

# 8<sup>th</sup> Shanghai - Kyushu - Yeungnam (SKY) Symposium & 23<sup>rd</sup> International Symposium on Clean Technology

2024.11.15-17, Gyeongsan, Yeungnam University, South Korea

E24, Chemical Engineering Building, Yeungnam University, Gyeongsan, South Korea

## 2024/11/15 (Fri.)

10:00 – 18:00 Local Tour and Hotel Check-In

18:00 – 20:00 Welcome Dinner (TBA)

## 2024/11/16 (Sat.)

### Session 1: Opening Ceremony and Keynote Speech

**09:30 – 11:30 Room 213**

Chair: Prof. Jintae Lee, Director, Institute of Clean Technology

09:00 Registration

09:30 Opening Address

Prof. Moonyong Lee  
(Director of BK program, Yeungnam University)

09:35 Congratulatory Address

Prof. Kyeong-Soo Lee  
(Vice President, Yeungnam University)

09:40 Photo time

09:50 **(Keynote)** Thermal Plasma Generation for Innovative Environmental Processing

Prof. Takayuki Watanabe  
(Kyushu University, Japan)

10:15 **(Keynote)** Design and Construction of Biomedical Polymer Self-assemblies

Prof. Hailong Che  
(Shanghai University, China)

10:40 **(Keynote)** The Use of Gas Self-Inducing Impeller in Alleviating High Hydrogen Pressure in a Semi-Batch Reactor of Hydrogenation of Alkenes

Prof. Dijan Supramono  
(Universitas Indonesia, Indonesia)

11:05 **(Keynote)** Insight into Adsorption Behaviors and Equilibrium Solubility using Deep Machine Learning and COSMO Theory

Prof. Uthaiporn Suriyapraphadilok  
(Chulalongkorn University, Thailand)

11:30 Lunch

### Session 2: Advanced Biological Technology

**12:30 – 13:50 Room 213**

Chair: Profs. Chang-Hyung Choi / Yusuke Sakai

12:30 **(Invited)** Liver reconstruction for regenerative medical science

Prof. Yusuke Sakai  
(Kyushu University, Japan)

12:50 Pharmaceutical Degradation in A Dual-Chambered Microbial Fuel Cell by Utilizing Natural Microbial Consortium from Sewage Sludge

Prof. Tania Surya Utami  
(Universitas Indonesia, Indonesia)

13:05 Capsule-based colorimetric temperature monitoring sensor for customizable cold chain management

Prof. Chang-Hyung Choi  
(Yeungnam University, Korea)

13:20 Whole Transcriptome Sequencing Reveals LncRNA/circRNA-miRNA-mRNA Networks in Bisphenol AF Induced Cardiac Inflammatory Response in Zebrafish

Ms. Qing Wei  
(Shanghai University, China)

13:35	Integrin-stimulating polymer-peptide for improved cell survival in a recellularized liver model	Mr. Mario Kokichi Uehara Uyeda (Kyushu University, Japan)
13:50	Break	
<b>Session 3: Catalysis and Process Control</b>		
<b>12:30 – 13:50 Room 214</b>		Chair: Profs. Minkyu Kim / Ampira Charoensaeng
12:30	<b>(Invited)</b> Improving Surfactant Efficiency Through Nanoparticle-Assisted Systems: Reducing Adsorption and Enhancing Interfacial Properties	Prof. Ampira Charoensaeng (Chulalongkorn University, Thailand)
12:50	Ethylene aromatization over zeolite catalyst with sulfur species	Prof. Kazuma Oshima (Kyushu University, Japan)
13:05	Revolutionizing Distillation Column Analysis with Artificial Intelligence and Digital Twins	Prof. Riezqa Andika (Universitas Indonesia, Indonesia)
13:20	Visible-light assisted hydrogen evolution over Cu-decorated polymeric carbon nitride nanostructures	Dr. Shalini Sahani (Yeungnam University, Korea)
13:35	A Comprehensive Solvent Design Framework for Amine-based CO <sub>2</sub> Chemical Absorption	Mr. Apri Wahyudi (Chulalongkorn University, Thailand)
13:50	Break	
<b>Session 4: Green Environmental and Energy Technology</b>		
<b>14:00 – 15:50 Room 213</b>		Chair: Profs. Woo Kyoung Kim / Dianursanti
14:00	<b>(Invited)</b> Microalgae: A Valuable Biomass Source for CO <sub>2</sub> Sequestration	Prof. Dianursanti (Universitas Indonesia, Indonesia)
14:20	Perfluorooctanoic acid efficient chain reaction degradation in multifunctional mineral augmentation geobiochemical remediation system	Prof. Wenbing Wang (Shanghai University, China)
14:35	Attenuation of phenylanthracenic acids related to oil sands process water using solar activated calcium peroxide	Prof. Ming Zheng (Shanghai University, China)
14:50	Fe(IV)=O/Fe(V)=O and [FeIVaqO] <sup>2+</sup> /[FeVaqO] <sup>3+</sup> cooperating with free radicals induced high-rate SMX-Cr(VI) simultaneous removal in Fe7S8-PS micro-nano catalytic system	Dr. Chunyang Li (Shanghai University, China)
15:05	Fabrication of conducting polymer nanostructures and their applications	Prof. Sunghun Cho (Yeungnam University, Korea)
15:20	Regulated Zn metal deposition by multi-channel carbon organic complex	Ms. Li Gao (Shanghai University, China)
15:35	TiO <sub>2</sub> : a highly potential support to reliable electrocatalysis for PEMFCs	Dr. Moonsu Kim (Yeungnam University, Korea)
15:50	Break	
<b>Session 5: Batteries and Supercapacitors</b>		
<b>14:00 – 15:35 Room 214</b>		Chair: Profs. Seho Sun / Yang Dai
14:00	<b>(Invited)</b> High performance CF <sub>x</sub> /Li battery: materials and cells	Prof. Yang Dai (Shanghai University, China)
14:20	Electrode Structure Engineering for All Solid State Batteries	Prof. Seho Sun (Yeungnam University, Korea)
14:35	Microwave-assisted synthesis of Co <sub>3</sub> O <sub>4</sub> /SnO <sub>2</sub> /reduced graphene oxide nanocomposites for supercapacitor applications	Dr. Sumanta Sahoo (Yeungnam University, Korea)

14:50	Synthesis of Garnet-Type Cubic-LLZO Solid-Electrolyte for All-Solid-State Lithium-Ion Batteries via a Combined Process of Induction Thermal Plasma and Sintering	Mr. Byeong-il Min (Kyushu University, Japan)
15:05	Redox-active “Structural Pillar” Molecular Doping Strategy To-wards High-Performance Polyaniline-based Flexible Supercapacitors	Ms. Wei Ding (Shanghai University, China)
15:20	N/O-bridge stimulated robust binding energy and fast charge transfer between carbon nanofiber and NiCo LDH for advanced supercapacitors	Mr. Yuancong Luo (Shanghai University, China)
15:35	Break	
<b>Session 6-1: Student’s Oral Presentation</b>		
<b>16:10 – 17:10 Room 213</b>		Chair: Prof. Minkyu Kim
16:10	Enhancing heterojunction interface charge transport efficiency in NiCo-LDHs@Co/CoO-CNFs for high-performance asymmetric and zinc-ion hybrid supercapacitors	Huicheng Ge (Shanghai University, China)
16:20	Superb green cycling strategies for microbe-FeO neural network-type interaction: Harnessing eight key genes encoding enzymes and mineral transformations to efficiently treat PFOA	Qifeng Fan (Shanghai University, China)
16:30	Selective Conversion of Ethane to Value Added Products on RhO <sub>2</sub> (110): A DFT and Microkinetic Simulation Study	Seongjun Lee (Yeungnam University, Korea)
16:40	Optimized chilling system design for precision cooling using mixed refrigerants cycle in semiconductor industry	Muhammad Islam (Yeungnam University, Korea)
16:50	Synthesize Vegan Leather Substrate using Agricultural Waste Extract Based Culture Medium	So Yeon Won (Yeungnam University, Korea)
17:00	Buckling-Induced Controlled Release from Asymmetric Shell Microcapsules	Hyo-Jin Kim (Yeungnam University, Korea)
<b>Session 6-2: Student’s Poster Presentation</b>		
<b>16:10 – 17:10 1<sup>st</sup> and 2<sup>nd</sup> Floor</b>		Chairs: Profs. Hailong Che / Takayuki Watanabe / Dijan Supramono / Uthaiporn Suriyapraphadilok
PP01	Synthesis and Characterization of Guanidinylated singlet oxygen Releasing polymersomes Based on Biodegradable Polycarbonate	Suzhen Wang (Shanghai University, China)
PP02	The research explores the application of multifunctional catalysts in alkaline electrochemical water splitting	Jinhu Wu (Shanghai University, China)
PP03	Nitric Oxide-Releasing Tubular Polymersomes toward Ad-vanced Gas Therapeutic Carriers	Zhezhe Li (Shanghai University, China)
PP04	Covalent Triazine Based Frameworks with Donor-Donor- $\pi$ -Acceptor Structures for Dendrite-Free Lithium Metal Batteries	Xiaomeng Lu (Shanghai University, China)
PP05	Revealing the effect of calcination temperature on the performance of MnOx-TiO <sub>2</sub> catalysts for ethanol oxidation at low temperatures	Xueqian Zhang (Shanghai University, China)
PP06	Enhancing Peptide Incorporation in Hydrogels for Dense and Sustainable Data Storage	Benxiang Luo (Shanghai University, China)
PP07	Coordination regulation of solvation structure assisting the wide-temperature sodium-ion batteries.	Xiangwu Chang (Shanghai University, China)
PP08	Controllable synthesis of p-NiO/n-ZnO heterojunctions with preferred orientation of ZnO (100) and (110) planes for enhancing n-butanol sensing performance	Xuan Li (Shanghai University, China)
PP09	Constructing functional organic interfacial layers with tethered electric double layer on Zn metal anodes for ultra-stable Zn-ion batteries	Limeng Sun (Shanghai University, China)

