb on the oppositely charged surface to desalinate water. Recently, studies have shown that pairing carbon with faradaic materials can change its surface characteristics and enhance its electrochemical and CDI performance. Manganese and nickel oxides/hydroxides are promising combination materials due to their low cost and high theoretical capacitance. In this work, commercial activated carbon (AC) was coated by Ni-Mn oxide/hydroxide to form a composite electrode (NM-AC). This was done through anodic electrodeposition at a constant current. Characterization shows an improvement in hydrophilicity and a reduction in charge transfer resistance due to its interconnected-nanowire morphology. Specific capacitance has also increased from 13.46 F g⁻¹ to 62.93 F g⁻¹. The desalination tests revealed that NM-AC obtained a higher salt removal efficiency and electrosorption capacity than AC (Figure 1). An increase in charge efficiency and electrosorption rate has also been observed. These enhancements are consistent at different applied voltages and NaCl salt concentrations. The improved performance is attributed to the high wettability and low charge transfer resistance of the composite electrode. Moreover, the pseudocapacitive nature of Ni-Mn oxide/hydroxide might have formed a synergistic effect with the double layer capacitance of activated carbon. Therefore, this study successfully enhanced the performance of activated carbon through the Ni-Mn oxide/hydroxide coating.

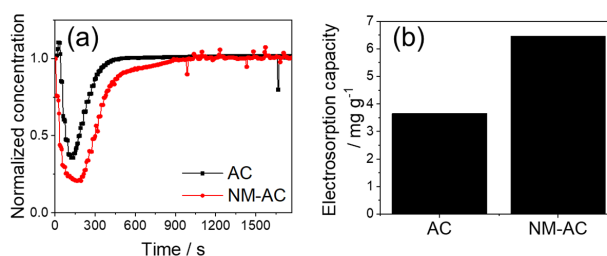


Figure (a) Adsorption profiles and (b) electrosorption capacity of AC and NM-AC using 200 mg L⁻¹ NaCl solution at 1.2 V.

References

- [1] F. Mohammadi, M. Sahraei, Y. Al-Abdullah, G.T. Heydt, Proceedings of the 2019 IEEE Global Humanitarian Technology Conference (GHTC), Seattle, WA, USA, Oct. 17-20, 2019; IEEE, 2019.
- [2] S. Porada, R. Zhao, A. van der Waal, V. Presser, P. M. Biesheuvel, *Prog. Mater. Sci.* **2013**, 58, 1388-1442.
- [3] M. A. A Mohd Abdah, N. H. N. Azman, S. Kulandaivalu, Y. Sulaiman, *Mater. Des.* **2020**, 186, 1-20.
- [4] G. Fu, Z. Hu, L. Xie, X. Jin, Y. Xie, Y. Wang, Z. Zhang, Y. Yang, H. Wu, *Int. J. Electrochem Sci.* **2009**, 4, 1052-1062.

Amphiphilic Porous Fe-N-C Catalyst for Advanced Power Performance of Alkaline Hydrazine Fuel Cells

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An alkaline hydrazine liquid fuel cell (AHFC) has been highlighted in terms of high power performance even with non-precious metal catalysts. To increase the non-noble catalyst utilization efficiency, many studies have been reported on the pore structure of the electrocatalysts. This study developed improved Fe-N-C catalysts for the oxygen reduction reaction (ORR) in the cathodes of alkaline hydrazine liquid fuel cells. Due to the well-known slow ORR kinetics, ORR electrocatalysts are essential for obtaining a high power performance in hydrazine fuel cells, which have emerged as promising potential backup power sources. Fe-N-C materials are currently the most promising non-noble-metal-based ORR electrocatalyst for alkaline hydrazine liquid fuel cells, but their low density of surface active sites compared with Pt/C necessitates improving their utilization via porous structures. To address this, we considered the importance of water as a connector for ionic conduction between the fuel cell electrode and electrolyte and thus aimed to alter the hydrophobicity of conventional Fe-N-C catalysts consisting mainly of graphitic carbon. We prepared Fe-N-C catalysts via sequential carbonization, steam activation, and acid treatment with reheating and analyzed their microstructures and electrochemical properties. We found that steam activation transformed the Fe₃C nanoparticles in Fe-N-C into larger Fe₃O₄ particles, which caused the electrode surface to become more hydrophilic. The modification of the inner pores with a hydrophilic material can help form the water networks for ionic conduction and water transfer between the membrane and catalytic active sites. We could conclude that the steam activation process for the electrospun Fe-N-C catalyst generated the amphiphilic pore surfaces that provide transfer paths for both water and O₂ gas that are connected to the active sites. It could increase the extent of triple-phase boundaries and eventually the catalyst utilization efficiency of the AHFC.

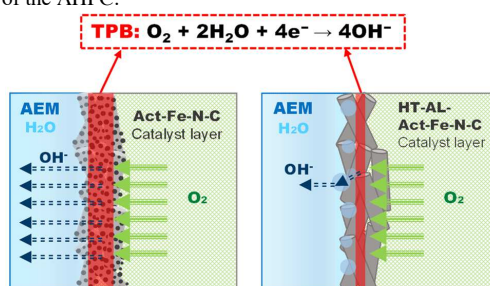


Figure Effects of hydrophilicity in the electrocatalyst layer: lower IR loss in the cell and extended triple-phase boundary for better catalyst utilization.

Methanol-tolerant Phosphorus-doped Carbon Layer on Platinum Cathode Catalyst for Direct Methanol Fuel Cell

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Global warming, which has become severe in recent years, is threatening human life, and fuel cells are excellent alternative energy for fossil energy. Among various types of fuel cells, direct liquid fuel cell, especially direct methanol fuel cell (DMFC) is quite attractive technology due to various advantages of rapid refueling and high energy density, which are crucial characteristics for portable applications. DMFC consists of methanol oxidation reaction at anode and oxygen reduction reaction (ORR) at cathode on PtRu-based and Pt-based catalyst, respectively. One of the most challenging problems toward DMFC is methanol crossover. Methanol at the anode permeates the cathode and reacts with cathode catalyst, resulting in voltage drop. Pt/C is an excellent catalyst, but it actively reacts with methanol at the cathode. Thus, methanol-tolerant property has great significance with Pt-based catalyst to increase the ORR selectivity at the cathode.

In our previous study, we synthesized Pt catalyst with P-doped carbon layer. We found out that Pt catalyst with phosphorus doped carbon layer has the potential for methanol tolerance, maintaining the ORR activity with addition of methanol. Therefore, we focus on Pt/C-P catalyst this time. Pt/C-P showed both lower activity in the methanol oxidation reaction and higher activity in ORR than pristine Pt/C. The excellent selectivity toward ORR of Pt/C-P would be originated from phosphorus-doped carbon layer, blocking the diffusion of methanol. Finally, we applied P-doped Pt/C on the cathode and confirm selectivity compared with pristine Pt/C. This approach suggests the way to design a Pt catalyst for ORR to improve performance in DMFC.

Formation of 1-Butanol from Gas-phase CO₂ Conversion on Phosphorus-rich Copper Cathode

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Electrochemical reduction of CO₂ to high value multi-carbon fuels using renewable energy is an attractive potential method that is alternative to fossil fuels. Many studies on copper based electrodes have reported the production of various oxygenated hydrocarbons such as methanol, ethanol, n-propanol, and 1-butanol below faradaic efficiency (FE) < 1%. Most of them mentioned *CO dimerization for C-C coupling reaction to C²⁺ multi-carbons. Herein, we report the first direct electrochemical reduction of CO₂ to 1-butanol on copper phosphide electrode (FE = 3.868 % at -0.6V vs RHE), without *CO dimerization instead combined reaction of faradaic and non-faradaic reaction. Possible produced intermediates with in-situ SEIRAS led us to propose a total reaction for the formation of oxygenated hydrocarbons, including formate, acetaldehyde, and 1-butanol. Our results point out an important view towards C-C coupling reaction to have a better product selectivity to multi-carbons.

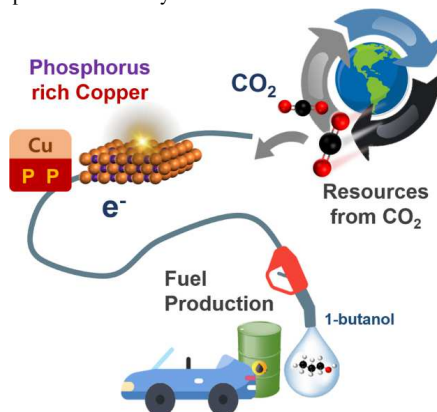


Figure Not combating with global warming gas, it has to be considered as unlimited resources for the continuous production of real fuel, 1-butanol on phosphorus-rich copper cathode catalyst by heterogeneous and autonomous chain growth processes.

References

- [1] G. Park, S. Hong, M. Choi, S. Lee, J. Lee, *Catalysis today*, in press
- [2] S. Lee, M. Choi, J. Lee, *The Chemical Record*, **2020**, 20, 89-101.
- [3] D. Kim, S. Lee, J.D., Ocon, B. Jeong, J.K. Lee, J. Lee, *J. Phys. Chem. Chem Phys.* **2015**, 17, 824.

