2024
International Symposium on Materials Chemistry
2024 충남대학교 소재화학연구소 국제학술대회

| 일시 | Time

2024년 10월 14일(월) 14:30~18:00
October 14th (Monday) 2024

| 장소 | Place

충남대학교 자연과학대학 4호관(W11-2) 109호
Room 109, Natural Science Building 4 (W11-2), Chungnam National University, Daejeon, Korea

| 주관 | Host

충남대학교 소재화학연구소
Research Institute of Materials Chemistry, Chungnam National University

| 후원 | Sponsors

충남대학교 화학과
Department of Chemistry, Chungnam National University

충남대학교 화학물질특성분석 핵심연구지원센터
CNU Chemistry Core Facility

충남대학교 뉴그린 에너지 · 환경화학 연구소
Institute of New Green Energy & Environment Chemistry, Chungnam National University

2024년도 CNU 선도학문분야 글로벌연구실 지원사업
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충남대학교 3단계 산학연협력 선도대학 육성사업단
Leaders in INdustry-university Cooperation 3.0 (CNU LINC 3.0)

Welcome Address

The hot summer has finally ended, and the beautiful autumn has arrived, providing the perfect setting for our 2024 International Symposium on Materials Chemistry. It is my great pleasure to welcome all of you to this event, hosted by the Research Institute of Materials Chemistry at Chungnam National University. This symposium offers a unique platform for academic and industry experts to come together, exchange ideas, and explore innovative solutions to some of the most pressing challenges in chemistry. I am confident that today's sessions will provide us with valuable knowledge and foster fruitful discussions that will contribute to the advancement of this field. I would like to extend my sincere thanks to all our speakers for their participation and for sharing their work with us. I hope that today's symposium will not only be an opportunity to gain knowledge but also to build lasting connections and collaborations among researchers from different countries and institutions.

Once again, welcome, and I wish you all a very successful and productive symposium. Thank you.

October 2024

Jeongkwon Kim, Ph.D.

Director of Research Institute of Materials Chemistry

2024 International Symposium on Materials Chemistry

Date: October 14th (Monday) 2024

Location: Room 109, Natural Science Building 4 (W11-2), Chungnam National University, Daejeon, Korea

〈 Program 〉

14:30-14:50 Registration

14:50-15:00 Opening Remarks :
Prof. Min Yong Jeon (Dean, CNS)
Prof. Jeongkwon Kim (Director, RIMC, CNU)

〈Session I〉

Chairperson : Prof. Ji-Hyun Cha (Chungnam National University, Korea)

15:00-15:30 Dr. Phu-Cuong Nguyen
(Department of Food Science and Technology, Chungnam National University)
"Novel Lipophilic Inotodiol–Oleic Acid Conjugates: Synthesis, Characterization, and Digestion/Absorption Behavior "

15:30-16:00 Dr. Mohamed A. Gab-Allah
(National Institute of Standards, Egypt)
"Synthesis of boronic acid-functionalized mesoporous nanomaterial for selective capture of glycopeptides from human serum"

16:00-16:30 Dr. Hyun Sik Kim
(ASTA Corporation, Korea)
“Development of Mass Spectrometers for Industrial and Medical Applications”

16:30-16:40 Coffee Break

〈Session II〉

Chairperson : Prof. Jinwoo Kim (Chungnam National University, Korea)

16:40-17:10 Prof. Jin-sil Choi
(Department of Chemical and Biological Engineering, Hanbat National University, Korea)
"Nanozyme: beyond the natural enzyme for a better detection system"

17:10-17:40 Prof. Boon Siang Jason YEO
(Department of Chemistry, National University of Singapore, Singapore)
"Electrosynthesis of Oxygenates and Hydrocarbons"

17:40 - 17:50 Photo Time

18:00 - 20:00 Dinner

CV's and Abstracts

Brief C.V.