PP10	Discharge Plasma-assisted ball milling is used to convert photovoltaic waste silicon into high-performance lithium-ion battery anode materials	Dingyi Zhang (Shanghai University, China)
PP11	Artificial Protective Layer Enhancing Stable Dendrite-Free Lithium Metal Batteries Enabled by Metal Organic Framework	Yibo Wu (Shanghai University, China)
PP12	Enabling Gradient-Structured Solid Electrolyte Interphase by a Hydrated Eutectic Electrolyte for High-Performance Zn Metal Batteries	Chenxu Jiang (Shanghai University, China)
PP13	Effect of electrical treatment on CFRP recycling by chemical dissolution method	Ryohei Kobayashi (Kyushu University, Japan)
PP14	Catalytic conversion of plastic pyrolysis gas into aromatics using zeolite	Yuki Takeda (Kyushu University, Japan)
PP15	Development of Tissue Engineering Scaffolds by Spatial Configuration Control of Wet Electrospun 3D Fibers	Zhenghao Li (Kyushu University, Japan)
PP16	Viscosity Reduction of Heavy Oil Using Bi-Metallic Catalyst in Low-Temperature Aquathermolysis Reactions	Sanfun Limprapaipong (Chulalongkorn University, Thailand)
PP17	CHA Zeolite/Cellulose Acetate Mixed Matrix Membranes for CO <sub>2</sub> /CH <sub>4</sub> Separation via Microwave-Assisted Synthesis	Weerawit Luewanichwong (Chulalongkorn University, Thailand)
PP18	Molecular Dynamics Simulation of Cationic Surfactant Adsorption for Steel Corrosion Protection in CO <sub>2</sub> -Rich and High-Salinity Conditions	Sitthikiat Boonchoo (Chulalongkorn University, Thailand)
PP19	Extraction, Purification, and Analysis of Carbonic Anhydrase from <i>Caulerpa lentillifera</i> (Sea Grapes): Evaluating Its Effectiveness in CO <sub>2</sub> Sequestration	Kattariy Srasamran (Chulalongkorn University, Thailand)
PP20	Coating effect of metal organic complex (Co-DTPMP) layer on enhancing PEC water oxidation performance of BiVO <sub>4</sub> photoanode	Alaa Magdy Saad (Yeungnam University, Korea)
PP21	Advancing Co-N-C electrocatalyst by enlarged accessible active sites for a highly efficient PEMFC cathode	Jinhyuk Baek (Yeungnam University, Korea)
PP22	Methane Pyrolysis using Molten salt	Dasol Bae (Yeungnam University, Korea)
PP23	Investigation of the Zn/Co ratio impact on water electrolysis activity using bimetallic selenides derived from zeolitic imidazolate frameworks	Hyeonwook Son (Yeungnam University, Korea)
PP24	A LiF-rich solid electrolyte interphase formation by fluorinated carbon host for anode-free lithium metal batteries	Yunji Jeong (Yeungnam University, Korea)
PP25	Synergistic Effect of 3D/2D Vanadium Diselenide/Tungsten Diselenide Hybrid Materials: Electrochemical Detection of 5-	Prajakta R. Chavan (Yeungnam University, Korea)
PP26	Synergistic Design of Processable Nb <sub>2</sub> O <sub>5</sub> -TiO <sub>2</sub> Bilayer Nanoarchitectonics: Enhancing Coloration Efficiency and Dual-band Electrochromic Energy Storage Stability	Rutuja U. Amate (Yeungnam University, Korea)
PP27	Simplifying nitridation of Li metal anode by direct Lewis acid-base reaction	Seokjun Kim (Yeungnam University, Korea)
PP28	Enabling uniform microstructure of dry electrode via pre-kneading process	Taehyeong Kim (Yeungnam University, Korea)
PP29	Determining the difference in conversion of CO by comparing the Gibbs free energy of CO to methanol in Cu, In/Cu, and In <sub>2</sub> O <sub>3</sub> surface with DFT	Yuna Song (Yeungnam University, Korea)
PP30	Halogenated Heterocyclic Scaffolds as Antimicrobial Agents against Uropathogenic <i>E. coli</i>	Bharath Reddy Boya (Yeungnam University, Korea)
PP31	Antimicrobial activities of flavonoids against <i>Vibrio</i> species	Olajide Sunday Faleye (Yeungnam University, Korea)
PP32	Antimicrobial Potentials of Iodinated Amino Acid against <i>Staphylococcus aureus</i>	Oluwatosin Oluwaseun Faleye (Yeungnam University, Korea)

PP33	Antibacterial Efficacy of Halogenated Phenol	Olanrewaju Rauf Olalekan (Yeungnam University, Korea)
PP34	Antibiofilm Characteristic of Crocetin against <i>Staphylococcus aureus</i>	Saurav Paramanya (Yeungnam University, Korea)
PP35	Phthalimide derivatives as antifungal agents	Shamshe Shaik (Yeungnam University, Korea)
PP36	Multi-halogenated Pyrimidines as Antibiofilm and Antimicrobial Agents Against <i>Staphylococcus aureus</i> .	MinHwi Sim (Yeungnam University, Korea)
PP37	Antibiofilm activities of halogenated pyrimidines against enterohemorrhagic <i>Escherichia coli</i>	Hyejin Jeon (Yeungnam University, Korea)
PP38	Analysis of Separation Mechanism on Photovoltaic Module with Sacrificial Layer	Jongwon Ko (Yeungnam University, Korea)
PP39	Enhanced Oxygen Evolution Reaction Performance Using a CNSe/FeOOH Bilayer Electrocatalyst	Sang-June Kwon (Yeungnam University, Korea)
PP40	Unveiling the Potential of High-Temperature Chemical Vapour Deposition Growth of Boron Carbide: Investigating Physicochemical, Mechanical and Electrical Properties	Namita A. Ahir (Yeungnam University, Korea)
PP41	Optimizing Isopropyl Alcohol – Water Separation: Modeling of Cyclic Heterogeneous Azeotropic Distillation	Raisa Aulia Hanifah (Yeungnam University, Korea)
PP42	Simulating Cyclic Dividing-wall Column for Enhanced Separation Efficiency in Alcohol Separation	Nguyen Nhu Nga (Yeungnam University, Korea)
PP43	Fabrication of Pepstatin A labeled Solid Lipid Nanoparticles for theranostic applications in Adenocarcinoma	Yumi Son (Yeungnam University, Korea)
PP44	Synergistic insights into the electrocatalytic mechanisms of ZIF-derived $\text{Co}_3\text{S}_4$ on 1T- $\text{WS}_2/\text{WO}_3$ Bifunctional Catalyst for overall water splitting	Nimisha Baby (Yeungnam University, Korea)
PP45	Multifaceted Binary Nanohybrids Integrated PLA Composite Films for Active Food Packaging Applications	Ajmal P Muhammed (Yeungnam University, Korea)
PP46	N-doped Carbon encapsulated Cobalt Vanadium Oxide Nanosheets as a Highly Efficient Bifunctional Electrocatalyst for Overall Water Splitting	Mohammad Kashif (Yeungnam University, Korea)
PP47	N-doped Holey CNT Ni-MOF Hybrid as a Bifunctional Electrocatalyst for Overall Water Splitting	Mrunal Bhosale (Yeungnam University, Korea)
PP48	Engineering heterojunction of multi-morphologies and bifunctional hybrid rGO- $\text{V}_2\text{O}_5$ embedded $\text{CeO}_2$ nanostructures for robust visible-light-driven dye degradation and supercapacitor	Sahil S Magdum (Yeungnam University, Korea)
PP49	Synthesis and Characterization of Polyimides with Different Main Chain Lengths according to Chain Length of Ethylene Oxide	Su Bin Park (Yeungnam University, Korea)
PP50	Characterization of Strict Chain Copolyimide Synthesized	JangHwan Park (Yeungnam University, Korea)
PP51	Utilizing an organic dye with a simple wet chemical coating of fluorine- $\text{TiO}_2/\text{WO}_3$ as an innovative photo-anode to improve the performance of photoelectrochemical cells	Dong-Hwan Kim (Yeungnam University, Korea)
PP52	The role of dye anchor counter electrode on solid state-DSSC to achieve enhanced efficiency: a mechanistic approach	Oh Joon Kwon (Yeungnam University, Korea)
PP53	Improved dye-sensitized photoelectrochemical water oxidation through the introduction of hydroxamic acid group in dye structure.	Seo Young Kim (Yeungnam University, Korea)
PP54	Solution-based synthesis and analysis of $\text{WO}_3$ film as an effective photo-anode for photoelectrochemical cells	Yujeong Hwang (Yeungnam University, Korea)
PP55	Designing Cost-Effective Alloy Catalysts for $\text{NH}_3$ Decomposition: Reducing Ruthenium Dependence Through DFT Calculations	Chaerin Son (Yeungnam University, Korea)
PP56	Red Mud as a Low-Cost Catalyst for Sulfur Removal and COS Decomposition: A Theoretical and Experimental Study	Ga-yeong Kim (Yeungnam University, Korea)

PP57	Rotating packed beds for CO <sub>2</sub> Capture: Efficiency Improvements and Cost Reduction Strategies	Junwoo Shin (Yeungnam University, Korea)
PP58	Development of a Movable Rotating Packed Bed System for Efficient VOCs Removal in Shipboard Operations	Uidong Jin (Yeungnam University, Korea)
PP59	A Customized Core/Shell Architecture: Co <sub>0.85</sub> Se Nanowires Encased in NiCo-LDH for Enhanced Battery-Type Supercapacitor Performance.	Sang-Jun Kwon (Yeungnam University, Korea)
PP60	Microwave-assisted Ultrafast Synthesis of Reduced Graphene Oxide/Mn <sub>3</sub> O <sub>4</sub> Nanocomposites Hydrogels for Bone Tissue Engineering Applications	Ritu Singhmar (Yeungnam University, Korea)

# Session 1

Opening Ceremony and Keynote Speech

# Thermal Plasma Generation for Innovative Environmental Processing

Takayuki Watanabe\* and Manabu Tanaka

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**Keywords:** thermal plasma • multiphase AC arc • water plasma • plasma diagnostics

## Abstract:

Thermal plasmas are expected to be utilized for a number of innovative industrial applications such as decomposition of harmful materials, recovery of useful materials from wastes, and synthesis of high-quality and high-performance nanoparticles. The advantages of thermal plasmas including high enthalpy to enhance reaction kinetics, high chemical reactivity, and oxidation or reduction atmospheres in accordance with required chemical reactions are beneficial for innovative processing.

The experimental and modeling efforts on thermal plasma characteristics has been devoted to industrial application. However, the thermal plasma characteristics remain to be explored in spite of these efforts. The arc fluctuation phenomena are one of the most considerable issues, because it determines the processing performance in thermal plasmas. The objective of the talk is to investigate the physical and chemical phenomena in thermal plasma processing for industrial application.

A multiphase AC arc (MPA) is one of the most attractive thermal plasmas due to its advantages such as large plasma volume with low gas velocity, which are favorable for material processing. Other advantages compared with other thermal plasmas include high energy efficiency and low cost. The most important phenomena to be explored are the arc stability, the temporal and spatial characteristics of the arc discharge.

Water plasma system has been scaled up into a mobile system in a vehicle with direct-current generator. This innovative in-vehicle plasma has great advantage to reduce the risk and cost caused by the transportation of harmful wastes. Recent studies have revealed the arc fluctuation and temperature field of the water plasma by high-speed visualization. The observation of arc fluctuation and the measurement of the arc temperature were conducted by employing the high-speed camera system. Water as plasma source was introduced from cathode nozzle to discharge area. The copper or iron as anode material rotates to reduce anode erosion.

## Reference

1. Investigation of Electrode Phenomena In An Innovative Thermal Plasma for Glass Melting, T Watanabe et al., *Plasma Chemistry and Plasma Processing* 34, 443-456 (2014), Enhanced Decomposition of Caffeine by Water Plasma Combined with Mist Generator, SH Kim, et al., *Chemosphere* 307, 136056 (2022)

## Biography



Prof. Takayuki Watanabe received his Ph.D at Tokyo Institute of Technology in 1991. Since 2013, he has been Professor of the Kyushu University. Professor Watanabe is an expert in the area of plasma processing science. He is the Board of Directors of International Plasma Chemistry Society, and he organized 25th International Symposium on Plasma Chemistry as the Chair in 2023.

## Oral presentation

# Design and Construction of Biomedical Polymer Self-assemblies

Zhezhe Li, Suzhen Wang, Hailong Che\*

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**Keywords:** polymer self-assembly • polymersomes • responsive materials

### Abstract:

Polymersomes also referred to as polymer vesicles, are hollow structures surrounded by bilayers self-assembled from amphiphilic block copolymers. Compared with their counterparts, liposomes, and polymersomes demonstrate improved structural stability and chemical versatility. In addition, the polymersome can not only encapsulate hydrophilic compounds in their aqueous lumen but also load hydrophobic cargos in the membranes. Considering the fascinating characteristics of polymersomes, they have found many potential applications in various fields, such as drug delivery, nanomedicine, nanoreactors, as well as artificial cells. In this study, we report the design and construction of biomedical polymersomes and explore their potential applications in gas (such as NO and CO) releasing nanocarriers, photodynamic therapy, and triggered delivery systems. The functional copolymers were prepared via ROP and post-modification strategy, and the polymersomes were constructed by self-assembly technology. We found that the polymersomes demonstrate controlled gas-releasing behavior upon stimuli treatment, and the in vitro study also confirms the excellent biomedical activity of polymersomes.