Enhancement of Photoelectrochemical Properties through α -Fe₂O₃ Deposition on a Modified Fluorine-doped Tin Oxide

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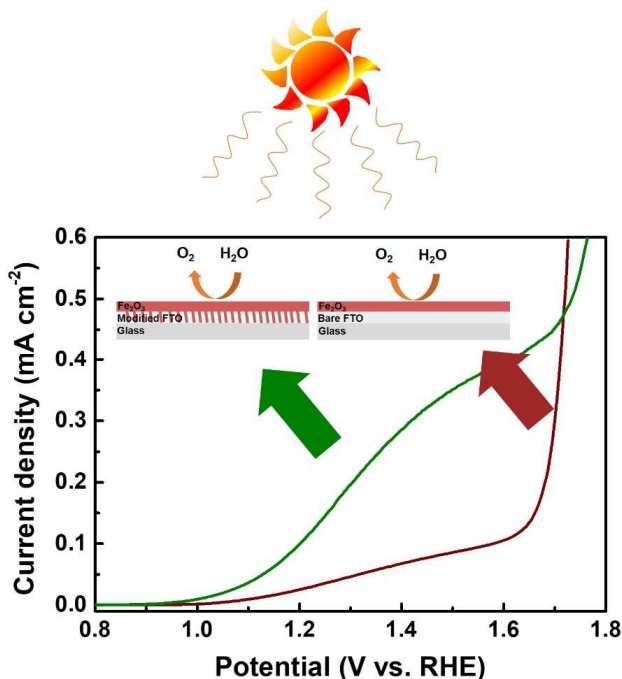
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Hydrogen is attractive energy resource for renewable energy. In order to produce H₂, several approaches are suggested. In particular, water splitting is well-known as an eco-friendly production approach. Moreover, electrochemical water splitting has a challenge that noble metal based catalyst. For this reason, photoelectrochemical (PEC) water splitting has been studied for a long time but not yet to reach a goal of society demand. For PEC water splitting, there are several materials has been considered such as Fe₂O₃, WO₃, TiO₂, BiVO₄ etc. Among them, Fe₂O₃ is the most attractive material due to cheap, abundant resources and smaller bandgap than other material. However, it has a demerits of short life time owing to short diffusion length.

In this research, we investigated enhancement of PEC performance with electrodeposited Fe₂O₃ on surface modified fluorine-doped tin oxide (FTO). The roughness of FTO substrates were increased with various electrochemistry method in acidic electrolyte. The modified FTO substrate area which leads to increasing electric conductivity. Under optimum condition photocurrent could be enhance with 20% in compare with α -Fe₂O₃ on pristine FTO substrate. Moreover, over-potential was also reduced with 100 mV.



Green Ammonia Synthesis under Neutral pH Condition using Mo Decorated Rh/C Nitrogen Reduction Catalyst

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Ammonia (NH₃), one of the important chemicals in the global economy, is generally used for the production of fertilizers, refrigerants and other chemical feedstock. Ammonia is also being considered as an effective carbon-free energy carrier due to its high volumetric density of hydrogen^[1]. Haber-Bosch process which is the main route for large-scale ammonia production, requires huge energy consumption and high purity hydrogen which generally comes from fossil fuel reforming. As an alternative route for green ammonia production, electrochemical method has been recently received much attention due to low energy consumption arising from ambient reaction condition. Herein, a molybdenum decorated rhodium electrode (Rh_{Mo}/C) is prepared by spray deposition and electrodeposition technique. With the dual active sites of Mo and Rh for nitrogen reduction reaction (NRR), the Rh_{Mo}/C electrode exhibits a higher yield of ammonia and higher faradaic efficiency in comparison with the pristine Rh/C electrode. Moreover, after optimizing pH of electrolyte and applied potential, hydrogen evolution reaction (HER) which is the competing reaction at cathode were successfully hindered due to the suppression of proton transfer. In this way, the selectivity towards NH₃ was dramatically improved while maintaining the performance on NH₃ yield rate. This study reveals the relationship between the reaction condition and the selectivity of ambient ammonia synthesis.

References

- [1] J. Gwak, M. Choun, J. Lee, *ChemSusChem*. **2016**, 9, 403

Effect of Annealing Temperature on the Performance of CuO Anode for LIB: Understanding the Formation of Solid Electrolyte Interphase Layer

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With the recent development of electric vehicles, portable electronic devices, and energy storage systems, high performance lithium ion batteries (LIBs), which have high energy density, high rate capability, and cycling stability, are highly required. However, graphite, widely employed as a commercial anode for LIBs with high conductivity and excellent cycling stability has a limitation for growing pursuit of high capacity energy storage devices due to its low theoretical capacity (372 mAh/g). In an attempt to solve this challenge, the intense researches on transition metal oxides such as copper oxide, cobalt oxide, iron oxide, and nickel oxide as anode materials with a relatively high theoretical capacity have been actively conducted. However, transition metal oxides still suffer from the pulverization of electrodes –peeling and degradation when they react with lithium ion due to large volume expansion.

In this study, the effect of annealing temperatures on the configuration of copper oxide nanostructures is investigated. We found that the electrochemical properties of copper oxide electrodes are affected by the grain size controlled by subsequent annealing temperature. These properties of the electrode can be attributed to the formation of stable SEI layer, which can endure the strain caused by the volume expansion of the electrode during charge/discharge processes. Copper oxide nanostructure annealed at 550 °C shows the relatively high gravimetric capacity (410 mAh/g) and high areal capacity (863 $\mu\text{Ah}/\text{cm}^2$) with superior capacity retention of 95 % after 200 cycles at 0.5 A/g.

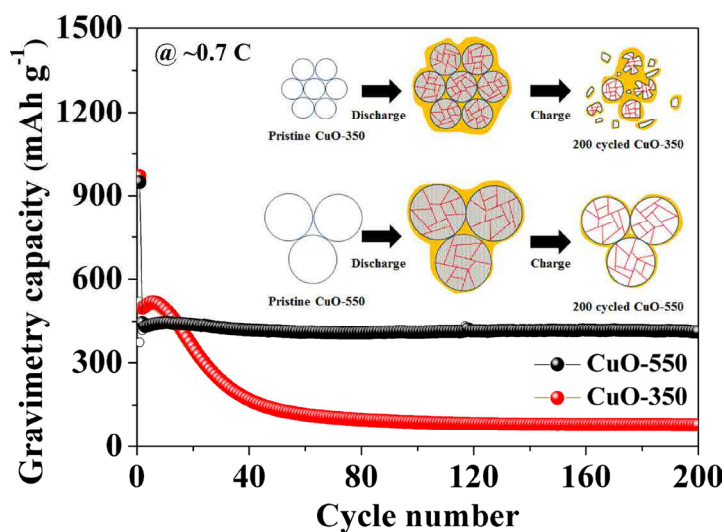


Figure Schematic image for the comparison of the cycling performance of CuO electrodes with different annealing temperatures.

Keywords: in-situ growth precipitation, lithium ion battery, copper oxide, SEI layer

Electrochemical Ammonia Production on RuO₂ Incorporated with Ionic Liquid

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Ammonia is an important building blocking for the production of fertilizers, fiber and explosive. In addition, Ammonia has received great attention as a promising energy storage medium and a fuel on behave of hydrogen gas, which has some issues of transportation and storage^[1]. However, the production of ammonia is limited to only Haber-Bosch process, which consumed 2 % of the global annual energy and generated 0.5 % of the CO₂ emission^[2]. Recent studies showed the feasibility of electrochemical ammonia production by the reduction of abundant N₂ gas in ambient pressure and temperature without CO₂ emission. But, the Faradaic efficiency for nitrogen reduction reaction (NRR) is only ~1 % due to both very close theoretical potential with hydrogen evolution reaction (HER) and difficult N₂ adsorption on the catalyst compared with proton^[3]. To enhance the Faradaic efficiency and ammonia production rate, we introduced ionic liquid to facilitate N₂ gas adsorption on the RuO₂ catalyst layer. The hydroxyl group in the ionic liquid helped the dispersion of RuO₂ onto gas diffusion layer, which increased electrochemically active surface area. The interaction between RuO₂ and imidazole in the ionic liquid could affect the stability of N₂ gas onto the catalyst layer and improve the ammonia production rate and Faradaic efficiency compared with pristine RuO₂ catalyst.

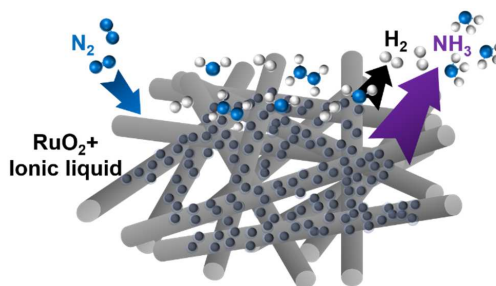


Figure Schematic image of the RuO₂ catalyst layer incorporated with ionic liquid for electrochemical ammonia production.

References

- [1] Neil V. Reesa, Richard G. Compton, *Energy Environ. Sci.* **2011**, 4, 1255.
- [2] Y. Yao, S. Zhu, H. Wang, H. Li, M. Shao, J. Am. Chem. So. **2018**, 140, 1496.
- [3] X. Guo, H. Du, F. Qu, J. Li, *J. Mater. Chem. A* **2019**, 7, 3531.