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Experience in reverse chronological order (latest first)

2024-present: Research Professor. Chungnam National University
2020-2023: KRF (Brain Pool)-Postdoctoral Research Fellowship. Chungnam National University
2014-2020: Graduate School Research Assistant. Chungnam National University
2009-2014: Researcher. Can Tho University, Vietnam.

Education in reverse chronological order (latest first)

Ph.D. in Food Science & Technology (2020). Chungnam National University.
M.S. in Food Science & Technology (2017). Chungnam National University.
B.S. in Food Technology (2009). Can Tho University, Can Tho, Vietnam.

Representative publications

1. Enzymatic synthesis and characterization of novel lipophilic inotodiol–oleic acid conjugates. (2024). Food Chemistry. Impact Factor: 8.5. (First-author).
2. Enhancement of bioavailability and anti-inflammatory activity of inotodiol through complexation with γ- cyclodextrin. (2024). Journal of Drug Delivery Science and Technology. Impact Factor: 4.5. (Co-author).
3. Isolation, physicochemical characterization, and biological properties of inotodiol, the potent pharmaceutical oxysterol from Chaga mushroom. (2023). Antioxidants. Impact Factor: 6.0. (First-author)
4. One-step synthesis of glycogen-type polysaccharides from maltooctaose and its structural characteristics. (2022). Carbohydrate polymers. Impact Factor: 10.7. (Co-author).
5. A novel maltoheptaose-based sugar ester having excellent emulsifying properties and optimization of its lipase-catalyzed synthesis. (2021). Food Chemistry. Impact Factor: 8.5. (First-author)
6. Enzymatic synthesis and characterization of maltoheptaose-based sugar esters. (2019). Carbohydrate polymers. Impact Factor: 10.7. (First-author).

Abstract

Title, author(s), affiliation(s), and body text

Novel Lipophilic Inotodiol–Oleic Acid Conjugates: Synthesis, Characterization, and Digestion/Absorption Behavior

Phu-Cuong Nguyen [a], My-Tuyen Thi Nguyen [b], So-Young Ban [a,c], Jaehan Kim [b], Jong-Tae Park [a,c,*]

[a] *Department of Food Science and Technology, Chungnam National University, Daejeon 34134, Republic of Korea*
[b] *Department of Food and Nutrition, Chungnam National University, Daejeon 34134, Republic of Korea*
[c] *CARBOEXPERT Inc., Daejeon 34134, Republic of Korea*

Inotodiol, a medicinal oxysterol derived from Chaga mushrooms, has garnered increasing research interest due to its multifunctional properties, including antioxidant, anti-cancer, anti-inflammatory, and anti-allergic activities. However, the oral bioavailability of inotodiol is poor due to its hydrophobic structure. In this study, we establish an efficient enzymatic approach for producing novel inotodiyl-oleates (IOs) from pure inotodiol and oleic acid to improve the properties of inotodiol. For the esterification between inotodiol and oleic acid, lipase A from *Candida antarctica* and n-hexane were the optimal biocatalyst and solvents for forming IOs with 80.17% conversion yield. These IOs comprised two distinct monoesters, the C3 or C22 ester forms of inotodiol. Intriguingly, no diesters were detected. The IOs had a melting point of 53.48 °C, much lower than that of inotodiol (192.06 °C). The *in vitro* digestion rate of IOs (25–28%) was significantly ($p < 0.05$) lower than that of cholesteryl-oleate (60%). Additionally, IOs exhibited much lower *in vivo* absorption than inotodiol when orally administered using different formulations ($p < 0.05$). The results indicated that IOs were resistant to enzymatic digestion in the small intestine, which could be advantageous in targeting the large intestine for disease treatments.

Brief C.V.

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ORCID ID: 0000-0002-0993-5991

Experience in reverse chronological order (latest first)

May 2012 – Present Researcher, National Institute of Standards, Egypt
Sept 2023- Present Post-doctoral fellow, Chungnam National University, Chemistry Department (South Korea).