### Reference

1. Yanyan Zhu, Zhezhe Li, Suzhen Wang, Jian Gu, Rui L. Reis, and Hailong Che\*, Synthesis and characterization of light-responsive biodegradable tubular polymersomes, *Polym. Chem.*, 2024, 15, 1026-1033.
2. Zhezhe Li, Suzhen Wang, Lili Zhao, Jian Gu, and Hailong Che\*, "Nitric Oxide-Releasing Tubular Polymersomes toward Advanced Gas Therapeutic Carriers", *ACS Macro Lett.*, 2024, 13, 87-93.
3. Yanyan Zhu, Shoupeng Cao, Meng Huo\*, Jan C. M. van Hest\*, and Hailong Che\*, "Recent advances in permeable polymersomes: fabrication, responsiveness, and applications", *Chem. Sci.*, 2023, 14, 7411-7437.
4. Zhezhe Li, Suzhen Wang, Lili Zhao, Shaofeng Feng, and Hailong Che\*, "Synthesis and Characterization of Guanidinylated CO-Releasing Micelles Based on Biodegradable Polycarbonate", *Biomacromolecules*, 2024, 25, 5149-5159.

### Biography



Dr. Hailong Che received his PhD degree from Eindhoven University of Technology (TU/e) in 2019 and then worked as a postdoctoral at TU/e. In 2021, he joined Shanghai University as a full professor in the College of Environmental Science and Engineering. Research interests: Polymer synthesis, self-assembly, biomedical materials

## Oral presentation

# The Use of Gas Self-Inducing Impeller in Alleviating High Hydrogen Pressure in a Semi-Batch Reactor of Hydrogenation of Alkenes

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**Keywords:** hydrogenation; non-oxygenated oil; pressure; self-inducing impeller; Ni/Al<sub>2</sub>O<sub>3</sub> catalyst.

## Abstract:

At the moment, high pressure of hydrogen gas is commonly employed in the hydrotreatment of alkenes to produce alkanes. The pressure used is rarely less than 20 bar and there has been few efforts of modifying the design of reactors applied to reduce the pressure. The reduction has some advantages such as safer reactor operation and avoidance of frequent leakage of hydrogen gas through the packing of reactor lid. A semi-batch hydrogenation reaction using a hydrogen gas self-inducing impeller to internally recirculate the hydrogen gas has been implemented in the present work to generate high shear of gas in liquid phase and to provide small hydrogen gas bubbles. This in turn highly improved the gas inventory in liquid phase and consequently intensified the dispersion of hydrogen gas in the liquid phase. The hydrogenation reaction in the present work was performed on polypropylene pyrolyzate at 185 °C with an impeller speed of 400 rpm. The pressure was varied from 2 to 8 bar. This technique was expected to improve the contact of small hydrogen bubbles with liquid phase of polypropylene pyrolyzate and Ni/Al<sub>2</sub>O<sub>3</sub> solid catalyst. At the pressure of 2 bar, the main reactions were hydrogenation of alkenes and cyclization of alkenes leading to cycloalkane formation, while at the pressures of 4, 6, and 8 bar, the main reactions were hydrogenation of alkenes and oligomerization of alkenes. The hydrogenation reaction shifted the carbon chain length in the oil towards the carbon chain length attributed to diesel fuel with more branching as the hydrogen pressure was increased. The gas inducement technique employed in the present work has succeeded in saturating almost all alkenes at moderate pressures (below 9 bar) and therefore alleviated high pressures of hydrogen gas.

## Reference

1. Moderate Hydrogen Pressures in the Hydrogenation of Alkenes using a Reactor with Hydrogen Gas Self-Inducing Impeller, Supramono, D., Yoandi, I. and Fauzi, M.R., Processes 2022, 10, 1662. <https://doi.org/10.3390/pr10081662>

## Biography



He completed BSc program in Chemical Engineering from Bandung Institute of Technology (ITB), gained his Master degree in Process Integration from University of Manchester, UK, and graduated from Doctorate program in the area of Co-pyrolysis of Polyolefin-Biomass from Universitas Indonesia. Currently, he is a full professor at the Department of Chemical Engineering of Universitas Indonesia. His current research areas are pyrolysis and biofuel synthesis.

# Insight into Adsorption Behaviors and Equilibrium Solubility using Deep Machine Learning and COSMO Theory

Achmad Anggawirya Alimin<sup>a</sup>, Apri Wahyudi<sup>a</sup>, Ampira Charoensaeng<sup>a,b</sup>, Bor-Jier Shiau<sup>c</sup>, and Uthaiporn Suriyapraphadilok<sup>a,b\*</sup>

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**Keywords:** Equilibrium Solubility, Artificial Neural Network Model, COSMO Theory, Sigma-Profiles

## Abstract:

This work aimed to utilize the COSMO (COnductor-like Screening Model) statistical thermodynamics model and the powerful Deep Machine Learning Tool to develop predictive models for equilibrium isotherms. Two systems were demonstrated: (1) surfactant/solid equilibrium adsorption, and (2) equilibrium solubility of aqueous amine-CO<sub>2</sub> systems. For each demonstrated system, apart from physical property and system's condition, COSMO was used to generate the surface charge distribution, so called the sigma-profile of each substance. Four types of potential interactions can be extracted including the contribution of the non-hydrogen bonding atoms, hydrogen bonding due to the hydroxyl groups, other possible hydrogen bonding atoms, and specifically in this work, the contribution of hydrogen bonding by nitrogen atoms. The system conditions and chemical features extracted from COSMO were fed as numerical features along with the equilibrium data into the artificial neural network model (ANN). The systems were evaluated and were found to capture the behavior of the equilibrium systems. This work has demonstrated that the use of deep neural network and the molecular descriptors extracted from COSMO shed light onto to prediction of equilibrium loading without knowing chemical reactions nor sophisticated thermodynamic models. The COSMO-based descriptors also provide a physical perspective for interpreting the behavior of various molecular configurations. The models can potentially be used to pre-screen the interest systems to reduce the screening time and expenditure on conducting experiments.

## Biography



Dr. Uthaiporn Suriyapraphadilok is currently an Assistant Professor at the Petroleum and Petrochemical College, Chulalongkorn University located in Bangkok, Thailand. She obtained her M.S. in Chemical Engineering and Ph.D. in Materials Science and Engineering from Pennsylvania State University, USA. Her research interests are in the areas of Enhanced Oil Recovery, Carbon Capture and Storage and Simulation & Modeling.

# Session 2

Advanced Biological Technology

## Oral presentation

# Liver reconstruction for regenerative medical science

Yusuke Sakai\* and Hiroyuki Ijima

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**Keywords:** liver • tissue engineering • hepatocyte • bilecanaliculi • bile duct

### Abstract:

The liver is a main organ of metabolism and has been attracting attention as a target for regenerative medicine and drug screening. It is known that the liver in the living body can regenerate after resection or injury, but this is difficult to do *in vitro*. Many researchers are challenging the reconstruction of liver tissue in regenerative medical science. In particular, the reconstruction of the bile excretion system of liver metabolites has been of interest to many researchers in recent years.

In this presentation, we will report on the formation of spherical cell tissues and the construction of a human liver with a vascular network that can lead to regenerative medicine, focusing on liver tissue culture technology. On the other hand, there is concern that the loss of the bile duct network will lead to a decrease in function due to cholestasis. In order to reconstruct the bile duct, which is one of the important metabolic product excretion pathways, we used chemically-induced liver progenitor cells (CLiPs). The composite hepatic tissue of hepatocytes and cultured bile ducts normalizes hepatocyte polarity and hepatic transporters, and maintains liver-specific functions for a long period of time. We expect this to be an organ model for drug screening and liver disease treatment.

### Reference

1. Vascularized subcutaneous human liver tissue from engineered hepatocyte/fibroblast sheets in mice, Sakai Y, *et al.*, *Biomaterials*, 65, 66–75, 2015.
2. Bioengineering of a CLiP-derived tubular biliary-duct-like structure for bile transport *in vitro*, Huang Y, Sakai Y, *et al.*, *Biotechnology and Bioengineering*, 118 (7), 2572–2584, 2021.

### Biography



I obtained my BS, MS, and PhD degrees in Engineering from The University of Kitakyushu, Japan. I obtained secondary PhD in Medical Science from Nagasaki University, Japan. After working at The University of Kitakyushu and Nagasaki University, I am currently an Associate Professor in the Department of Chemical Engineering at Kyushu University, Japan. My research topics are in the areas of liver reconstruction for regenerative medicine and cell-based assay system. And I am interested in materials and devices for efficient cell transplantation processes.

## Oral presentation

# Capsule-based colorimetric temperature monitoring sensor for customizable cold chain management

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**Keywords:** colorimetric detection • temperature responsive release • microcapsule • microfluidic • cold chain

### Abstract:

The COVID-19 pandemic and its impact on supply chains have highlighted the need for improved systems to safely store and transport critical items. Current temperature monitoring technologies for cold chain management, however, often lack reliability, cost-effectiveness, and flexibility, making them unsuitable for handling a variety of products with different temperature requirements. In this study, we introduce a new capsule-based colorimetric temperature monitoring system that allows for precise and easily adjustable temperature detection. This system employs a microfluidic technique to create uniform microcapsules containing an interstitial phase-change oil (PCO) layer with accurately controlled dimensions and composition. When the PCO layer undergoes a liquid-solid phase transition at its freezing point, it releases the encapsulated contents, leading to a noticeable color change. This offers a highly sensitive, visual way to monitor temperature changes. The system's adaptability allows users to adjust the PCO layer's composition to expand the temperature range accurately. This simple yet effective approach can detect both increases in temperature in frozen environments and instances of freezing, making it possible to monitor multiple temperatures. Overall, this advancement represents a significant step toward developing a customizable and precise colorimetric temperature monitoring system suitable for a wide range of temperature-sensitive applications in cold chain management.

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### Biography



I obtained my BS, MS and Ph.D degrees from Chungnam National University and performed postdoctoral studies at Harvard University. Currently, I am an assistant professor in the School of Chemical Engineering at Yeungnam University, Korea, I published more than 100 papers (h-index 30) and 20 patents. My research interests are in the development of functional hydrogel materials using microfluidic technology and their applications in the biomedical field.

## Oral presentation

# Whole Transcriptome Sequencing Reveals LncRNA/circRNA-miRNA-mRNA Networks in Bisphenol AF Induced Cardiac Inflammatory Response in Zebrafish

Qing Wei,<sup>1</sup> Junlang Liang,<sup>1</sup> Zhong Chen,<sup>\*2</sup> Ming Yang<sup>\*1</sup>

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**Keywords:** cardiotoxicity • bisphenol AF • long non-coding RNA • gene regulatory networks • zebrafish

## Abstract:

Bisphenol AF (BPAF) is a fluorinated derivative of bisphenol A and widely used as BPA alternative in industry currently. Among all bisphenol analogues, BPAF ranks one of the most detected ones in various environmental media. Previous studies have shown cardiovascular toxicity of bisphenols, however, there are still many unknowns about how epigenetic regulation play roles in bisphenol-induced cardiotoxicity. In the present study, we first found the acute BPAF exposure exerts dose-dependent toxic effects on cardiac development, morphology, and function in zebrafish embryos and larvae during their early developmental stages. And then, following a 28-day exposure of adult zebrafish to an environmentally relevant concentration of BPAF, we observed the long-term BPAF exposure induces cardiac inflammation in both male and female zebrafish, and paternal exposure has a more significant impact on the cardiac function of F1 generation. The BPAF exposed zebrafish adult hearts were further subjected to high-throughput RNA sequencing, obtaining a comprehensive transcriptome database of the hearts from both sexes. These results reveals significant changes in the expression patterns of mRNA, miRNA, lncRNA, and circRNA in the hearts of both sexes upon the long-term of BPAF exposure. Utilizing bioinformatics and RNA molecular regulatory network analysis, we investigated the biological processes and signaling pathways involved in target genes regulated by non-coding RNAs. It was showed that the mRNAs in the lncRNA/circRNA-miRNA-mRNA regulatory networks are significantly enriched in various metabolic processes, myocardial contraction, ion transmembrane transport, cell contraction and multiple hydrolase activities. The above findings should help to better understand the toxicity and action mechanisms of bisphenols, and also provide scientific data for screening specific biomarkers further applied for assessing pollutant-induced cardiac toxicity.