How to Enhance Ammonia Synthesis and Selectivity in Aqueous Media

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In this study, we have investigated electrochemical ammonia synthesis with high production rate using Mo oxide decorated Rh electrocatalyst (RhMo/C) as nitrogen reduction reaction (NRR) electrode. We have fabricated RhMo/C electrode via spray deposition of Rh/C and subsequent electrodeposition of Mo oxide. Due to the favourable N₂ adsorption and reduction mechanism which is confirmed by DFT calculation, RhMo/C shows a high NH₃ production rate and good stability during 30 hrs continuous electrochemical test under strong alkaline conditions. For the enhancement of the NRR selectivity towards NH₃ synthesis, the competing HER process was successfully suppressed under neutral pH conditions, exhibiting an outstanding NH₃ yield rate of 57.2 $\mu\text{g h}^{-1} \text{mg}_{\text{cat}}^{-1}$ at -0.6 V vs. RHE and a high Faradaic efficiency of 22% at -0.2 V vs. RHE. Furthermore, our approach is generic and replicable. The results will be of significant interest to researchers in a plethora of fields such as electrochemical engineering, materials science, nanotechnology scientists, and physicists.

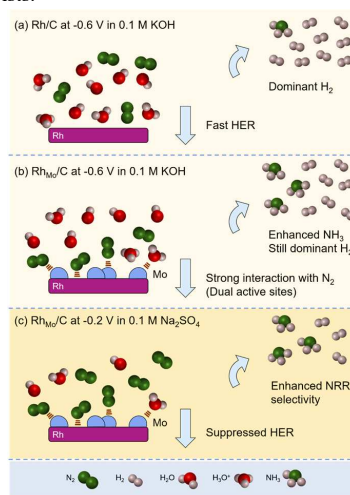


Figure A A schematic illustration of the NRR mechanism for Rh/C and RhMo/C catalysts.

Moderate Oxophilic CoFe in Carbon Nanofiber for the Oxygen Evolution Reaction in Anion Exchange Membrane Water Electrolysis

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We propose corrosion-resistant carbon-coated $\text{Co}_{0.9}\text{Fe}_{0.1}$ alloy nanoparticles as highly active and durable electrocatalysts for the oxygen evolution reaction (OER) in anion exchange membrane water electrolysis (AEMWE). In the presence of 10% Fe atoms, the oxophilicity of Co metal is modulated in a direction to facilitate OH^- adsorption on Co^{3+} ; thus, $\text{Co}_{0.9}\text{Fe}_{0.1}$ -carbon nanofiber (CNF) can exhibit smaller overpotentials than other metal ratios in $\text{Co}_{1-x}\text{Fe}_x$ -CNF. Additionally, we confirm catalytic degradation from the oxidation of the carbon layer, which is triggered by defects in the carbon originating from Fe during the pyrolysis step. The $\text{Co}_{0.9}\text{Fe}_{0.1}$ metal is further optimized by increasing graphitization to simultaneously achieve superior activity and durability for application on AEMWE. This work not only demonstrates the role of Fe in Co metal for controlling the proper oxophilicity but also shows the importance of graphitized carbon as a catalyst support for stable water oxidation.^[1]

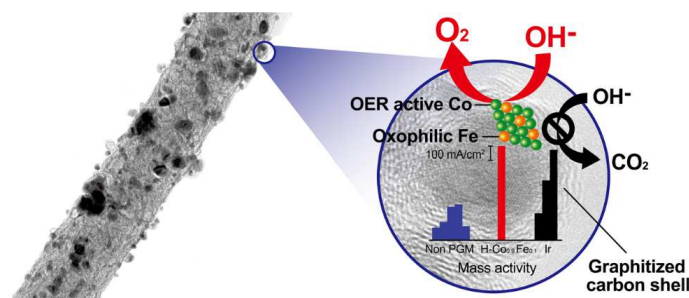


Figure Incorporation of Fe on Co embedded carbon nanofiber, successfully tune the oxophilicity, the ability to adsorb hydroxyl ion. Regarding stable operation issues, minimized amount of Fe has to be contained to maximize the degree of graphitization of carbon that prevents harsh carbon corrosion. H- $\text{Co}_{0.9}\text{Fe}_{0.1}$ -CNF led the high mass activity (0.5 mg cm^{-2} , 794 mA cm^{-2} @ 1.7 V) of anion exchange membrane water electrolysis with 290 hr stable operation.

References

- [1] S. Kang, K. Ham, J. Lee, *Electrochim. Acta* **2020**, 353, 136521.

Enhanced Charging Capability for Aluminum Ion Batteries with Surface Modified Graphite Cathode

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High demand for batteries applying to the mobiles, electric vehicles, and energy storage systems (ESS) requires a new battery system. Aluminum-ion batteries (AIBs) are promising alternative batteries for post-lithium-ion batteries as aluminum is abundant and non-flammability. In general, aluminum used as anode material and carbon material, metal oxide/sulfide used as cathode materials in an ionic liquid electrolyte ($\text{AlCl}_3/[\text{EMIm}]\text{Cl}$). However, the large size of aluminum ions (AlCl_4^- and Al_2Cl_7^-) is difficult to move in the graphite layers for fast charging, long cycling, and good rate capability. Therefore, modified graphite is essential to enhance the movement of aluminum ions of AIBs for a new battery system.

In this study, AEG (Acid expanded graphite) and BEG (Base etched graphite) are prepared by the acid and base solution. The inter-layers of AEG can be expanded up to about 0.1 nm, leading to facilitate the aluminum ions movement and more easily intercalate to the graphite. The BEG expanded layers and pores improve the performance of AIB due to the easy movement of the aluminum ions. The crystallinity and morphology are analyzed by the X-ray diffraction (XRD) and scanning electron microscope (SEM). The electrochemical performance is investigated by the cyclic voltammetry (CV) and charge/discharge test at each current densities.

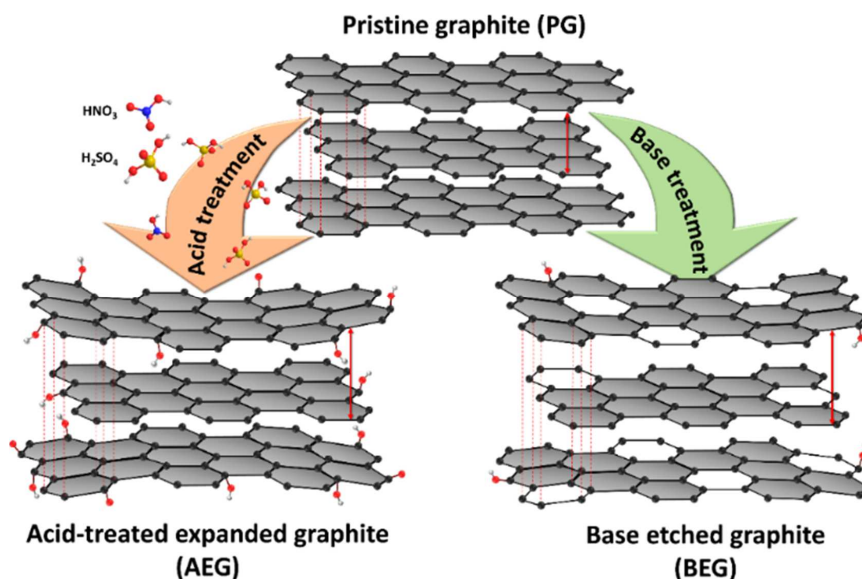


Figure Schematic images of surface treated graphite (AEG, BEG).

Anodically Prepared Nanoporous Stainless Steel Electrocatalysts: A Self-activated and Ultra-stable Catalysts for the Hydrogen Evolution Reaction

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Hydrogen appears as a sustainable and clean energy carrier and has thus gained a lot of interest over the past few years. One of the most promising methods to produce high-purity hydrogen is electrocatalytic water splitting, which primarily involves hydrogen evolution reaction (HER). Stainless steel was well-known as the material containing electrocatalytic elements such as Fe and Ni, which are distinguished as excellent catalysts for hydrogen reduction reaction. In this study, the performance of anodic nanoporous stainless steel as electrocatalyst for HER is investigated. Nanoporous stainless steel electrode with large surface area provides a lot of active sites for electrochemical hydrogen evolution. Furthermore, thermal annealing treatment applied to prevents the deterioration of the anodic oxide layer offers ample oxygen vacancies accelerating the reaction kinetics without forming thermal oxide layer under Ar/H₂ atmosphere. Remarkably, the overpotential for the hydrogen evolution is additionally reduced from 370 to 348 and 244 mV after linear sweep voltammogram measurement at 10 mA cm⁻² for 5000 and 10000 cycles, respectively. The improved catalytic performance along with ultrastability is attributed to the self-activation of stainless steel electrocatalyst – hydroxylation of the anodic film during repeated cycles. This surface phenomenon is explored by the physical characterizations including x-ray diffraction (XRD), x-ray photoelectron spectroscopy (XPS), and Raman spectroscopy.