- Proteomics (glycopeptide enrichment and analysis in human biofluids using nano-LC-MS/MS).
- Analysis of organic contaminants and nutrients (i.e., mycotoxins, antibiotic residues, and vitamins) in foods using multi-analyte methods (LC-MS/MS).

Education in reverse chronological order (latest first)

Ph.D. in Analytical Chemistry (2023), University of Science and Technology/Korea Research Institute of Standards and Science (South Korea).
M.Sc. in Analytical Chemistry (2017), Cairo University (Egypt)
B.Sc. in Chemistry (2010), Menoufia University (Egypt)

Representative publications

1- **Gab-Allah, M. A.**, & Kim, J.* (2024). A Comprehensive Review of Recent Advances in the Enrichment and Mass Spectrometric Analysis of Glycoproteins and Glycopeptides in Complex Biological Matrices. Mass Spectrometry Letters, 15(1), 1-25.
2- **Gab-Allah, M. A.**, Lijalem, Y. G., Yu, H., Lim, D. K., Ahn, S., Choi, K.,* & Kim, B.* (2023). Accurate determination of four tetracycline residues in chicken meat by isotope dilution-liquid chromatography/tandem mass spectrometry. *Journal of Chromatography A*, 463818.
3- **Gab-Allah, M. A.**, Lijalem, Y. G., Yu, H., Lee, S., Baek, S., Han, J., Choi, K.*, & Kim, B.* (2022) Development of a certified reference material for the accurate determination of type B trichothecenes in corn. *Food Chemistry*, *404*, 134542.
4- **Gab-Allah, M. A.**, Choi, K.*, & Kim, B.* (2022). Development of isotope dilution–liquid chromatography/tandem mass spectrometry as a candidate reference method for the accurate determination of patulin in apple products. *Analytical and Bioanalytical Chemistry*, *414*(5), 1867-1879.
5- **Gab-Allah, M. A.**, Choi, K.*, & Kim, B.* (2021). Accurate determination of type B trichothecenes and conjugated deoxynivalenol in grains by isotope dilution–liquid chromatography tandem mass spectrometry. Food Control, 121, 107557.
6- **Gab-Allah, M. A.**, Choi, K.*, & Kim, B.* (2021). Development of isotope dilution-liquid chromatography/tandem mass spectrometry for the accurate determination of type-A trichothecenes in grains. Food Chemistry, 344, 128698.
7- **Gab-Allah, M. A.**, Mekete, K. G., Choi, K.*, & Kim, B.* (2021). Occurrence of major type-B trichothecenes and deoxynivalenol-3-glucoside in cereal-based products from Korea. Journal of Food Composition and Analysis, 99, 103851.

Abstract

Title, author(s), affiliation(s), and body text

Synthesis of boronic acid-functionalized mesoporous nanomaterial for selective capture of glycopeptides from human serum

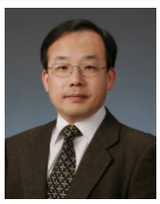
Mohamed A. Gab-Allah[a,b], Jeongkwon Kim[b]*

[a]*National Institute of Standards, Egypt*
[b]*Department of Chemistry, Chungnam National University, Daejeon, Republic of Korea*