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## Oral presentation

# Integrin-stimulating polymer-peptide for improved cell survival in a recellularized liver model

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**Keywords:** liver tissue engineering • primary hepatocytes • anoikis • recellularization • PEG polymer-peptide

### Abstract:

In liver tissue engineering it is considered that primary hepatocytes are one of the best candidates for the repopulation of decellularized scaffolds. However, previous research has found that many of the seeded hepatocytes die once the recellularization process is completed. This cell death is likely due to anoikis, or cell death from the loss of cell-cell and cell-extracellular matrix (cell-ECM) interactions. Our hypothesis is that binding to the RGD-integrin followed by mechanical stimulation could mimic cell-ECM binding to ensure their survival and maintain their functionality. To address this, we have synthesized a molecule named PEG-GRGDS (PG). This polymer-peptide consists of a polyethylene glycol chain functionalized with a GRGDS peptide, which contains the RGD cell-adhesion sequence. In this study, we have evaluated the effects of the treating hepatocytes with PG (PG-treatment) when cells are cultured in suspended conditions, as well as within decellularized liver tissue. Our results have shown that PG-treatment has promise in prolonging the time non-adherent dispersed hepatocytes remain viable. This unique approach offers a simple method to improve cell conditions during recellularization and can help close the gap between recellularized liver technology and its implementation.

### Biography



I obtained a BS in Chemical Engineering from the University of Guadalajara, Mexico, followed by a Certificate in New Ventures Leadership from the Massachusetts Institute of Technology, USA. After working in Mexico for 3 years as a Plant Design Engineer, I moved to Japan, where I obtained a MS degree in Chemical Engineering from Kyushu University, where I am currently pursuing a PhD degree. My research interests are in the areas of cell culture, tissue engineering, and bioreactors.

# Session 3

Catalysis and Process Control

## Oral presentation

# Improving Surfactant Efficiency Through Nanoparticle-Assisted Systems: Reducing Adsorption and Enhancing Interfacial Properties

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**Keywords:** Surfactant, Adsorption, Nanoparticle, dispersion stability, Interfacial tension

### Abstract:

Surfactants are widely used in applications such as cleaning, detergency, enhanced oil recovery (EOR), oil decontamination, and site remediation. A significant challenge in these applications is the loss of surfactants due to adsorption onto solid surfaces (e.g., soil, fabrics, metals), which impacts both the economic viability of operations and raises environmental concerns regarding residual surfactants. To address this, nanoparticle-assisted surfactant systems have been introduced to reduce surfactant losses and enhance overall performance. In this study, surfactant formulations designed to achieve ultra-low interfacial tension with model oil (e.g., crude oil) were developed using Winsor Type III (middle-phase) microemulsions. The research investigated the effects of nanoparticles on surfactant behavior, including surface and interfacial properties, as well as microemulsion formation. Furthermore, the influence of various nanoparticle types (hydrophobic and hydrophilic silica) on surfactant adsorption onto solid surfaces, such as clay and sand, was examined. The findings revealed the mechanisms of surfactant-nanoparticle interactions, particularly the competitive adsorption between nanoparticles and solid surfaces. In EOR applications, incorporating nanoparticles into ultra-low interfacial tension formulations reduced surfactant adsorption onto various soil media by 40% to 60%.

### Reference

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### Biography

Ampira Charoensaeng is an assistant professor at the Petroleum and Petrochemical College (PPC), Chulalongkorn University, with 20 years of experience in surfactant science and technology. She holds a Ph.D. and M.S. in Environmental Management from Chulalongkorn University. Her research focuses on surfactant-based solutions for industrial and environmental applications, colloid chemistry; environmental and carbon management, and Life Cycle Analysis (LCA).



## Oral presentation

# Ethylene aromatization over zeolite catalyst with sulfur species

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**Keywords:** ethylene aromatization • MFI-type zeolite • Ga modification • sulfur species • stability

### Abstract:

Natural gas and biogas ( $\text{CH}_4+\text{CO}_2$ ) contain trace amounts of sulfur species such as hydrogen sulfide ( $\text{H}_2\text{S}$ ) and methanethiol ( $\text{CH}_3\text{SH}$ ), which cause equipment corrosion and catalyst deactivation. While these sulfur species are typically removed before chemical processes, in our project, we try to utilize these sulfur species as feedstocks for various reactions for future utilization of heavy fossil resources. In this study, we investigate the influence of a trace amount of  $\text{H}_2\text{S}$  or  $\text{CH}_3\text{SH}$  on ethylene aromatization, which is an olefin production, using an MFI-type zeolite catalyst. Results showed that while  $\text{H}_2\text{S}$  did not affect the reaction and the catalyst,  $\text{CH}_3\text{SH}$  led to significant degradation of the reaction. To improve the stability, we investigated the metal modification onto the zeolite. Among them, the gallium (Ga) modification, particularly at a concentration of 2-8 wt%, improved the stability regardless of the presence of  $\text{CH}_3\text{SH}$ . The role of the Ga modification is to promote the decomposition reaction of  $\text{CH}_3\text{SH}$ , which is strongly adsorbed on the reaction site of the zeolite. This finding contributes to the effective utilization of biogas to produce olefins in carbon neutrality.

### Reference

1. Influence of sulfur contamination on ethylene aromatization over a Ga-modified MFI-type zeolite, K Oshima, E Konishi, R Watanabe, C Fukuhara, M Kishida, Chemical Engineering Journal 480, 148241 (2024)

### Biography



I obtained my BS, MS, and PhD degrees in Applied Chemistry from Waseda University, Japan. After working at Numazu College and Seikei University, I am currently an Assistant Professor in the Department of Chemical Engineering at Kyushu University, Japan. I received the Advanced Technology Award from the Fuji-Sankei group in 2013. My research topics are in the areas of material circulation using catalysts or electrical activation. In addition to catalytic conversion of hydrocarbons, I investigate the electrical recycling of carbon composites such as CFRP and feedstock recycling of plastics.

# Revolutionizing Distillation Column Analysis with Artificial Intelligence and Digital Twins

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**Keywords:** ethylene aromatization • MFI-type zeolite • Ga modification • sulfur species • stability

## Abstract:

This research delves into the integration of artificial intelligence (AI) and digital twin (DT) technologies in process systems engineering, with a specific focus on a distillation column as the case study. The approach combines process simulators with real-time data collection systems, establishing a comprehensive DT framework. This integration allows for the validation of simulation results against historical sensor data, facilitating the early detection of operational anomalies. Additionally, the DT provides real-time monitoring capabilities for key process parameters that are typically not measured by standard sensors, such as percentage flooding. From an AI perspective, advanced methodologies like online bias learning (OBL), noise reduction techniques, and deep learning algorithms are utilized to enhance predictive performance. These improvements exceed benchmarks from previous research (Qin et al., 2021), showcasing the role of AI in boosting the efficiency and reliability of distillation column processes.

## Reference

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## Biography



I received my Bachelor's degree from Universitas Indonesia and my MS-PhD from Yeungnam University. Currently, I am an Assistant Professor in the Department of Chemical Engineering at Universitas Indonesia. My research interests focus on process simulation and the application of artificial intelligence, particularly in green energy and process.

# Visible-light assisted hydrogen evolution over Cu-decorated polymeric carbon nitride nanostructures

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**Keywords:** Photocatalytic water splitting; Polymeric carbon nitride; Heterostructure, Visible light; Hydrogen evolution

## Abstract:

CuO/polymeric carbon nitride-based heterostructure confines the band alignment which harvests solar light in the visible range. A series of Cu-doped polymeric graphitic carbon nitride photocatalysts were prepared using copper nitrate and melamine as precursors. Hydrogen production via photocatalytic water splitting was investigated by Cu-doped polymeric carbon nitride under visible light irradiation. The physicochemical properties of the synthesized samples were characterized by X-ray diffraction (XRD), Fourier transform infrared spectroscopy (FT-IR), scanning electron microscopy (SEM), transmission electron microscopy (TEM), UV-Vis diffuse reflectance spectra (DRS). The results showed that Cu-doped substrate exhibited higher hydrogen production in the visible range than bare polymeric carbon nitride. The apparent quantum yield of Cu-doped PCN's hydrogen generation is 18.23% at 420 nm.

## Biography



Dr. Shalini Sahani is an international research professor in the School of Chemical Engineering at Yeungnam University in Korea. She got his PhD Degree from the Department of Chemistry, Indian Institute of Technology (Banaras Hindu University), Varanasi, India.

# A Comprehensive Solvent Design Framework for Amine-based CO<sub>2</sub> Chemical Absorption

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**Keywords:** Amine-based solvents•Chemical absorption•Graph neural network•Multiobjective optimization

## Abstract:

Solvent properties are crucial for the design and operation of a carbon capture unit. In this work, we proposed a novel framework for designing amine-based solvents for CO<sub>2</sub> chemical absorption, utilizing graph neural networks (GNNs) to model the intricate behavior of multicomponent systems. The framework aims to develop three individual models that predict essential solvent properties, including equilibrium CO<sub>2</sub> loading, rate of reaction, and heat of absorption, across various process conditions. Once these models are constructed, multi-objective optimization will be performed to identify the system with the most optimal properties. Preliminary findings demonstrated that the non-physically-constrained GNN successfully predicts equilibrium CO<sub>2</sub> loading with promising accuracy. Future developments will incorporate thermodynamic constraints such as Gibbs-Duhem equation and sets of equilibrium reaction equation to enhance the model's physical consistency and predictive reliability. Furthermore, we will also include models for predicting the rate of reaction and heat of absorption, with physical constraints integrated. This approach offers a versatile method for managing solvent mixtures in CO<sub>2</sub> capture systems, regardless of the number of amine types in the mixture. The proposed framework shows promise for advancing the efficiency and effectiveness of amine-based carbon capture technologies and has the potential to significantly reduce the need for excessive experimental repetitions.

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## Biography



My name is Apri Wahyudi, and I hold a Bachelor of Engineering in Chemical Engineering from Universitas Islam Indonesia and a Master of Science in Petrochemical Technology from the Petroleum and Petrochemical College, Chulalongkorn University. I am currently pursuing a Doctor of Philosophy in Petrochemical Technology at the same institution. My research interests include amine-based CO<sub>2</sub> capture, mathematical modeling, and machine learning-driven modeling.

# Session 4

Green Environmental and Energy Technology

## Oral presentation

# Microalgae: A Valuable Biomass Source For CO<sub>2</sub> Sequestration

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**Keywords:** microalgae • carbon capture • CO<sub>2</sub> fixation • climate change • microalgae utilization

### Abstract:

Global warming, which is partly caused by rising levels of carbon dioxide in the atmosphere, is a main trigger for sustainable methods of sequestering carbon. This is due to the fact that excessive carbon dioxide (CO<sub>2</sub>) emissions into the atmosphere have become a dire threat to humanity and environmental sustainability. However, existing carbon capture and storage (CCS) methods are still considered economically complicated, and their long-term environmental implications remain unclear. The biological capture of carbon dioxide (CO<sub>2</sub>) using microalgae has recently been seen as an attractive medium to address these problems. Moreover, through microalgae, CO<sub>2</sub> can be captured and recycled into biomass, which in turn can be utilized as a carbon source to produce lipids for bioenergy production and other value-added products. Here we review carbon capture, utilization, and storage with microalgae, as well as microalgal species currently used for CO<sub>2</sub> capture.