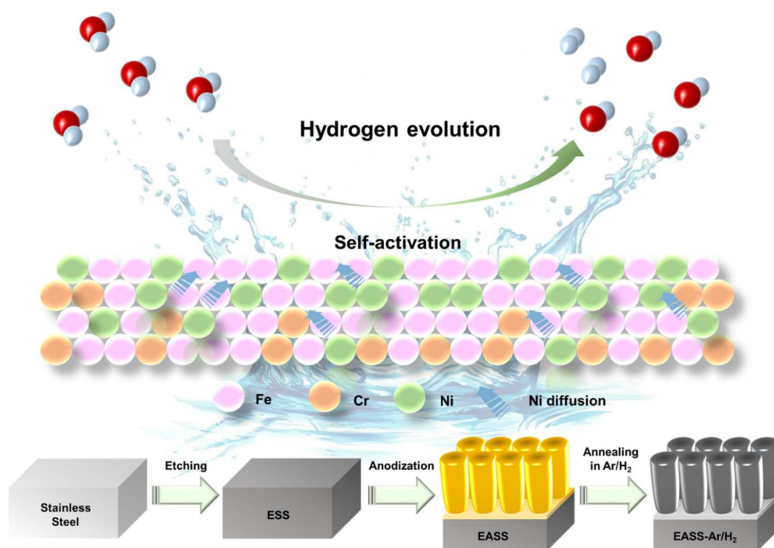


Figure Scheme of the self-activation and preparation of the catalysts.

Keywords: anodization, water splitting, hydrogen evolution reaction, stainless steel, self-activation, ultrastability

Electrochemical Study of an Aluminum Battery Operating with an Aqueous Electrolyte

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Aluminum ion batteries, a promising next-generation energy storage system gained attention due to their low cost, fast charging performance, excellent cycle performance and stability. Specifically, aluminum a naturally abundant trivalent metal exhibits a high theoretical volume capacity (8046 mAh cm^{-3}), which is about four times greater than lithium. However, ionic liquid ($\text{AlCl}_3[\text{EMIM}]\text{Cl}$) which have been mainly used as electrolyte for aluminum ion batteries, are expensive and its strong acidity nature have a high corrosion. To overcome this drawback, an alternative safe and inexpensive aqueous electrolyte is being studied. In aqueous aluminum ion batteries, graphitic materials, transition metal oxides, transition metals that can reversibly charge/discharge aluminum ions is widely used as an electrode.

In this study, an aqueous aluminum ion battery is fabricated and studied using various aqueous electrolytes. Aqueous aluminum ion batteries exhibit different performance depending on the type and concentration of the electrolyte. In addition, various cathode materials were applied to study the properties of aqueous aluminum ion batteries. The morphology was studied using a FE-SEM and TEM. The physical properties of the materials were investigated by XPS and XRD. Their electrochemical characteristics were studied by cyclic voltammetry, electrochemical impedance spectroscopy.

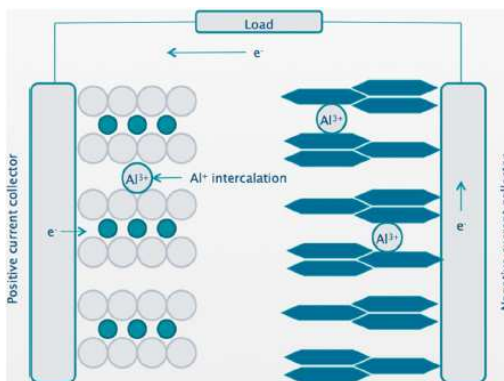


Figure Scheme of the aqueous aluminum ion battery^[1].

References

- [1] A. Holland et al., *J. Appl. Electrochem.* **2018**, 48, 243

Limits of Single-Atom Catalysts in Electrochemical Nitrogen Reduction Reactions: A DFT Study

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The electrochemical nitrogen reduction reaction (NRR) is one of the most attractive and emerging chemical process in clean hydrogen storage and transportation. As NRR catalysts, the single-atom catalysts (SACs) have been spotlighted as a promising candidate. But while we are studying on the Ru SACs, single-atom Ru showed its limits. We studied sub-nanoscale Ru catalysts embedded in modified defective graphene (Ru_x/YC , Ru: Ruthenium, x: 1 to 3, Y: Nitrogen and Boron, C: Carbon) using density functional theory (DFT) computation. First, we systematically investigated the energetically optimized geometries of Ru_x/YC . And the free energy of dissociative nitrogen adsorption on each catalyst was calculated to determine which mechanism to follow for NRR on Ru_x/YC . In addition, we calculated the adsorption energy of possible reaction intermediates to identify detailed reaction mechanism and the limiting potential for NRR on each catalyst. It was found that Ru SACs showed poor activity compared to diel-atomic and triple-atomic Ru catalysts. This is because the adsorption energy of reaction intermediates, including N_2H^* , has been adjusted to an appropriate level. We found Ru_2/NC as the most promising candidates for NRR catalyst due to the highest NRR activity and the selectivity.

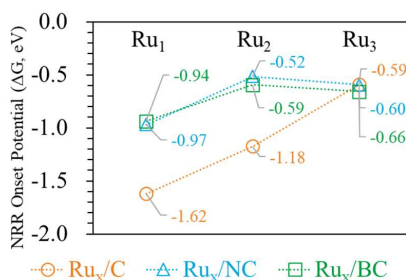


Figure Reaction free energy change on Ru_x/NC for NRR.

References

- [1] J. Zhao, Z. Chen, *J. Am. Chem. Soc.* **2017**, 139, 12480-12487.
- [2] C.H. Christensen, T. Johannessen, R.Z. Sørensen, J.K. Nørskov, *Catal. Today* **2006**, 111, 140-114.
- [3] B. Huang, N. Li, W.-J. Ong, N. Zhou, *J. Mater. Chem. A* **2019**, 7, 27620-27631.
- [4] B. Qiao, A. Wang, X. Yang, L.F. Allard, Z. Jiang, Y. Cui, J. Liu, J. Li, T. Zhang, *Nat. Chem.* **2011**, 3, 634-641.
- [5] J. Cho, S. Lee, S.P. Yoon, J. Han, S.W. Nam, K.-Y. Lee, H.C. Ham, *ACS Catal.* **2017**, 7, 2553-2562.
- [6] Y. Abghoui, E. Skúlason, *J. Phys. Chem. C* **2017**, 121, 6141-6151.

Porous V_2O_5 Nanostructures Prepared by Anodization: Effect of Annealing Temperature on the Performance of Lithium Ion Batteries

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Nowadays, commercially available lithium ion batteries (LIBs), which can convert chemical energy into electrical energy that can be applied from portable electronic to electric vehicles, are one of the most promising energy storage system exhibiting the features of high power and energy density, long cycle life, and environmental friendliness. To meet the ever-growing demands for electrified transportation and large-scale energy storage solutions, the development of novel electrodes beyond traditional cathode materials including the $LiCoO_2$, $LiFePO_4$ and $Li(NiCoMn)O_2$ generally deliver low capacity less than 200 mAh g^{-1} is essential for next-generation LIBs.

Vanadium pentoxide (V_2O_5), which has the most stable state of V^{5+} of the multiple valence states, is considered to be a promising candidate for the next generation cathode material due to its layered crystal structure and high output voltage, leading to high theoretical specific capacity up to 294 mAh g^{-1} (assuming intercalation of two lithium ions) and mass energy density to 1218 mWh g^{-1} (assuming a nominal 2.75 V discharge voltage). In this study, porous vanadium oxide nanostructures are prepared by straightforward anodization method using vanadium metal as substrate, enabling a binder-free type electrode without the use of any kinds of binder or conductive agents, and subsequent thermal annealing treatment to generate the desired phase and develop (001) plane promoting Li ion diffusion. We found that development of the (001) plane of V_2O_5 by thermal annealing above 300 °C leads to a significant enhancement in the specific discharge capacity of the electrodes due to the low energy barrier for diffusion of Li ions. Furthermore, irreversible generation of the V_3O_7 phase at 300 °C and over-development of the (001) plane at 500 °C result in severe capacity fading during the charge/discharge process.

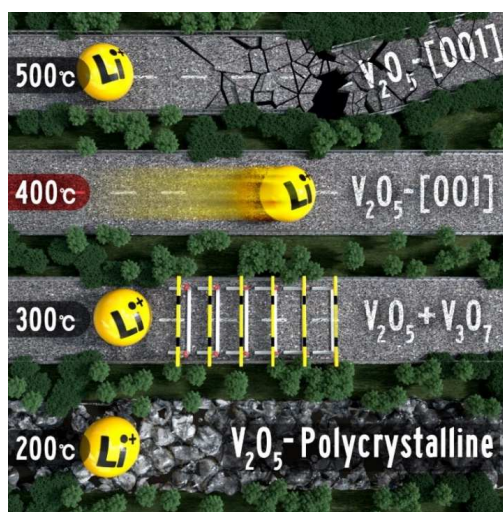


Figure Effect of thermal annealing treatment temperatures on the performance of lithium ion batteries for anodically prepared porous V_2O_5 cathode material.