As an important and widespread post-translational modification of proteins, glycosylation plays a key role in regulating a variety of complicated biological reactions. Because glycopeptides are low abundant and the ionization efficiency could be suppressed in mass spectroscopic detection, highly efficient and selective enrichment methods are essential to identify protein glycosylation by mass spectrometry. Boronate affinity materials, as unique sorbents, have emerged as important media for the selective separation and molecular recognition of cis-diol-containing biomolecules including glycopeptides. In this study, we propose a new enrichment strategy using a boronic acid (BA)-functionalized mesoporous nanomaterial for isolating intact glycopeptides from human serum. The material was prepared by using a two-step post-grafting method. Firstly, the 3-glycidyloxypropyltrimethoxysilane (GLYMO) and 3-aminophenylboronic acid monohydrate (APB) were reacted to prepare boronic-acid bonded GLYMO (denoted as GLYMO-APB). Secondly, the nanocomposite was added to the prepared GLYMO-APB solution to prepare the final product. This as-prepared material was characterized by FT-IR, and the results showed that the boronic acid groups were successfully grafted to the nanocomposite material. The attractive features of this composite, including high surface area, hydrophilic interaction of silica, and the reversible covalent binding with BA enable the effective and specific enrichment of glycopeptides. The glycopeptide enrichment efficacy was evaluated by the enrichment of IgG N-glycopeptides. In total, 29 glycopeptides enriched from IgG digests were identified by nanoLC-MS/MS, and 180 glycopeptides corresponding to 84 glycoproteins were enriched from merely 2 μL serum using this material, indicating a great potential of the material for glycoproteomic research.

Brief C.V.

General information (Name, e-mail, homepage, google scholar ID, ORCID iD, etc)



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Experience in reverse chronological order (latest first)

2022 – 2024	ASTA Corporation R&D Center, Director : Development of Gas monitoring TFO-MS & TGA TOF-MS
2003 – 2021	Division of Scientific Instrumentation & Management, Principal Researcher, Director : Instrument Development of FT-ICR MS, & portable MS
1996 – 2003	Principal Research Scientist, LG Chemical Ltd / Research Park : Proteomics & characterization of Pharmaceutical protein drugs
1995 - 1996	Post-doctoral Research Fellow, California Institute of Technology : Development of MALDI/FT-ICR MS

Education in reverse chronological order (latest first)

1990 - 1994	Ph.D. in Physical & Analytical Chemistry with Prof. Alan G. Marshall. Department of Chemistry, **The Ohio State University**, Columbus, Ohio.
1983 - 1985	M.S. in Physical Chemistry with Prof. Kwan Kim. Department of Chemistry, **Seoul National University**, Seoul, Korea.
1979 - 1983	B.S. in Chemistry. Department of Chemistry, College of Education, **Seoul National University**, Seoul, Korea.

Representative publications

1. Kim, H.S.; Wood, T.D.; Lee, J ; Marshall, A.G.*, "Production of Gold Cluster Ions by Laser Desorption/Ionization Fourier Transform Ion Cyclotron Resonance Mass Spectrometry", ***Chem. Phys. Letter.*** **224(5,6)**, *1994,* 589-594.
2. Kim, H.S.; Marshall, A.G.*, "Magnitude-Mode Multiple-Derivative Spectra for Resolution Enhancement without Loss in Signal-to-Noise Ratio in FT-ICR Mass Spectrometry", ***J. Mass Spectrom.*** **30**, *1995,* 1237-1244.
3. Myoung Choul Choi, Kyu Hwan Park, Sunghwan Kim, Jong Shin Yoo*, Hyun Sik Kim*; "Improved Ion Transmission through the Gate Valve of a New Hybrid Ion Guide for Fourier Transform Ion Cyclotron Resonance Mass Spectrometry", ***Rapid Comm.Mass Spectrom.***. **2010**, **24,** 469-472
4. Hyun Sik Kim, Seung Yong Kim, and Mo Yang*; "Cold Electron Source with an Electron Multiplier Illuminated by Ultraviolet Photons", ***Anal. Chem.*** **2012, 84**, 3635−3639
5. Wanseop Jeong, Hyun Sik Kim*, Byeongwon Kang*, "Development of a portable time-of-flight mass spectrometer prototype using a cold electron source" ***Rev. Sci. Instrum.*** 93, 023302 (2022
6. Si Hyun Seong, Hyun Sik Kim, Yong-Moon Lee, Jae-Seok Kim, Sangwoo Park, Jieun Oh*; "Exploration of Potential Breath Biomarkers of Chronic Kidney Disease through Thermal Desorption-Gas Chromatography/Mass Spectrometry". ***Metabolite*** **2023 13(7) 837**. doi: 10.3390/metabo13070837