### Reference

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2. Effects of the light intensity and the reactor geometry on the microalgae yield in a bubble-column photobioreactor. in E Kusriani & IGD Nugraha (eds), Muharam, Y, Dianursanti, Pramadana, AB & Supit, S, *4th International Tropical Renewable Energy Conference, i-TREC 2019.*, 0300411, AIP Conference Proceedings, vol. 2255, American Institute of Physics Inc., 4th International Tropical Renewable Energy Conference 2019, i-TREC 2019, Bali, Indonesia, 14/08/19 (2022). <https://doi.org/10.1063/5.0013968>

### Biography



I am a lecturer and researcher in the Bioprocess Engineering Study Program, Department of Chemical Engineering at Universitas Indonesia. I hold undergraduate, graduate, and postgraduate degrees in Chemical Engineering from Universitas Indonesia. My research focuses on Biomass production and CO<sub>2</sub> Fixation of Microalgae.

# Perfluorooctanoic acid efficient chain reaction degradation in multifunctional mineral augmentation geobiochemical remediation system

Wenbing Wang

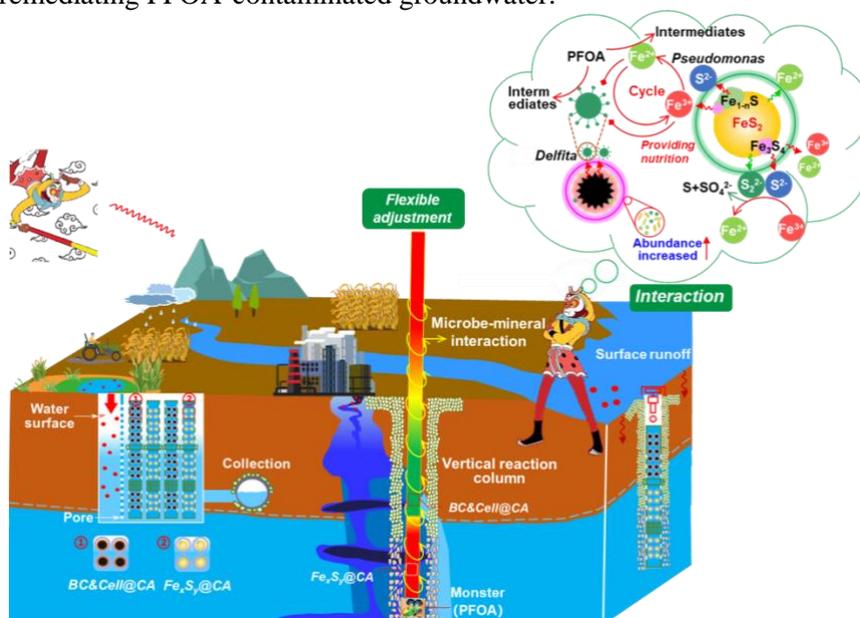
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**Keywords:** perfluorooctanoic acid • microbe • mineral • interaction • degradation

## Abstract:

Serious contamination of perfluorooctanoic acid (PFOA) has aroused global concern. General biotransformation or iron-based materials did not meet efficient PFOA removal. Here, specific green and low-carbon microorganism-biochar pellets, multi-component and multifunctional iron-sulfur ( $\text{Fe}_x\text{S}_y$ ) mineral pellets, and a microbe- $\text{Fe}_x\text{S}_y$  interaction geobiochemical remediation device were developed to solve this problem. The multi-scale (molecular, interface, and column scales) research method combined with the physical-chemical-biological multi-process reaction model was constructed to explore the PFOA removal and mechanism. Results revealed that the microbe- $\text{Fe}_x\text{S}_y$  interaction achieved excellent PFOA degradation performance and retention effect, with degradation rate  $\lambda$  ( $0.213 \text{ h}^{-1}$ ) increased by 113% than the  $\text{Fe}_x\text{S}_y$  ( $0.100 \text{ h}^{-1}$ ) device. The distribution coefficient  $K_d$  and kinetic adsorption  $\alpha$  increased by 18.54% and 22.61%; the fraction of kinetic sorption increased by 63.83% in the microbe- $\text{Fe}_x\text{S}_y$  device (77%) compared to alone  $\text{Fe}_x\text{S}_y$  (47%) device. High-throughput sequencing showed that microbe- $\text{Fe}_x\text{S}_y$  interaction increased the abundance of bacteria and archaea in the aqueous phase. *Delftia* and *Pseudomonas* combined with  $\text{Fe}^{2+}$  drove an efficient cycle chain reaction for PFOA. Liquid chromatograph mass spectrometer (LC-MS) results and quantitative structure-activity relationship (QSAR) model indicated that intermediates exhibited lower biotoxicity than PFOA. The bioaccumulation factor of intermediates decreased by 40.09%-99.24% than PFOA. Furthermore, the  $\text{NO}_3^-$  further increased the retention effect of the microbe- $\text{Fe}_x\text{S}_y$  device for PFOA with little reaction rate fluctuation, making it promising for eliminating PFOA contamination, especially in  $\text{NO}_3^-$  type of groundwater. It provided an efficient technology and device based on microbe-mineral interaction in remediating PFOA-contaminated groundwater.



## Reference

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2. Wenbing Wang\*, Meng Zhang, Qifeng Fan, Chunyang Li, and Hui Li\*. Dual Role of Microbe-FexSy Interaction to Drive Perfluorooctanoic Acid Multipath Chain Reaction Decay Cycles and Secondary Minerals-Ions (Fe<sup>2+</sup>/Fe<sup>3+</sup>) Transformation Cycles [J]. *ES&T Water* 2024 4 (5), 2123-2134.
3. Meng Zhang, Wenbing Wang\*, Tiantian Gong, Yulin Wu, Guangyao Chen. Cutting-edge technologies and relevant reaction mechanism difference in treatment of long- and short-chain per- and polyfluoroalkyl substances: A review[J]. *Chemosphere* 354 (2024) 141692.

## Biography



Prof. Wenbing Wang has been engaged in contamination remediation of soil and groundwater and numerical simulation for a long time, and is good at interdisciplinary research based on materials, microbiology, and mathematics disciplines; such as material interface reaction, microbial molecular mechanism, and static and dynamic reactive transport models. In-depth and extensive research has been done in the fields of site contaminants transport and transformation, accurate identification of contaminants spatial distribution and spatial-temporal evolution technology (algorithm), and microbial-chemical modular low-carbon remediation technology. So far, Dr. Wang has published more than 40 papers, and he has authored 22 SCI papers as first author and corresponding author. Here, he proposed a project to study the composition of emerging contaminant PFAS in the site, accurate identification of spatial distribution and green and low-carbon prevention and control; to construct a high-precision site sampling system, optimize PFAS step inversion calibration technology, interpolation method, and improve the green and low-carbon characteristics of technologies.

# Attenuation of phenyl-naphthenic acids related to oil sands process water using solar activated calcium peroxide

Ming Zheng<sup>1,2</sup>, Isaac Sánchez-Montes<sup>1</sup>, Jia Li<sup>1</sup>, Xiaodi Duan<sup>2</sup>, Bin Xu<sup>3</sup>, and Mohamed Gamal El-Din<sup>1,\*</sup>

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**Keywords:** naphthenic acids • solar activation • calcium peroxide • kinetics modeling • genotoxicity

## Abstract:

Refractory naphthenic acids (NAs) are among the primary toxic compounds in oil sands process wastewater (OSPW), a matrix with a complex chemical composition that poses challenges to its remediation. This study evaluated the effectiveness of calcium peroxide (CaO<sub>2</sub>) combined with solar radiation (solar/CaO<sub>2</sub>) as an advanced water treatment process for degrading model NAs (1,2,3,4-tetrahydronaphthalene-2-carboxylic acid, pentanoic acid, and diphenylacetic acid) in synthetic water (STW) and provide preliminary insights in treating real OSPW. Solar light and CaO<sub>2</sub> acted synergistically to degrade target NAs in STW (>67 of synergistic factor) following a pseudo-first-order kinetic ( $R^2 \geq 0.95$ ), with an optimal CaO<sub>2</sub> dosage of 0.1 g L<sup>-1</sup>. Inorganic ions and dissolved organic matter were found to hinder the degradation of NAs by solar/CaO<sub>2</sub> treatment; however, the complete degradation of NAs was reached in 6.7 hours of treatment. The main degradation mechanism involved the generation of hydroxyl radicals ( $\cdot\text{OH}$ ), which contributed ~90% to the apparent degradation rate constant ( $K$ ), followed by H<sub>2</sub>O<sub>2</sub> (4-5%) and <sup>1</sup>O<sub>2</sub> (0-5%). The tentative transformation pathways of three NAs were proposed, confirming an open-ring reaction and resulting in short-chain fatty acid ions as final products. Furthermore, a reduction in acute microbial toxicity and genotoxic effect was observed in the treated samples, suggesting that solar/CaO<sub>2</sub> treatment exhibits high environmental compatibility. Furthermore, the solar/CaO<sub>2</sub> system was successfully applied as a preliminary step for real-world applications to remove natural NAs, fluorophore organic compounds, and inorganic components from OSPW, demonstrating the potential use of this technology in the advanced treatment of oil-tailing-derived NAs.

## Reference

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## Biography



Dr. Ming Zheng, is an associate professor at Shanghai University since April 2023. He conducted postdoctoral research at Shanghai University, China (2020.1-2021.7) and the University of Alberta, Canada (2021.8-2023.7), focusing on recycling of harmful biomass, and control of emerging contaminants and pathogenic microorganisms in water. In 2019, he had a Ph.D. from Tongji University, jointly supervised by the University of Arizona (2016-2017). He has published 32 scholarly papers with H index of 17, presided 3 national or provincial level projects, participated in 4 national projects, and won the Shanghai Pujian talent program, Shanghai Postdoctoral Daily funding, etc.

## Oral presentation

# Fe(IV)=O/Fe(V)=O and $[\text{Fe}^{\text{IV}}_{\text{aq}}\text{O}]^{2+}/[\text{Fe}^{\text{V}}_{\text{aq}}\text{O}]^{3+}$ cooperating with free radicals induced high-rate SMX-Cr(VI) simultaneous removal in Fe<sub>7</sub>S<sub>8</sub>-PS micro-nano catalytic system

Chunyang Li<sup>1</sup>, Wenbing Wang<sup>\*1</sup>, Qifeng Fan<sup>1</sup>, Yunhui Zhang<sup>2</sup>, Meng Zhang<sup>1</sup>, Qianling Dong<sup>1</sup>, Ghebretensae Aron Kifle<sup>1</sup>, and Hui Li<sup>\*1</sup>

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**Keywords:** Fe(IV)/Fe(V) • Fe<sub>7</sub>S<sub>8</sub> • SMX-Cr(VI) • kinetic control • free radicals

## Abstract:

Conventional persulfate-based (PS-based) catalytic systems that resolve single-pollutant sulfamethoxazole (SMX) problems depends on free radicals. However, research on the contribution or cooperative effect of non-free radical Fe(IV)/Fe(V) species and the interaction of co-contamination Cr(VI)-SMX have not been enough sufficiently elucidated. The production source of Fe(IV)/Fe(V) species requires further exploration and expansion. Here, a pyrrhotite-PS (Fe<sub>7</sub>S<sub>8</sub>-PS) micro/nanocatalytic system was independently constructed to stimulate the production of Fe(IV)/Fe(V) species, which were identified by Mössbauer spectroscopy. In the Fe(IV)/Fe(V) species cooperating with the free-radical-induced high-rate reaction system, kSMX (0.0304 min<sup>-1</sup>) raised 152.0 times to kSMX (0.0002 min<sup>-1</sup>) in the sole Fe<sub>7</sub>S<sub>8</sub> system. SMX has five possible degradation pathways, in which the fractures of the S-N and N-C bonds are the two main chain scission degradation pathways confirmed through density functional theory (DFT) calculations. Furthermore, Cr(VI) was dominated by rapid reduction (0.0227 min<sup>-1</sup>) to low-toxicity Cr(III), which was eventually adsorbed by the dynamically transformed Fe<sub>7</sub>S<sub>8</sub> and secondary iron-oxide minerals. The SMX reaction path and degradation rate were increased by the  $[\text{FeaqIVO}]^{2+}/[\text{FeaqVO}]^{3+}$  in the solution (reacting with SMX and accelerating the transformation of free radicals). Hence, the Fe<sub>7</sub>S<sub>8</sub>-PS micro/nanocatalytic system provides a new strategy for treating high-concentration SMX-Cr(VI) co-contaminated wastewater and groundwater.