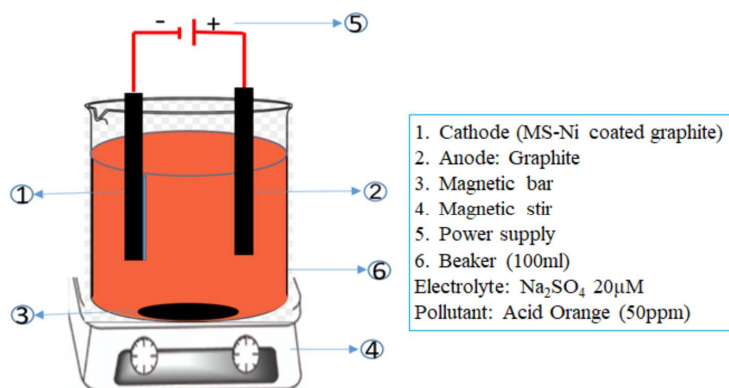
Sulfur-modified Metal Oxides for the Electro-Fenton System

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An electro-Fenton (EF) system was developed and investigated for Acid Orange 7 (AO7) degradation in wastewater. The cathode was prepared by mesoporous sulfur-modified metal coated graphite. The effect of sulfur doping was evaluated and the degradation pathway of AO7 was discussed. Both sulfur-modified and non-sulfur-modified metal oxides are abundant with pores, cracks, and have large surface areas. The effects of the operation parameters, such as voltage, catalyst dose, pH, electrolyte concentration, pH, and AO7 concentration were optimized. Results showed that MS-Ni exhibited a good activity for degradation of 50ppm AO7, achieving 94% removal efficiency after 4 hours under the optimal conditions, which was approximately three times higher than the value obtained by bare graphite (31%) as cathode.



Schematic of the degradation of AO7 by EF process

Figure Schematic of the degradation of AO7 by electro-Fenton process.

Keywords: Nanoporous Gold, Supercapacitors, Fuel Cells

Cobalt-Metal Hetero Double Atom Catalysts for Oxygen Evolution Reaction: A DFT Study

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Single-atom catalysts (SACs) have been extensively investigated in oxygen evolution reaction (OER) due to the maximized atomic efficiency and high catalytic activity. However, development of SACs surpassing conventional OER catalytic activity is still challenging. In this study, we first investigated Co@N₄/graphene as a referential SAC having an overpotential of 0.90V for electrocatalytic water oxidation through density functional theory (DFT) calculations. Then, we considered a hetero-double atom on the N-doped defective graphene (Co-M@N₄/graphene, M=In, Pd, Cu, Ga) instead of a single-atom in order to enhance OER activity, and estimated the effect of M towards the OER overpotentials. The DFT calculations revealed that the overpotentials of Co-Pd, -Cu, -Ga@N₄/graphene are 0.76, 0.84 and 1.12V respectively, and a hetero Co-In double atom exhibited the highest activity with the overpotential of 0.74V. This improvement is most likely due to the change of electronic structure on active sites. Consequently, this work could be used to explore promising hetero-double atom catalysts with high efficiency for water electrochemical oxidation in the future.

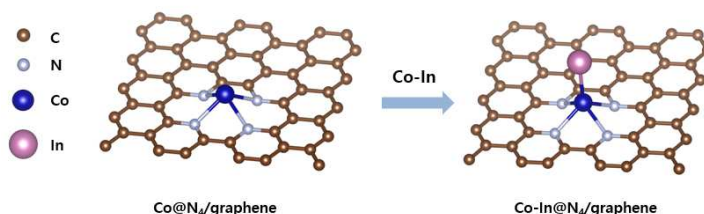


Figure Structure of Co-In@N₄/graphene.

Formation of NiO@Ni₃S₂ Heterostructure with Excellent OER Performance by Anodization and Hydrothermal Method

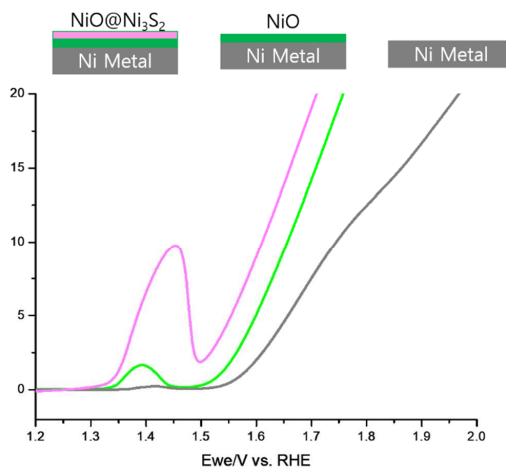
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Nickel based electrode materials are attracting attention as promising water electrolysis catalysts due to their low-cost, earth-abundant and excellent OER activity. In basic condition, most nickel based materials such as Ni oxides, sulfides, nitrides, phosphides, selenides, borates and MOFs can be converted from Ni(II) to Ni(III), which can easily form NiOOH having excellent OER activity. Especially, heterostructures with NiO and NiS binary chemical compositions can achieve better chemical properties than single species.

In this research, OER active materials were synthesized by anodization and hydrothermal method. First, porous NiO was fabricated on Ni foil by anodization method. Then, a sulfide layer was attached through hydrothermal method. Various parameter such as anodization conditions, annealing temperature and hydrothermal conditions were adjusted. The synthesized NiO@Ni₃S₂ heterostructure could be achieve a large number of active area and a uniform structure. Furthermore, in order to provide better active sites, oxygen vacancy was imparted through heat treatment in a reducing atmosphere.



Carbon-Supported IrRu Alloy Catalyst with High Performance for the Hydrogen Oxidation Reaction in Alkaline Membrane Fuel Cell

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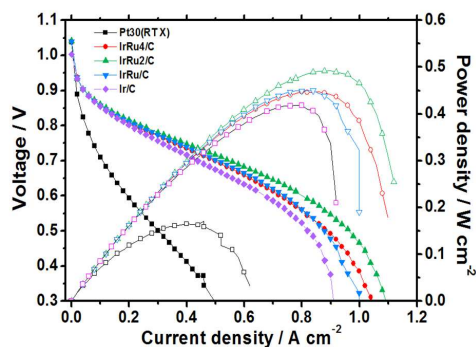
Anion exchange membrane fuel cell (AEMFC) has an advantage of the high efficiency of energy conversion and it is possible that use of the non-Pt catalyst^[1]. However, in alkaline media hydrogen oxidation reaction (HOR) kinetics on Pt are much more sluggish, being over 100 times slower than in acidic media. The development of electrocatalysts with higher activity than Pt/C for alkaline HOR is the key to improve the overall performance of AEMFC.

There is the recent development of PGM (precious group metal)-based (e.g., IrRu, PtRu)^[2] and PGM-free (e.g., NiMo, Ni/N-CNT)^[3] alkaline HOR catalysts. For PGM-free based HOR catalysts, the challenge originates from the demand to maintain a partly oxide-free metal surface up to an anode potential of 0.1 V. In this regard, the development of PGM-based HOR catalysts such as IrRu has been suggested.

In this study, to investigate the HOR activities of the IrRu/C catalysts with various compositions, the catalysts were prepared by the polyol method under the acidic condition for the first time. It could be possible that IrRu/C catalysts are prepared by the one-step and one-pot without any surfactant and stabilizer.

HOR activities were evaluated by chronoamperometry (at 20 mV_{RHE}) with various rotating speeds. HOR activity order is IrRu₂/C > Ir₂Ru/C > Ir₃Ru/C > IrRu₄/C > IrRu/C > Ir/C > Pt/C. It is shown that the HOR activity of the IrRu₂/C is superior to Pt/C, which is attributed to the oxophilic effect of the IrRu₂/C catalyst, as suggested by the XPS analysis.

To reveal an enhanced catalytic activity for HOR, membrane electrode assembly (MEA) tests are performed. The MEA performance (mA·cm⁻² at 0.6V) is following the order of IrRu₂/C (800) > IrRu/C (718) = IrRu₄/C (716) > Ir/C (678) > Pt/C (195), which is well agreed to the half-cell results.



References

- [1] D. R. Dekel, *J. Power Sources* **2018**, 375, 158-169
- [2] J. Ohyama, D. Kumada, A. Satsuma, *J. Mater. Chem. A*, **2016**, 4, 15980-15985
- [3] S. Kabir, K. Lemire, K. Artyushkova, A. Roy, M. Odgaard, D. Schlueter, A. Oshchepkov, A. Bonnefont, E. Savinova, D.C. Sabarirajan, P. Mandal, E.J. Crumlin, I.V. Zenyuk, P. Atanassov, A. Serov, *J. Mater. Chem. A*, **2017**, 5, 24433-24443

A study on the Effect of Including Co^{2+} Capturing Layer in PEMFC Cathode for Durability of PtCo/C Catalyst

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Proton exchange membrane fuel cell (PEMFC), one of the fuel cell types, needs catalysts due to high overpotential of oxygen reduction reaction. Therefore, Pt-based metal catalysts are commonly used for fastening oxygen reaction rate (ORR) rate. Both ORR activity and price competitiveness are need to be enhanced, 4d transition metals (e.g. Co, Ni, Fe) are alloyed with Pt. While its better performance, transition metals are easier to be dissolved than Pt in PEMFC operating condition, they cause deactivation of PEMFC performance.

In this study, we tried to get higher durability of the PtCo/C catalyst in PEMFC cathode by capturing dissolved Co^{2+} ion. N-doped carbon layer is added to capture dissolving Co^{2+} ion. We confirmed Co^{2+} ions are captured on capturing layer and compared ORR performance difference depending on the amount of N-doped carbon. Also, accelerated stress test was conducted to evaluate the durability of catalyst with N-doped carbon.