Abstract

Title, author(s), affiliation(s), and body text

Development of Mass Spectrometers for Industrial and Medical Applications

Hyun Sik Kim

ASTA Corporation., Suwon-si, Gyeonggi-do, Korea

As a small company producing research instruments, ASTA Corporation was established on the instrumentation techniques of time-of-flight mass spectrometers (TOF-MS). The mass spectrometer business market is highly competitive, with advanced technologies already invented and adopted by global big companies. Therefore, all ASTA Corporation business projects focus on niche markets of medical and industrial application of mass spectrometers.

In this presentation, I will introduce the TOF-MS products that ASTA Corporation has developed and is currently developing. In the early stage, we developed the simplest structured linear MADLI TOF-MS for the identification of microorganisms, targeting the domestic hospital market for diagnosing human blood using a protein profile database of disease-related microorganisms in 2015. After that, we developed a high resolution reflectron MALDI TOF-MS for advanced research including the analysis of proteins, carbohydrates and nucleic acids. Later, a domestic display company asked us to developed a MALDI TOF-MS for the analysis of OLEDs. The high-performance imaging LDI TOF-MS, IDSys *Premier*, is designed to provide micrometer-scale mass spectrometry imaging for quality control of OLED performance in the display industrial applications. IDSys *Premier* offers a variable mass spectrometry imaging size from a minimum of 5 microns to a maximum of 100 microns. Several IDSys *Premiers* have been adopted by domestic display companies and have shown powerful performance for quality control of their products. Years ago, a semiconductor company ask us to develop a portable TOF-MS to monitor the gas reagents used in semiconductor production. We developed an electron ionization TOF-MS to monitor gas molecules and are testing it in the field of semiconductor production to meet their requirements for on-site monitoring of processing gases. One of the main issue in these tests is that most of gases used in semiconductor fabrication are very toxic and difficult to ionized compared to well-known VOCs. Therefore, we need to protect the ionization source and improve the sensitivity of our RT-GMS (Real-Time Gas Monitoring System). RT-GMS was enhanced with a high stability ionization filament and a differential pumping system for the electron ionization source to achieve higher sensitivity and stability. Recently, a rechargeable battery company call us to produce a mass spectrometer for quantitative analysis of gas molecules during the thermal analysis of materials composing the battery. For advanced materials comprising parts that require significant thermal stability, such as secondary batteries, it is crucial to analyze the chemical composition of gases generated during physical property changes at high temperatures. Qualitative and quantitative analysis of gases generated from each thermal decomposition process during ThermoGravimetric analysis (TGA) can be performed by integrating TGA with Time-of-Flight Mass Spectrometer (TOF-MS). In the case of NCM (Nickel Cobalt Manganese) ternary metal Li-ion battery cathode materials, the higher the proportion of Ni, the lower the thermal stability becomes. Using TGA TOF-MS, the stability of designed NCM cathode materials can be evaluated by monitoring the onset temperatures at which thermal decomposition occurs, as well as the amount and composition of evolved gases. TGA TOF-MS provides a reliable quality control method for assessing thermal stability.

Brief C.V.

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Experience in reverse chronological order (latest first)

2022.10~	Associate Professor, Hanbat National University
2018.09~2022.09	Assistant Professor, Hanbat National University
2017.10-2018.08	Senior Researcher, Y-IBS, Yonsei University
2013.09-2017.01	Post-doc, UCLA
2011.09-2013.08	Post-doc, Yonsei University

Education in reverse chronological order (latest first)

2006.03~2011.08	Ph.D., Yonsei University, ,
2004.03~2006.02	M.S., Yonsei University
1999.03~2004.02	B.S., Yonsei University