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## Biography



My name is Chunyang Li and I am a postdoctor from the School of Environmental Science and Chemical Engineering, Shanghai University. I am currently primarily engaged in researching the optimization of advanced oxidation processes (AOPs) and its practical application in actual contaminated sites. The primary research focuses on the development and preparation of highly efficient iron-based activators, optimizing iron-sulfur transformation to enhance pollutant removal, as well as achieving simultaneous and effective elimination of heavy metal and organic compound co-pollution. I have published two articles in Journal of Hazardous Materials (IF=13.6) and ACS ES&T Engineering (IF=7.4), as the first author.

# Fabrication of conducting polymer nanostructures and their applications

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**Keywords:** Conducting polymer • Nanomaterial • 3D structures • Electrode material • Chemical oxidative polymerization

## Abstract:

Conducting polymer (CP) nanomaterials are a distinguishable class of organic semiconducting materials that can achieve high electrical conductivity and unique electrochemical behaviors. In addition to their inherent advantages, they are also lightweight, processable, and low-cost. These advantages of CP nanomaterials can be enhanced by manufacturing them into three-dimensional (3D) structures and complexing them with other materials, such as metal oxides and carbon nanomaterials. In this work, we report fabrications and applications of various conducting nanomaterials through the solution processes. The CP nanomaterials in our work have been fabricated into 3D hydrogels/aerogels, conducting inks, thin films, and 3D-printed sculptures. The as-prepared CP nanomaterials are expected to be applied to various fields, including sensors, energy storage/conversion devices, thermoelectric devices, and OLEDs.

## Biography



Prof. Sunghun Cho received his Ph.D. in the School of Chemical and Biological Engineering at Seoul National University under the guidance of Prof. Jyongsik Jang in 2015. After carrying out postdoctoral research in Department of Chemistry and Biochemistry at University of California at Los Angeles (UCLA), Prof. Cho has been serving as a professor at Yeungnam University since 2016. In 2018, Prof. Cho received the Minister of Science and Technology Award of the Republic of Korea for the best safety environment laboratory. In 2019, he received the Excellence in Teaching Award from the President of Yeungnam University. Prof Cho's research interests include new fabrication methods for conducting hydrogel/aerogels, conducting inks, laser-scribed graphenes for chemical/pressure sensors, supercapacitors, thin-film solar cells, thermoelectric materials, and antistatic materials.

# Regulated Zn metal deposition by multi-channel carbon organic complex

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**Keywords:** Artificial interface layer, Multi-channel regulation, Inorganic-organic composite layer, Zinc anode, Water zinc-ion battery

## Abstract:

Rechargeable water-based zinc-ion batteries (AZIB) have become one of the most promising technologies in post-lithium battery technology due to their low cost, high safety and environmental friendliness. However, their practical development has been hampered by problems with zinc metal anodes, including dendrite growth, passivation, hydrogen evolution, and other side reactions. In order to solve these problems, a simple preparation strategy of artificial interface layer is proposed in this paper. Organic-inorganic composite artificial interface layer with multi-channel regulating zinc deposition is constructed on zinc foil as the anode of high performance AZIB. The results of density functional theory (DFT) theoretical calculation, in situ optical visualization and spectral analysis confirm that the organic composite layer has multi-channel directional deposition, so that the CMK-5/PS@Zn anode can promote homogeneous Zn deposition and inhibit hydrogen evolution reaction, and can be stably cycling for about 2000 hours. CMK-5/PS@Zn//NH<sub>4</sub>V<sub>4</sub>O<sub>10</sub> full battery still has a high specific capacity of 120.4 mAh g<sup>-1</sup> after 1000 cycles at 5.0 A g<sup>-1</sup>. This work proposes an innovative method of carbon-based organic composite layer protection for zinc anodes as an advanced design strategy for AZIB and beyond.

## Biography



Gao Li, PhD candidate in Chemical Engineering and Technology, School of Environmental and Chemical Engineering, Shanghai University. Main research interests: Design of new energy materials and their applications in lithium and water zinc batteries. Published 1 SCI paper in ACS Applied Materials & Interfaces as the first author.

## Oral presentation

# TiO<sub>2</sub>: a highly potential support to reliable electrocatalysis for PEMFCs

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**Keywords:** TiO<sub>2</sub> • Support material • Durability • Oxygen reduction reaction • proton exchange membrane fuel cells

### Abstract:

The low durability of Pt/C catalysts induced by the carbon corrosion is an important challenging area of a polymer electrolyte membrane fuel cell (PEMFC). To overcome this limitation, This study investigates the enhancement of support materials in PEMFCs through Nb and Si co-doping into TiO<sub>2</sub> (NSTO), targeting a breakthrough in electrocatalytic performance while circumventing the vulnerabilities associated with carbon corrosion. By integrating silicon—a dopant that modifies the electronic band structure and maximizes surface chemistry notably enhancing the Strong Metal-Support Interaction (SMSI) and oxygen vacancy concentration—these improvements bolster the interaction with platinum, significantly boosting oxygen reduction reaction (ORR) performance and durability without suffering from carbon corrosion risks. Quantitative achievements highlight the promising shift in operational roles from NSTO, delivering notably enhanced performance metrics in half-cell (10.135 A g<sub>Pt</sub><sup>-1</sup> of mass activity and 23.92 m<sup>2</sup> g<sub>Pt</sub><sup>-1</sup> of ECSA after 10,000 ADT) and single-stack cell tests (1.25 A cm<sup>-2</sup>/1.1 W cm<sup>-2</sup> after 5,000 ADT) with nearly zero-degradation under assorted conditions.

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### Biography



Dr. KIM, Moonsu obtained his B.S. degree from the Department of Chemistry at Inha University, followed by M.S. and Ph.D. degrees from the Department of Chemical Engineering at the same institution. Before pursuing his Ph.D., he worked in the industrial field at Samsung Electronics Co., Ltd. He also served as a visiting scholar at the Fritz-Haber-Institut der Max-Planck-Gesellschaft in Berlin, Germany, and performed postdoctoral research at the Institut des Sciences Chimiques de Rennes (ISCR) - UMR CNRS 6226 in Rennes, France. Currently, he is a postdoctoral fellow in the School of Chemical Engineering at Yeungnam University, Korea, authoring 33 publications focused on materials electrochemistry, and energy storage & conversion. His research interests include electrodeposition (plating), anodizing processes, and energy storage & conversion: fuel cells, electrochemical water electrolysis, secondary batteries (Li<sup>+</sup>, Na<sup>+</sup>, K<sup>+</sup>, Al<sup>3+</sup>), and metal-air batteries.

# Session 5

Batteries and Supercapacitors

# High performance CF<sub>x</sub>/Li battery: materials and cells

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**Keywords:** CF<sub>x</sub>/Li battery • rate-performance 2 • low-temperature performance

## Abstract:

Li/CF<sub>x</sub> batteries possess the highest theoretical energy density of 2180 Wh·kg<sup>-1</sup> among the primary batteries, which play essential roles in implantable medical-biological devices, tire-pressure monitoring systems, deep underground devices, and spacecraft. Unfortunately, the limited rate-performance and low-temperature performance of the battery confine its practical application.

In this oral, I will present our strategies on improving the rate-performance and low-temperature performance of Li/CF<sub>x</sub> batteries (materials and cells) during last 10 years. I will also briefly introduce our work on high-voltage all-solid-state batteries.

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## Biography



Yang Dai obtained his Ph.D. degree in materials science and engineering at Shanghai Institute of Microsystem and Information Technology, CAS. in 2009. And then he worked as a senior engineer at Shanghai Institute of Space Power Sources for 6 years. After that he joined the Depart of Chemical Engineering, Shanghai University as an associate professor since 2015. His researches focus on materials and devices for electrochemical energy storage. He studied the lithium-rich layered material by spherical aberration corrected transmission electron microscope under the direction of Dr. Lijun Wu and Prof.

Yimei Zhu in Brookhaven National Laboratory, NY, United State during 2018-2019. He

has published 40 more articles in peer-reviewed international journals.

# Electrode Structure Engineering for All Solid State Batteries

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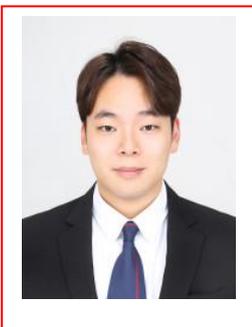
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**Keywords:** All-Solid-State Battery • Anode-free • Li deposition • Solid Electrolyte • Creep Behavior

## Abstract:

All-solid-state batteries (ASSBs) with sulfide-based solid electrolytes with high ionic conductivity are regarded as the ultimate next-generation energy storage systems due to their enhanced safety and energy density by enabling the use of metallic anodes. Li metal is considered a promising anode material for ASSBs because of its high theoretical specific capacity (3860 mAh/g) and the lowest electrochemical potential (-3.04 V versus standard hydrogen electrode). However, its practical use has been hindered by several issues related to the interface, such as contact loss during cycling, which accelerates Li dendrite growth, and chemical instability between Li and sulfide-based solid electrolytes. In this talk, the fundamental degradation mechanisms of the ASSBs underlying electrochemical and mechanical aspects are introduced first. Subsequently, we introduce our strategies to stabilize the Li metal and sulfide-based solid electrolytes interface. The designed ASSBs could effectively retard the Li dendrite growth and unwanted side reaction and shows much enhanced electrochemical performance.

## Biography



Seho Sun is an assistant professor in the School of Chemical Engineering at Yeungnam University in Korea. He got his Ph.D. in the Department of Energy Engineering at Hanyang University in 2022 and was appointed as a senior engineer in the Memory business division at Samsung electronics in 2022. In 2023, he joined Yeungnam University as a professor. His research interest is mainly focused on the design of nano materials for energy device and semiconductor applications. He is actively conducting research in energy-related fields such as batteries and electrocatalysts, and making significant contributions to these fields. He has collaborated with global companies such as Samsung Electronics, Samsung SDI, and LG Chem, and made significant contributions to the industry.