Layer-by-Layer Assembled Electrochemical Sensors for Low Molecular Weight Biomolecules

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Sensing technology is a fast-growing technology due to its urgent demand in various fields including medical diagnosis, food, and environmental monitoring^[1]. Therefore, it is important to detect biomolecules to prevent the spread of and cure diseases. In this poster, we demonstrate biosensing platforms using layer-by-layer (LbL) self-assembly of positively charged layer and negatively charged layer for biomolecules analysis on screen-printed carbon electrodes. Both cyclic voltammetry and differential pulse voltammetry were used for quantification analysis of biomolecules such as uric acid^[2], serotonin etc.... The electrode surface morphology was investigated by scanning electron microscope and atomic force microscopy while the surface composites was performed using X-ray photoelectron spectroscopy. The electron transfer property across the electrode-electrolyte interface was studied by electrochemical impedance spectroscopy. After the optimization of the LbL including layers, concentration of positive layer and negative layer, the LbL biosensor was further applied to evaluate the concentration of biomolecules in human normal serum and biomolecules related patients' serum samples. Preliminary results will be presented.

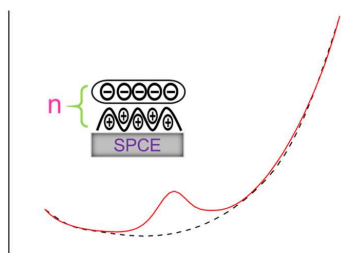


Figure Differential pulse voltammetry of biomolecules analysis in buffer without and with biomolecule using LbL biosensor.

References

- [1] T. Lakshmipriya, S.C. Gopinath, An introduction to biosensors and biomolecules. In Nanobiosensors for Biomolecular Targeting; *Elsevier*, **2019**, pp 1-21.
- [2] Y. Si, Y. E. Park, J. E. Lee, H. J. Lee, *Analyst* **2020**, *145*, 3656-3665.

Enhancement of Photogenerated Charge Transport by TiO₂ Modified WO₃/BiVO₄ Core-Shell Heterojunction

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Photoelectrochemical (PEC) water oxidation is a promising approach to generate hydrogen using solar light. For the purpose, several candidate materials are considered that are mostly semiconductive materials including metal oxide. Among various metal oxides, WO₃ has been regarded as a prospective resource because of their suitable band position, relatively higher photocorrosion resistance, and low cost. WO₃ allows photogenerated electrons and provide easy electron pathway to current collector through the conduction band. Furthermore, BiVO₄ deposition on WO₃ can attract hole from WO₃ that plays a key role for oxygen evolution reaction. Nevertheless, BiVO₄ has a drawback to be solved with respect to stability. For this reason, blocking layers with high band gap energy are suggested to protect the unstability. In particular, TiO₂ has not only high band gap energy but also chemical/physical stability. Moreover, TiO₂ blocks solution-mediated recombination at surface of WO₃/BiVO₄ core-shell heterojunction, which helps to improve PEC efficiency.

In the present work, we achieve facile approach to modify WO₃/BiVO₄ with TiO₂ deposition. As a result, photoinduced current density is recorded as 0.83 mA cm⁻² at 1.23 V vs. reversible hydrogen electrode (RHE) under AM 1.5 G illumination. This value makes 78.8 μL cm⁻² of H₂ evolution, which indicates almost 3.60 times higher than the WO₃ nanoplates.

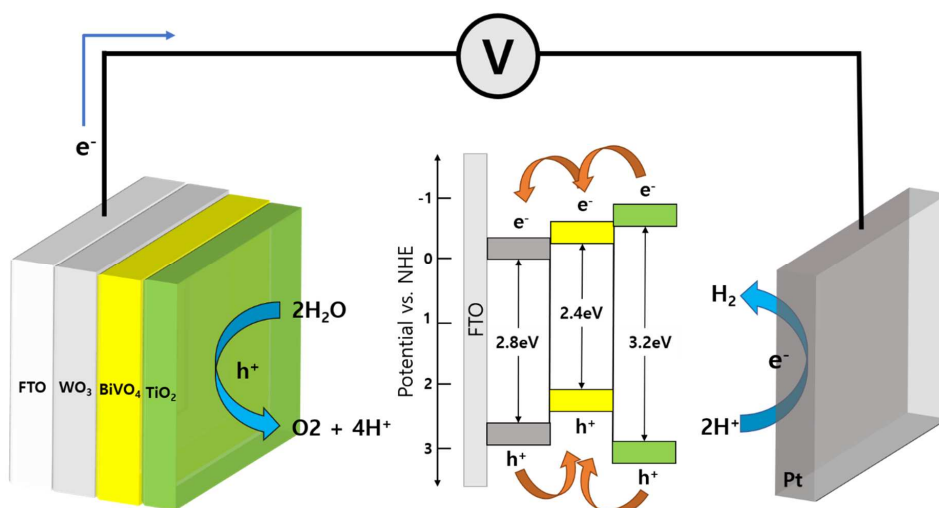


Figure Schematic illustration of a circuit with WO₃/BiVO₄/TiO₂ heterojunction.

The Morphological Transitions of Ni/C Catalyst for Hydrazine Oxidation

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Hydrazine fuel cell is one of the promising liquid fuel cells because of high theoretical voltage, high energy density, and no green gas emission. However, hydrazine can be decomposed chemically or electrochemically as a function of the type of catalyst used. Platinum, despite a noble metal, is an ambiguous catalyst due to faradaic reaction catalyst of hydrazine as well non-faradaic reaction. Therefore, in the aspect of the fuel efficiency, platinum is not suitable for hydrazine catalyst. Nickel, which is the same family with platinum, is non-noble metal and has quite good performance for hydrazine oxidation due to its similar structure to platinum. In these aspects, hydrazine fuel cell is further important, not requiring the expensive noble metal. Here, we synthesized Ni nanoparticles via polyol method changing the type of Ni precursor, since chemical, physical, and electro-chemical properties of a metal nanoparticle depend on its morphology and size. When using nickel nitrate, Ni nanoparticle size is smallest with shapeless morphology, whereas using nickel chloride, size is somewhat big but particles are well-spreaded on carbon support. Then, in order to confirm hydrazine electro-oxidation performance, catalyst ink was loaded on the rotating disk electrode (RDE), linear sweep voltammetry (LSV) was carried out (Fig. 1).

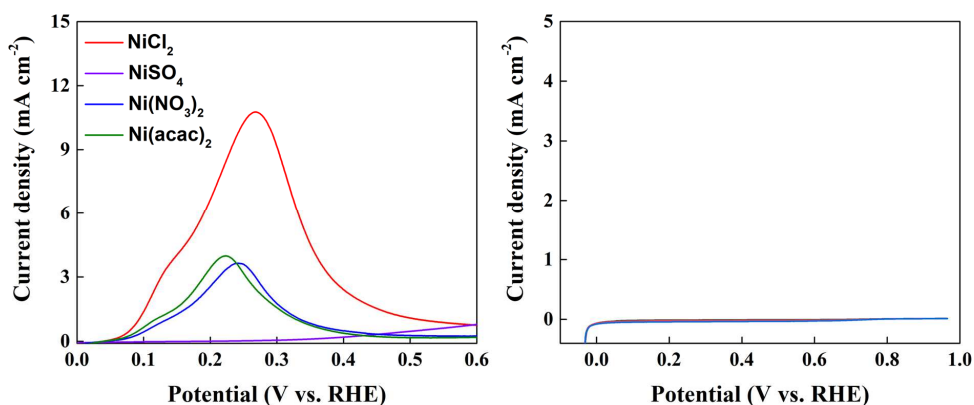


Figure Current – voltage plot as a function of Ni precursor with (left) and without (right) 0.1 M N₂H₄ with 1.0 M KOH solution.

Preparation of Ion-Conducting Composite Membranes for Low Temperature Fuel Cells

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Most of electrochemically driven energy conversion devices consist of anodic reaction, ion movement and cathodic reaction to complete full electrochemical cells. Ions move from anode to cathode or vice versa for electron exchanges. Pathway for ions is normally in an aqueous phase. Regardless, the introduction of any aqueous phase in energy conversion devices causes many problems during fabrication, operation, maintenance, and so on. Thus, much efforts have been devoted to develop quasi-solid electrolytes such as gel polymer, ion exchangeable polymers, impregnation of ions in porous matrix and so on. One of major disadvantages to use polymeric electrolytes is significant Ohmic voltage decay due to high areal resistance compared to aqueous phases. An approach to minimize areal resistance of film-type polymeric electrolytes is to make film thickness as thin as possible. Free standing polymeric electrolytes, however, show low mechanical properties. Thus, composite membranes could be used by impregnating polymeric electrolytes into thin porous substrates. The reinforced composite membrane is manufactured by impregnating an ionomer into support that provides mechanical strength. Currently, polytetrafluoroethylene (PTFE) is the most widely used as substrate for reinforced composite membranes. However, it is difficult to uniformly impregnate the hydrophilic ionomer solution because the PTFE surface has a hydrophobic nature. In this study, compatibility with hydrophilic ionomer solution was confirmed by hydrophilizing PTFE substrate which is hydrophobic, and the characteristic was analysed by producing composite membranes. A technique to impregnate polymeric electrolytes into porous substrates were intensively developed so as to prepare void-free composite membranes. Characterization in terms of ion conductivity, ion exchange capacity, water uptake, dimensional stability, mechanical strength was carried out.