Representative publications

1. "Ultrasmall Mn-doped Iron Oxide Nanoparticles with Dual Hepatobiliary and Renal Clearances for T1 MR Liver Imaging"
   Nanoscale Advances **2024**,
2. "Colorimetric mercury detection with enhanced sensitivity using magnetic-Au hybrid nanoparticles."
   Nanoscale Advances **2023**, *5*, 3084 - 3090.
3. “Enhancing catalytic efficiency of carbon dots by modulating their Mn doping and chemical structure with metal salts”
   RSC Advances **2023**, *13*, 8996 - 9002
4. "Zn-assisted modification of the chemical structure of N-doped carbon dots and their enhanced quantum yield and photostability"
   Nanoscale Advances **2022**, *4*, 2029-2035.
5. "Mag-spinner: A next-generation Facile, Affordable, Simple, and porTable (FAST) magnetic separation system"
   Nanoscale Advances **2022**, *4*, 792 - 800.
6. “Distance-dependent Magnetic Resonance Tuning (D-MRET) as a Versatile MRI Sensing Platform for Biological Targets”
   *Nature Mater.***2017**, *16*, 537–542.
7. “Cross-Linked Fluorescent Supramolecular Nanoparticles as Finite Tattoo Pigments with Controllable Intradermal Retention Times”
   ACS Nano, **2017**, *11*, 153–162.

Abstract

Title, author(s), affiliation(s), and body text

Nanozyme: beyond the natural enzyme for a better detection system

Jin-sil Choi

Department of Chemical and Biological Engineering, Hanbat National University, Daejeon, Korea

Nanozymes are a broad category of nanomaterials that mimic the catalytic functions of natural enzymes. In the biomedical field, various enzyme-based detection systems have been developed, but natural enzymes often face challenges related to storage and cost. Nanozymes offer advantages in terms of cost and ease of storage, leading to increasing interest from researchers.

Nanozymes can enhance their enzyme-like activity by modifying their physicochemical properties, such as composition, shape, structure, and surface coating. For instance, iron oxide nanozymes demonstrate that their enzyme-like activity diminishes with increasing particle size. Instead, the activity is more influenced by the size and crystallographic arrangement of individual particles within clusters. Similarly, carbon dots exhibit varying enzyme effects depending on factors such as the size of the sp^2 domain, functional groups, chemical structure, and component ratios. Doping carbon dots with metals can further enhance their enzyme-like activity, with the chemical structure and composition varying based on the metal used.

Despite these benefits, nanozymes generally have lower target selectivity compared to natural enzymes. Natural enzymes possess a three-dimensional structure allowing specific interactions with target substances. In contrast, nanozymes often require additional modifications, such as attaching target-specific molecules like DNA or peptides, to achieve selectivity. In this study, we propose a novel probe system that leverages the combined enzyme-like effects of iron oxide and carbon dot nanozymes. The hybrid system provides a synergistic enzyme-like effect compared to individual components. By using a linker that can be altered (e.g., broken, combined, bent, or unfolded) in response to interactions with a target substance, we aim to create a new detection system with enhanced target selectivity. This approach could lead to a next-generation nanozyme platform with improved detection capabilities, potentially transforming applications in fields such as treatment, environmental monitoring, and catalysis.

Brief C.V.

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Experience in reverse chronological order (latest first)

Jan 2019 – Present Associate Professor (tenured) in the Department of Chemistry, National University of Singapore Deputy Head, Education (2021–Present), Assistant Head (2020-2021) in the Department of Chemistry, NUS
Dec 2015 – Mar 2021 Group Leader of the Solar Fuels Lab in the Solar Energy Research Institute of Singapore (SERIS)
Apr 2012 – Dec 2018 Assistant Professor (tenure-track) in the Department of Chemistry, National University of Singapore

Education in reverse chronological order (latest first)

Feb 2009 – Jan 2012 Chemist Postdoctoral Fellow in the Lawrence Berkeley National Laboratory and University of California, Berkeley
Jan 2005 – Jan 2009 Dr. Sc. in Chemistry, ETH Zürich
Jul 2001 – Jul 2004 M.Sc. in Chemistry, National University of Singapore Gold Medal for the Most Outstanding M.Sc. Thesis in Chemistry
Jul 1997 – Jun 2001 B.Sc. with Honors (First Class) in Chemistry National University of Singapore