## Oral presentation

# Microwave-assisted synthesis of $\text{Co}_3\text{O}_4/\text{SnO}_2$ /reduced graphene oxide nanocomposites for supercapacitor applications

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**Keywords:** Supercapacitor • Microwave process • Perovskite hydroxide • Cycling stability

### Abstract:

Supercapacitor (SC) is one of the electrochemical energy storage devices that significantly advances the modern automobile industry. Graphene materials have been extensively utilized as the SC electrodes along with metal oxides (MOs). In recent times, Microwave (MW)-assisted dry synthetic approaches have been extensively studied for fabricating SC electrodes. Herein, we synthesized a ternary nanocomposite based on  $\text{Co}_3\text{O}_4$ ,  $\text{SnO}_2$ , and reduced graphene oxide (rGO) through MW irradiation within the reaction time of 30 s. The synthetic approach is suitable for converting perovskite hydroxides to MOs within a short time. Compared to the common time-consuming synthetic approaches, the MW-assisted synthetic approach is highly beneficial in terms of short reaction time, cost-effectiveness, and straightforwardness. The synthesized hybrid electrode displayed a good capacity (146.4 C/g) and enhanced cycling stability (103.2% after 15,000 cycles). Moreover, the corresponding aqueous hybrid supercapacitor device with MW-synthesized rGO as a negative electrode displayed a maximum energy density of 27 Wh/kg and promising cycling stability of 102.4% after 10,000 cycles.

### Biography



Sumanta Sahoo is an assistant professor in the School of Chemical Engineering at Yeungnam University in Korea. He got his Ph. D. degree from the Indian Institute of Technology, Kharagpur, India in the year 2013. His work is mainly focused on fabricating supercapacitor electrodes based on graphene, MXene, and metal oxide-based nanocomposites.

## Oral presentation

# Synthesis of garnet-type cubic-LLZO solid-electrolyte for all-solid-state lithium-ion batteries via a combined process of induction thermal plasma and sintering

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**Keywords:** induction thermal plasma • all-solid-state lithium-ion battery • solid electrolyte • garnet-type cubic-LLZO

### Abstract:

All-solid-state lithium-ion batteries (ASSLBs) are widely considered the most effective solution to overcoming the energy density and safety limitations of conventional lithium-ion batteries (LIBs) by replacing liquid electrolytes with solid electrolytes. Garnet-type cubic- $\text{Li}_7\text{La}_3\text{Zr}_2\text{O}_{12}$  (c-LLZO) is regarded as a promising solid electrolyte due to its high chemical stability and excellent  $\text{Li}^+$  conductivity. The most common method for synthesizing c-LLZO is the solid-state reaction (SSR) method, which involves an overconsumption of lithium precursors (to compensate for lithium loss) and requires long-duration sintering (10–36 hours) at high temperatures (1273–1673 K). However, the bulk particle and pellet forms of c-LLZO produced by the SSR method fail to meet the thin-film structural requirements of less than 100 micrometers, which are essential for the practical implementation of ASSLBs. Therefore, to enable the practical application of c-LLZO, exploring more efficient and advanced synthesis methods is urgent and necessary.

This study presents a facile and advanced method for synthesizing c-LLZO through combined process of induction thermal plasma and sintering. The c-LLZO was successfully synthesized via thermal plasma treatment of the precursors for several milliseconds, followed by subsequent one-hour calcination. The structure and chemical composition of the plasma treated intermediates and fabricated c-LLZO were analyzed using X-ray diffractometry (XRD) and scanning transmission electron microscopy-energy dispersive X-ray spectroscopy (STEM-EDS). The morphology was examined through bright field (BF) and annular dark field (ADF) images obtained via STEM. Additionally, the formation mechanism of plasma-treated intermediates and c-LLZO was elucidated by consideration of thermodynamic analysis and homogeneous nucleation theory. This study presents advanced and promising method for synthesizing c-LLZO thin films with thicknesses below tens of micrometers through short-time sintering, utilizing plasma-treated nano-sized intermediates.

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### Biography



Byeong-II Min is currently pursuing his Ph.D. in the Department of Chemical Engineering at Kyushu University, Japan. His research focuses on the synthesis and application of materials for all-solid-state lithium-ion batteries using thermal plasma technology

## Oral presentation

# Redox-active “Structural Pillar” Molecular Doping Strategy Towards High-Performance Polyaniline-based Flexible Supercapacitors

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**Keywords:** wearable supercapacitors • directional freezing • large-sized molecular dopant • pseudocapacitance • redox active

## Abstract:

To coordinate flexibility to electrodes without sacrificing their electrochemical properties is critical for the development of wearable supercapacitors (SCs)[1–3]. Polyaniline (PANI) is well-known pseudocapacitive electrode material due to its high conductivity and different oxidation states upon switchable structures[4,5]. However, its rigid conjugated backbone and structural instability caused by repeated doping/de-doping during cycling severely impede its utilization in flexible SCs. Herein, we deploy a directional freezing and redoxactive “structural pillar” molecular doping strategy to boost PANI-based flexible SCs with high performance. The directional freezing strategy constructs an interconnected 3D honeycomb hydrogel structure with PANI nanofibers, which guarantees fast ion diffusion and electron transport and meanwhile exposes abundant active sites. The large-sized dopant 2-amino-4-bromoanthraquinone-2-sulfonic acid sodium (AQNS) is used as the structural pillar to alleviate the structural instability of PANI during cycling and provides additional pseudocapacitance arising from its redox active quinone groups. Moreover, the negatively charged  $-SO_3^-$  on AQNS can further interact with  $H^+$  in the electrolyte to act as an internal proton reservoir, assisting the protonation of  $-NH-$  and  $-N=$  in PANI to facilitate its charge storage process. Consequently, the PANI-AQNS electrode achieves a high specific capacitance of  $578\text{ F g}^{-1}$  at  $1\text{ A g}^{-1}$  and its symmetric SCs exhibit a specific capacitance of  $199\text{ F g}^{-1}$  at  $0.5\text{ A g}^{-1}$  with an energy density of  $13.61\text{ W h kg}^{-1}$  at a power density of  $175\text{ W kg}^{-1}$ . Upon 2000 cycles of dynamic deformations, the SCs can still maintain above 90% of the initial capacitance, verifying their excellent flexibility-relevant property.

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## Biography



Ding Wei received her M.S. in 2024 majoring in Materials and Chemicals from Shanghai University. Currently, she is pursuing her Ph.D. degree in the School of Environmental and Chemical Engineering at Shanghai University. Her research interests focus on organic electrode materials and hydrogel electrolyte materials for supercapacitors, flexible wearable supercapacitors.

## Oral presentation

# N/O-bridge stimulated robust binding energy and fast charge transfer between carbon nanofiber and NiCo LDH for advanced supercapacitors

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**Keywords:** NiCo LDH • carbon nanofiber • binding energy • interfacial electrical field • supercapacitor

## Abstract:

Layered double hydroxide (LDH)-carbon composites effectively mitigate the inherent issues of agglomeration and poor conductivity in LDH. However, the weak binding energy and insufficient charge transfer capability between LDH and carbon substrate significantly compromise the active substance loading, cyclic stability and practical capacity of the composites. Herein, N/O co-doping porous carbon nanofibers (NOPCNFs) are first prepared by blending diminutive zinc imidazolate framework-8 nanoparticles with polyacrylonitrile for electrospinning, and then densely packed NiCo LDH nanosheets are homogeneously anchored on NOPCNFs to form NiCo LDH@NOPCNFs heterostructure via a hydrothermal method. The experimental findings and density functional theory calculation results indicate that N/O atoms exhibit robust binding forces with metal atoms through enhanced electrostatic adsorption and p-d covalent hybridization, which facilitates the nucleation and development of NiCo LDH on carbon nanofibers. Meanwhile, these heteroatoms also serve as the bridge for electron transfer from NiCo LDH to NOPCNF, leading to a strong interfacial electric field, thus accelerating charge transfer behaviors. Benefitting from the synergistic interaction between NiCo LDH and NOPCNF, the obtained NiCo LDH@NOPCNFs demonstrate an elevated mass loading of active substance (55 wt%), an impressive specific capacitance of 1340 F g<sup>-1</sup> at 1 A g<sup>-1</sup> (based on the mass of NiCo LDH, 2463 F g<sup>-1</sup>), and good cyclic durability for 5000 cycles. Moreover, an all-solid-state asymmetric supercapacitor using NOPCNFs and NiCo LDH@NOPCNFs shows promising practical application prospects. This work gives insights into the important influence of heteroatom doping in carbon, and provides a feasible approach for the efficient integration of electroactive and carbon material.

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## Biography



Luo Yuancong, a PhD student at the School of Environmental and Chemical Engineering, Shanghai University, specializes in research on energy storage and electrocatalytic electrode materials. To date, Luo has published 10 SCI papers, including two as the first author and one as a co-first author. In November 2023, Luo participated in an academic exchange at the National University of Singapore. Luo has received several honors, including the First-Class Academic Scholarship and Innovation Scholarship at Shanghai University, and Third Prize in the China Graduate Carbon Neutrality Innovation and Creativity Competition.

# Session 6-1

Student's Oral Presentation

## Oral presentation

# Enhancing heterojunction interface charge transport efficiency in NiCo-LDHs@Co/CoO-CNFs for high-performance asymmetric and zinc-ion hybrid supercapacitors

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**Keywords:** Carbon nanofiber • NiCo-LDHs • Heterointerface • Flexible asymmetric supercapacitor • Zn ion hybrid supercapacitors

## Abstract:

The lack of active groups and poor dispersion of pristine carbon substrates lead to their inability to composite with other materials effectively, so that the electron transfer between them is inefficient. Therefore, in order to design carbon-based composites with high conductivity and electrochemical properties, the electron transfer between them must be enhanced first. Herein, the Co/CoO quantum dots doped carbon nanofiber (Co/CoO-CNF) materials with mesopore, high degree of graphitization and mechanical flexibility are synthesized via an electrospinning method. Then, ultrathin NiCo-LDHs are uniformly loaded on the Co/CoO-CNFs in situ to form NiCo-LDHs@Co/CoO-CNFs. Benefiting from the Fermi energy level difference and heterointerface between Co/CoO-CNFs ( $E_F = -4.44$  eV) and NiCo-LDHs ( $E_F = -2.12$  eV), electrons can be transferred rapidly from NiCo-LDHs to Co/CoO-CNFs during the electrochemical reaction, so that NiCo-LDHs@Co/CoO-CNFs exhibit the excellent specific capacitance of  $2055 \text{ F g}^{-1}$  at  $1 \text{ A g}^{-1}$ . When using in a flexible asymmetric supercapacitor, NiCo-LDHs@Co/CoO-CNFs shows a high energy density of  $54.0 \text{ Wh kg}^{-1}$  at  $760.0 \text{ W kg}^{-1}$ . Furthermore, assembled as the Zn-ion hybrid supercapacitor, NiCo-LDHs@Co/CoO-CNFs can also display an ultra-high energy density of  $108 \text{ Wh kg}^{-1}$  at  $914.8 \text{ W kg}^{-1}$ , as well as outstanding work durability (the capacitance of 98.2% after 10000 cycles).

## Biography



I am Ge Huicheng, a master's student in the Environmental Functional Materials Group. My research focuses on aqueous zinc ion batteries and supercapacitors. Currently, I have published an academic paper as the first author in Carbon (JCR Q1 Top Journal IF: 10.5) titled "Enhancing Heterojunction Interface Charge Transport Efficiency in NiCo-LDHs@Co/CoO-CNFs for high-performance asymmetric and zinc-ion hybrid supercapacitors". The work "Design Manual of a High Energy Density, Impact-Resistant Wearable Zinc-Ion Hybrid Energy Storage Device" won the the Grand Prize in the School Competition of the 16th Energy Conservation and Emission Reduction Social Practice and Technology Competition. Additionally, I won the Third Prize in the National Competition of the First China Postgraduate "Dual Carbon" Innovation and Creativity Competition.