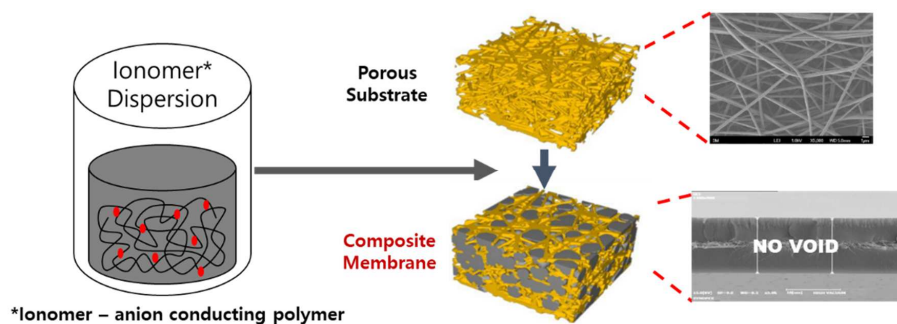


Figure Schematic diagram of showing the preparation of composite membranes.

Acknowledgement

This research was supported by the Technology Development Program to Solve Climate Changes of the National Research Foundation (NRF) funded by the Ministry of Science, ICT & Future Planning (NRF-2018M1A2A2063866).

Microstructure-Reactivity Relationships in the Electrocatalytic Oxygen Evolution Reaction of Cobalt Iron Oxide Catalysts Prepared by Microemulsion Assisted Co-precipitation

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Conventional co-precipitation at constant pH is a well-known technique for the synthesis of microcrystalline layered double hydroxides (LDHs) with platelet morphology. To achieve the formation of more isotropic colloids of these compounds, reverse micelles acting as nanoreactors can be used to confine the co-precipitation within the water droplets. This work establishes a new synthesis method with accurate online pH-control for the preparation of CoFe-LDHs and the corresponding spinels, which are accessible through calcination. Different pH values were applied to elucidate the effect of this synthesis parameter on CoFe-LDHs and the calcination products for both synthesis approaches. For samples prepared by microemulsion-assisted co-precipitation (MACP) a distinct trend in pore size was found with variation of pH. Both synthesis series revealed low overpotential in the electrocatalytic oxygen evolution reaction (OER). The microemulsion based series followed a clear trend towards a plateau, whereas no clear correlation with precipitation pH or porosity was found for the conventional samples. Upon calcination, a pronounced decrease in activity is observed for the spinels derived from the conventional synthesis, whereas the performance of the spinels obtained after thermal decomposition of the LDHs synthesized by MACP remains almost unaffected, which is a uniqueness of this synthesis technique. The higher OER activity of the microemulsion-based spinels might be explained by differences in bulk structure, a higher amount of Co²⁺ at the surface and a higher Co:Fe ratio as shown by *operando* X-ray absorption spectroscopy and quasi *in-situ* X-ray photoelectron spectroscopy.

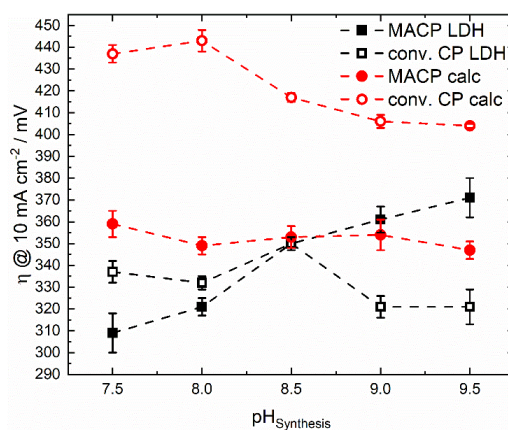


Figure Overpotential at 10 mA cm⁻² for LDHs and spinels derived from both synthesis approaches.

Electrochemical Determination of Catechol Polymerization Catalysed by Laccase/ABTS System

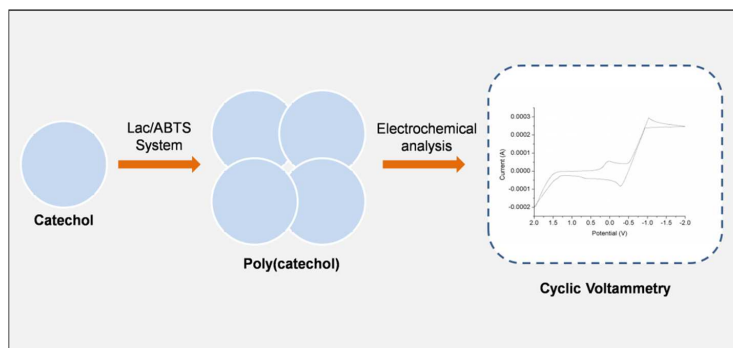
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The phenolic compound catechol has found various applications in the industry and is often discharged untreated in industrial effluents. The non-degradable toxic nature of the compound makes it an environmental hazard, which has led researchers to use the enzyme laccase for its ability to detect and polymerize catechol into a much lesser harmful compound. In the present study, we focus on studying the polymerization conditions of catechol electrochemically in reaction with laccase and the redox mediator 2,2'-azino-bis(3-ethylbenzothiazoline-6-sulfonic acid) (ABTS). The reactions carried out over a range of concentrations provided a thorough insight into ABTS' as well as laccase' differential effect on the compound. The characteristics of electron transfer in the reactions provided insight into the role the electroactive species of ABTS play in the polymerization of catechol. But, in comparison laccase brings about a high rate of oxidation coupled with a high rate of reduction along with polymerization. The evaluation of the cathodic and anodic reactions' changes in relation to concentration, in presence of the laccase/ABTS system verified their impact is concentration-dependent and is more gradual as the redox nature of the mediator enhances the electron transfer activity between the enzyme and substrate. Therefore, the ability of the laccase/ABTS system to polymerize catechol could serve as a building block in developing technologies including the treatment of wastewater and biosensors.



Synthesis of Hydrophilic Ionic Liquid for Future Energy Related Applications

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To meet the increasing demand for clean and sustainable energy, ionic liquids electrolytes are becoming alternate electrolytes in fuel cell due to less corrosive comparing to alkali metal based electrolytes like KOH^[1,2]. Room temperature ionic liquids (RT-ILs) of which the melting temperature is less or at room temperature can be used because they are consisted of organic or inorganic anions and organic cations having many exclusive properties such as high conductivity, low volatility, high thermal and electrochemical stabilities^[3]. In this work, we synthesized hydrophilic alkaline ionic liquid (IL) having hydroxide ion as anion part. Different parameters such as thermal stability and electrolyte performance were investigated via thermogravimetric analysis (TGA), differential scanning calorimetry (DSC), ionic conductivity, viscosity and cyclic voltammetry (CV)^[4]. In addition, the structure was examined through Fourier transform infrared spectroscopy (FTIR) and ¹H-NMR. The results indicate that the IL is promising for future energy related applications.

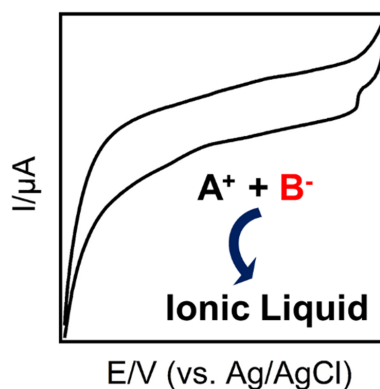


Figure A preliminary cyclic voltammogram data showing electrochemical potential window of ionic liquid.

References

- [1] J. L. A. C. Cadena, J. K. Shah, T. I. Morrow, J. F. Brennecke, E. J. Maginn, *J. Am. Chem. Soc.* **2004**, *126*, 5300.
- [2] R. D. M. E. D. Bates, I. Ntai, J. H. Davis, *J. Am. Chem. Soc.* **2002**, *124*, 926.
- [3] Y. F. H. Nakagawa, S. Kozono, Y. Katayama, T. Nukuda, H. Sakaebe, H. Matsumoto, K. Tatsumi, *J. Power Sources* **2007**, *174*, 1021
- [4] M. Salman, H. J. Lee, *J. Appl. Chem.*, **2020** in press.

Chicken Manure-Based Synthesis of Hierarchical Porous Carbons as ORR Electrocatalysts in Low Temperature Fuel Cells

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Chicken manure is a heteroatoms-rich biomass material, which is abundant in nature and is mainly used as manure for agricultural purposes. However, the real potential of this material has been explored after mixing it with kitchen waste for the design of an efficient electrocatalyst for the oxygen reduction reaction in fuel cell applications. The mixture of kitchen waste and chicken manure has been processed into organic compost in soil under environmental conditions (temp. 22-37 °C; humidity: 70-90 %). The organic compost was then treated at high temperature (700-1100 °C) under an inert gas atmosphere to prepare different samples, and the sample synthesized at 900 °C showed the best electrocatalytic performance. This electrocatalyst comprises of mesoporous carbons with pore size 32.670 nm and also includes multiple (N, P and S) heteroatoms. A more positive onset potential (-0.0806 V) and a higher limiting diffusion current density (-3.07 mA cm^{-2}) that is comparable to the commercial Pt/C electrocatalyst has been observed. The higher ORR performance has been explained to be due to the versatility of the biomass materials used, multiple heteroatoms-induced active sites, and the existence of mesoporous carbonaceous architecture. The performance of these materials based on chicken manure and kitchen waste can be further improved and can result in an environment-friendly strategy for developing high performance electrocatalysts for fuel cell applications along with green management of these wastes.