Representative publications

1. M.P.L. Kang, H. Ma, R. Ganganahalli and B.S. Yeo. Surfactant-Enhanced Formation of Ethylene from Carbon Monoxide Electroreduction on Copper Catalysts. ACS Catal. 14, 116. 2024.
2. H. Ma, E. Ibáñez-Alé, R. Ganganahalli, J. Pérez-Ramírez, N. López, and B.S. Yeo. Direct Electroreduction of Carbonate to Formate. J. Am. Chem. Soc. 145, 24707. 2023.
3. C.Y.J. Lim, M. Yilmaz, J.M. Arce-Ramos, A.D. Handoko, W.J. Teh, Y. Zheng, Z.H.J. Khoo, M. Lin, M. Isaacs, T.L.D Tam, Y. Bai, C.K. Ng, B.S. Yeo, G. Sankar, I. Parkin, K. Hippalgaonkar, M. Sullivan, J. Zhang, Y.F. Lim. Surface Charge as Universal Activity Descriptors for Electrochemical CO2 Reduction to Multi-Carbon Products on Organic-Functionalised Cu. Nature Comm. 14, 235. 2023. (WoS Highly Cited Paper)
4. Y. Zhou, R. Ganganahalli, S. Verma, H.R. Tan, B.S. Yeo. Production of C3 – C6 Acetate Esters via CO Electroreduction in a Membrane Electrode Assembly Cell. Angew. Chemie Int. Ed. 61, e202202859. 2022 (HOT Paper).
5. Y. Zhou, A.J. Martín, F. Dattila, S.B. Xi, N. López, J. Pérez-Ramírez, B.S. Yeo. Long-chain hydrocarbons by CO2 electroreduction using polarized nickel catalysts. Nature Catal. 5, 545. 2022. (WoS Highly Cited Paper)
6. O. Pique, Q.H. Low, A.D. Handoko, B.S. Yeo and F. Calle-Vallejo. Selectivity Map for the Late Stages of CO and CO2 Reduction to C2 Species on Copper Electrodes. Angew. Chemie Int. Ed. 60, 10784. 2021 (HOT Paper).

Abstract

Title, author(s), affiliation(s), and body text

Electrosynthesis of Oxygenates and Hydrocarbons

B.S. Yeo

National University of Singapore, Department of Chemistry. 3 Science Drive 3. Singapore 117543
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Currently, more than 80 % of the world's energy needs are met by burning fossil fuels. Supplies of these fuels are intrinsically limited and will eventually run out. In this presentation, we share our recent works related to the development of catalysts for the electroreduction of CO_2, CO, CO_3^{2-} and other feedstocks to oxygenates and long-chain hydrocarbons, which can be used as fuels. We shall first show how C_1-C_6 alkanes and alkenes such as *n*-hexane could be formed. The catalyst that was found to work well was unexpectedly based on nickel, rather than copper (which is generally considered to be the catalyst-of-choice for reducing CO_2 to multi-carbon molecules). We shall also show how carbonate anions (CO_3^{2-}), long thought to be electrochemically inert, could be directly reduced to formate on a copper catalyst using pulse electrolysis. The nature of the active sites generating the adsorbed carbonate species and the mechanism for the pulse-enabled reduction of carbonate to formate were elucidated.

References

1. H. Ma, E. Ibáñez-Alé, R. Ganganahalli, J. Pérez-Ramírez, N. López, and B.S. Yeo. *J. Am. Chem. Soc.* **2023**, 145, 24707.
2. Y. Zhou, A.J. Martín, F. Dattila, S.B. Xi, N. López, J. Pérez Ramírez, B.S. Yeo. *Nature Catal.* **2022**, 5, 545.

충남대학교 소재화학연구소