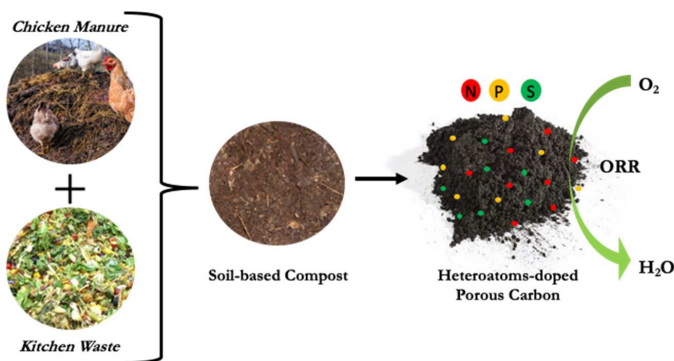


Figure Schematic details of the synthesis of heteroatom-doped porous carbon from chicken manure.

Acknowledgements

This research work was supported in part by Brain Pool Program through the National Research Foundation of Korea (NRF) funded by the Ministry of Science and ICT (2019H1D3A2A02102086) and in part by the Hydrogen Energy Innovation Technology Development Program of the National Research Foundation of Korea (NRF) funded by the Ministry of Science, ICT, & Future Planning (2019M3E6A1063677).

Enhancement of Electrochemical Redox Reaction by Transition Metal Oxalates for High-Performance Lithium-Sulfur Battery

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As the growth of global EVs market and continuous advances of IT devices' functionality, higher capacity and cycle stability of secondary batteries are being demanded. Lithium-sulfur(Li-S) battery is one of the promising next-generation batteries due to high theoretical capacity (1,672 mAh/g), natural abundance, and environmental nontoxic compare to conventional active materials of lithium-ion batteries. However, lithium polysulfide(PS) dissolution issue which causes capacity fade inevitably must be overcome for commercialization. In this study, we introduced metal oxalates synthesized with the first transition metal series as cathode additives. They have a high polar surface area which is able to enlarge the electrocatalytic interfacial boundary enabling LiPS redox reactions to occur. Furthermore, physicochemical interactions between LiPS and metal oxalates were verified by UV-vis, X-ray Photoelectron Spectroscopy, and Electrochemical Analysis. As a result, the modified cathode by the best candidate effectively decreased cell overpotential and improved the cycle stability by maximized electrochemical sulfur utilization.

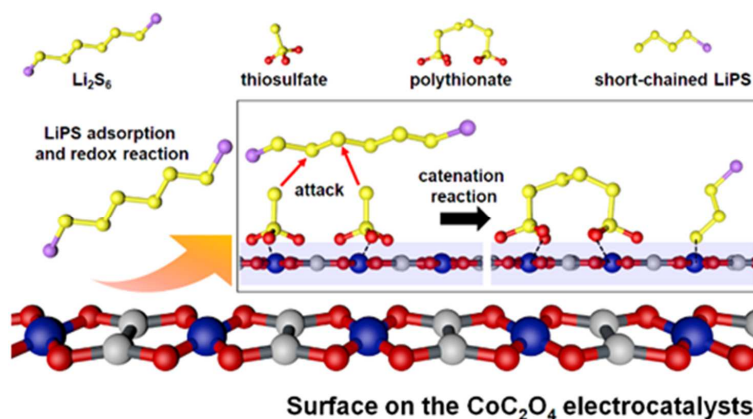


Figure Schematic illustration of LiPS redox reaction on the surface of CoC₂O₄ placed on the interfacial boundary contacted with a conductive carbon, CoC₂O₄ and LiPS reactor (blue:cobalt, red:oxygen, grey: carbon, yellow:sulfur, and purple:lithium atom).

References

- [1] David Sichen Wu, Feifei Shi, Guangmin Zhou, Chenxi Zu, Chong Liu, Kai Liu, Yayuan Liu, Jiangyan Wang, Yucan Peng, Yi Cui, *Energy Storage Mater.* **2018**, 13, 241–246.
- [2] Joyce S. Yeoh, Ceilidh F. Armer, Adrian Lowe, *Mater. Today Energy* **2018**, 9, 198–222.

Portable Electrochemical Sensors for Monitoring Alkaline Fuel Concentrations

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The global energy crises has led to an increase in the search for alternative environmentally friendly energy sources and there is increasing demand for the development of sensors to monitor the concentrations of the fuel in such systems^[1,2]. The combined effects of inorganic-organic hybrid nanomaterials have made this route for a new generation of electrochemical sensors with improved flexibility and mold-ability over organic materials and high heat stability and chemical resistance over inorganic materials. Herein, we report recent efforts made on the fabrication of a portable electrochemical sensor by the modification of a screen-printed carbon electrode using conducting polymers and metal alloy nanoparticles for potential application in monitoring fuel concentration. The surface morphology of the developed sensor was first characterized by scanning electron microscope (SEM) and the electrochemical characteristics and sensing performance of the fabricated sensor were evaluated by cyclic voltammetry (CV) and chronoamperometric measurements. The results obtained indicates that the developed electrochemical sensor could be a promising tool for alkaline fuel detection.

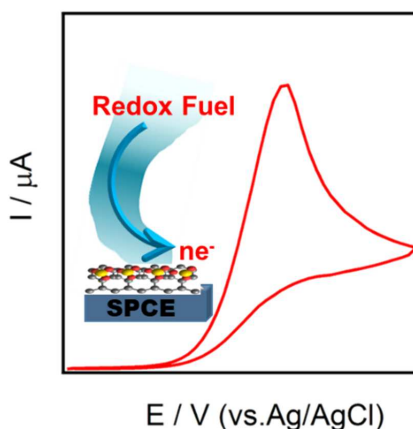


Figure A preliminary cyclic voltammogram for alkaline fuel concentration in 0.1 M KCl using a metal alloy modified electrode.

References

- [1] M. Liu, R. Zhang, L. Zhang, D. Liu, S. Hao, G. Du, A.M. Asiri, R. Kong, X. Sun, *Inorganic Chemistry Frontiers* **2017**, 4(3), 420-423.
- [2] X. Liu, J. He, S. Zhao, Y. Liu, Z. Zhao, J. Luo, G. Hu, X. Sun, Y. Ding, *Nat Commun* **2018**, 9(1), 4365.

Amine-Functionalized Zeolitic Imidazolate Framework-8 (ZIF-8) Nanocrystals for Adsorption of Radioactive Iodine

Xuan Huy Do^{a,b}, Yu-Ri Lee^a, Baek Kyung-Youl^{a,b,c*}

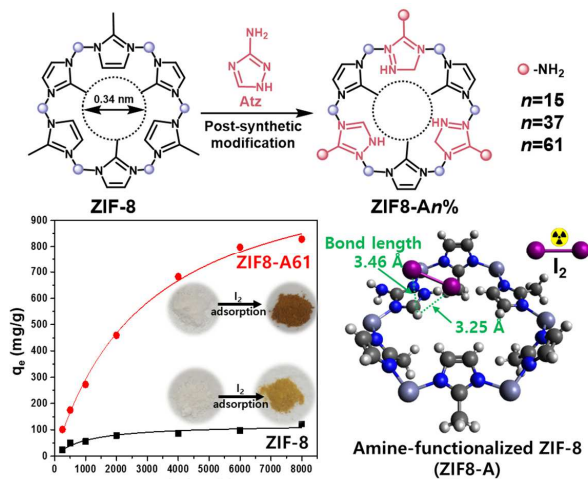
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The efficient removal of radioactive iodine (I_2) has drawn worldwide attention because of the severe effects of radiotoxicity on the environment and human health. As a result, efficient porous materials for the capture and safe storage of radioactive iodine are required. In this work, nanoscale zeolitic imidazolate framework-8 (ZIF-8) and its amino-functionalized ZIF-8 derivatives with 3-amino-1,2,4-triazole (Atz), denoted as ZIF8-A, were prepared via post-synthetic modification, and their performance for I_2 removal from n-hexane was investigated. The abundant amine functionalities in ZIF8-A structure including the primary and secondary amine groups ($-NH_2$ and $-NH$), and triazole ring ($-C=N-NH-$) not only serve as effective adsorption sites but form strong interactions with I_2 via electron transfer from the nitrogen atom of the ligand to I_2 . The adsorption isotherms and the kinetics were well-fitted by the Langmuir model and the pseudo-second order kinetic model, respectively, suggesting a monolayer chemisorption process. ZIF8-A61 achieved an adsorption capacity of more than 870% compared to the pristine ZIF-8. Based on the experimental and computational results, a plausible mechanism for the adsorption of I_2 on ZIF8-A nanocrystal is proposed by considering the host-guest interactions, specifically, those between the amine functional groups and I_2 . In addition, the reusability and structural stability of the adsorbents were investigated.



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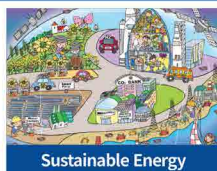
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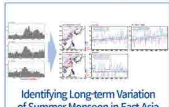
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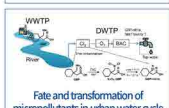
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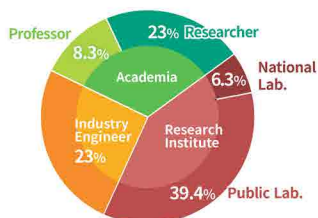


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