## Oral presentation

# Superb green cycling strategies for microbe-Fe<sup>0</sup> neural network-type interaction: Harnessing eight key genes encoding enzymes and mineral transformations to efficiently treat PFOA

Wenbing Wang<sup>1</sup>, Qifeng Fan<sup>1</sup>, Tiantian Gong<sup>1</sup>, Meng Zhang<sup>1</sup>, Chunyang Li<sup>1</sup>, Yunhui Zhang<sup>2</sup>, Hui Li<sup>1\*</sup>

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**Keywords:** Functional gene • Metabolic pathway • Microbe-Fe<sup>0</sup> • PFOA • Remediation

## Abstract:

To address time-consuming and efficiency-limited challenges in conventional zero-valent iron (ZVI, Fe<sup>0</sup>) reduction or biotransformation for perfluorooctanoic acid (PFOA) treatment, two calcium alginate-embedded amendments (biochar-immobilized PFOA-degrading bacteria (CB) and ZVI (CZ)) were developed to construct microbe-Fe<sup>0</sup> high-rate interaction systems. Interaction mechanisms and key metabolic pathways were systematically explored using metagenomics and multi-process coupling model for PFOA under microbe-Fe<sup>0</sup> interaction. Compared to Fe<sup>0</sup> (0.0076 day<sup>-1</sup>) or microbe (0.0172 day<sup>-1</sup>) systems, PFOA removal-rate (0.0426 day<sup>-1</sup>) increased by 1.5 to 4.6 folds in batch microbe-Fe<sup>0</sup> interaction system. Moreover, *Pseudomonas* accelerated transformation of Fe<sup>0</sup> into Fe<sup>3+</sup>, which profoundly impacted PFOA transport and fate. Model results demonstrated microbe-Fe<sup>0</sup> interaction improved retardation effect for PFOA in columns, with decreased dispersivity  $a$  (0.48 to 0.20 cm), increased reaction rate  $\lambda$  (0.15 to 0.22 h<sup>-1</sup>), distribution coefficient  $K_d$  (0.22 to 0.46 cm<sup>3</sup>·g<sup>-1</sup>), and fraction  $f'$  (52% to 60%) of first-order kinetic sorption of PFOA in microbe-Fe<sup>0</sup> interaction column system. Moreover, intermediates analysis showed that microbe-Fe<sup>0</sup> interaction diversified PFOA reaction pathways. Three key metabolic pathways (ko00362, ko00626, ko00361), eight functional genes and corresponding enzymes for PFOA degradation were identified. These findings provide insights into microbe-Fe<sup>0</sup> “neural network-type” interaction through unveiling biotransformation and mineral transformation mechanisms for efficient PFOA treatment.

## Reference

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## Biography



I'm Qifeng Fan, a senior graduate student majoring in Environmental Science and Engineering in Shanghai University. My research interests lie in the field of transport and fate of PFOA under microbial interaction with iron-based minerals. In my current research, I am focusing on the development of iron-based functional materials and their application in remediation of contaminated soil and groundwater. Anyway, I am dedicated to pursuing a career in the field of environmental science and engineering. I am confident that my passion, skills and knowledge will enable me to make contributions to the society and the environment.

## Oral presentation

# Selective Conversion of Ethane to Value Added Products on RhO<sub>2</sub>(110): A DFT and Microkinetic Simulation Study

Seongjun Lee<sup>1‡</sup>, Jungwon Yun<sup>2‡</sup>, Dasol Bae<sup>1</sup>, Minkyu Kim<sup>1\*</sup>

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**Keywords:** RhO<sub>2</sub>(110) • Selective Conversion • Micro Kinetic Simulation • DFT

### Abstract:

The selective transformation of small alkanes into value-added products represents a significant challenge in catalysis due to the propensity for complete oxidation. In this work, we utilize DFT calculations and TPRS simulations to explore the oxidation of ethane on the RhO<sub>2</sub>(110) surface. We compare the reactivity and selectivity of RhO<sub>2</sub>(110) with that of the extensively studied IrO<sub>2</sub>(110) surface. Our findings demonstrate that the moderate reactivity of RhO<sub>2</sub>(110) enhances selectivity towards ethylene formation. This selective behavior arises from a delicate balance between C-H bond cleavage and C<sub>2</sub>H<sub>4</sub> desorption on the RhO<sub>2</sub> surface. These results identify RhO<sub>2</sub>(110) as a promising catalyst for the selective oxidation of small alkanes, offering a potential route to increased yields of value-added products. Our study lays the foundation for further experimental and theoretical exploration of Rh-based catalysts for the activation and selective conversion of small alkanes.

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### Biography



I hold a B.S degree from Yeungnam University and am currently pursuing a Master's in Chemical Engineering under the guidance of Prof. Minkyu Kim at the same institution. With 7 published papers, over 36 citations, and an h-index of 3, my research focuses on advancing environmental catalysis through the application of Density Functional Theory (DFT) and experimental methods.

## Oral presentation

# Optimized chilling system design for precision cooling using mixed refrigerants cycle in semiconductor industry

Muhammad Islam<sup>1</sup>, Ahmad Naquash<sup>1</sup>, Moonyong Lee\*<sup>1</sup>

<sup>1</sup>School of Chemical Engineering, Yeungnam University, 38541, Gyeongsan-si, Republic of Korea  
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**Keywords:** Chilling system; Semiconductor industry; mixed refrigerants; cooling circuit

### Abstract:

In semiconductor manufacturing, etching is a critical process where unwanted parts are removed from the circuit sketch created during photolithography. This process requires precise cooling, typically provided by a chiller system using a vapor compression refrigeration cycle. The chilling system includes an evaporator, compressor, condenser, and expansion device, circulating refrigerants to manage the temperature of the process water system. The given study include the development of an integrated mixing unit and an ultra-low temperature, high-efficiency chiller capable of reaching temperatures as low as -85 °C using a mixed refrigerant system. The design allows for rapid and precise temperature control, crucial for maintaining the integrity of the cooling process during etching. Additionally, the selection of refrigerants was based on their thermophysical and environmental properties, aiming to optimize both performance and sustainability. The proposed chilling system addresses the specific refrigeration needs of semiconductor manufacturing, enhancing efficiency and control.

### Biography



Muhammad Islam, PhD candidate in Chemical Engineering, School of Chemical Engineering, Yeungnam University. Main research interest: Design of cryogenic energy systems, with applications aimed at enhancing compactness and optimization in chilling, liquefaction, and separation processes within the hydrocarbon and semiconductor industries. Contributed to the field through the publication of two SCI-indexed papers, one featured in the International Journal of Hydrogen Energy and the other in Energy, an open access journal.

## Oral presentation

# Synthesize Vegan Leather Substrate using Agricultural Waste Extract Based Culture Medium

So Yeon Won<sup>1</sup>, Seong Min Kim, Won Yi Jung, Da Eun Yeo, Sung Soo Han\*

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**Keywords:** Sustainable materials, Bacterial Cellulose, Agricultural Waste, Leather Substrate

### Abstract:

The rapid changes in climate, pest infestations, and supply-demand imbalances have led to an annual increase in discarded agricultural products, which in turn causes significant soil and water pollution due to improper disposal. Additionally, the production of natural leather involves animal sacrifice and generates large quantities of wastewater, prompting research into eco-friendly alternatives like synthetic leather.

This study developed an ethical and eco-friendly leather alternative by using extracts from discarded agricultural products as a culture medium to grow microorganisms, producing bacterial cellulose as the substitute material. Bacterial cellulose is gaining attention due to its high purity and strength compared to plant-based cellulose, and it can be produced without resource depletion. The physical properties of the cultured bacterial cellulose were analyzed using SEM, DSC, UTM, XRD, and FT-IR, while its toxicity was assessed through cell experiments. This research demonstrates the potential to repurpose agricultural waste as a vegan leather alternative, adding value to waste and offering both academic and economic benefits.

### Biography



So Yeon Won is a Graduate students in the School of Chemical Engineering at Yeungnam University in Korea. She got her Bachelor's and Master's Degree in the School of Chemical Engineering at Yeungnam University.

## Oral presentation

# Dual core microcapsule for Time-Temperature monitoring system

Hyo-Jin Kim, Hye-Seon Jeong and Chang-Hyung Choi\*

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**Keywords:** dual core microcapsule • microfluidic • controlled release • osmotic pressure • time monitoring

### Abstract:

This study proposes a novel release system that allows control over the release timing and profile using microcapsules with asymmetric shells in a simple manner. The capsule with this unique structure is produced with monodispersity using microfluidic technology based on a double emulsion (W/O/W), and microcapsules with asymmetric shell thicknesses are fabricated via rapid photopolymerization. This release occurs through the buckling and rupture of the shell caused by osmotic pressure. For example, when the continuous phase transitions to hypertonic conditions, the osmotic pressure difference between the interior and exterior of the capsule causes buckling at the thinner part of the asymmetric shell, leading to cracks once the rupture point is exceeded, and releasing the encapsulated cargo. By adjusting the capsule geometry or using shell materials with different mechanical properties, it is possible to control the trigger point, occurrence, and profile. This system can be applied in various fields requiring time monitoring, particularly in cold chain logistics, and improves stability and reliability through the irreversible rupture of the capsules.

### Reference

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2. Controllable Fabrication of Inhomogeneous Microcapsules for Triggered Release by Osmotic Pressure, W. Zhang et al. *Small* (2019)

### Biography



I am currently studying as a master's student in the School of Chemical Engineering at Yeungnam University, Korea. I am learning about developing functional hydrogel materials using microfluidic technology and applying them in the biomedical field.

# Session 6-2

Student's Poster Presentation

# Synthesis and Characterization of Guanidinylated singlet oxygen Releasing polymersomes Based on Biodegradable Polycarbonate

Suzhen Wang,<sup>1</sup> and Hailong Che\*<sup>1</sup>

<sup>1</sup>Department of Chemical Engineering, School of Environmental and Chemical Engineering, Shanghai University, Shanghai, 200444, China  
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**Keywords:** Polymer self-assembly • Polymersomes • guanidine groups • Anti-tumor

## Abstract:

Photodynamic therapy (PDT), a therapeutic modality that harnesses photosensitizers to convert surrounding oxygen into singlet oxygen ( $^1\text{O}_2$ ) upon laser irradiation, holds significant potential as a non-invasive approach for tumor ablation. Nevertheless, in the design and preparation of novel porphyrin-based photosensitizers, challenges such as aggregation-induced quenching, premature drug release, and hypoxia-induced resistance are conspicuously present. Herein, we have prepared functionalized poly(trimethylene carbonate) (PTMC) copolymers using pentafluorophenyl derivatives of TMC to obtain polymers with embedded photosensitizers. Moreover, the functionalization of guanidine groups endows polymersomes with enhanced cellular uptake efficiency via specific interactions with the cell surface, which synergistically augments the anticancer efficacy of the system. Polymersomes were prepared by direct hydration. We employed nuclear magnetic resonance spectroscopy ( $^1\text{H}$  NMR,  $^{19}\text{F}$  NMR) and gel permeation chromatography (GPC) to characterize the structure of amphiphilic block copolymers. The prepared polymersomes were confirmed to possess a uniform particle size distribution and a specific morphology by means of transmission electron microscopy (TEM) and dynamic light scattering (DLS). We evaluated the  $^1\text{O}_2$  release capacity of the polymersomes using a UV-visible absorption spectroscopy system and also investigated their cytotoxicity to tumor cells under dark and light conditions respectively. It was demonstrated that the polymer generates singlet oxygen under near-infrared light, and the copolymer containing guanidine groups exhibits a stronger anti-proliferative effect on cancer cells.

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## Poster presentation

# The research explores the application of multifunctional catalysts in alkaline electrochemical water splitting

Jinhu Wu,<sup>1</sup> and Yufei Zhao\*<sup>2</sup> and Hao Liu\*<sup>2</sup>

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**Keywords:** oxygen evolution reaction • multifunctional catalysts • water splitting

### Abstract:

The efficient oxygen evolution reaction (OER) process crucially depends on the rational design and synthesis of high-performance electrocatalysts. OER plays a vital role in energy conversion and storage devices. Nonetheless, the current state-of-the-art electrocatalysts are predominantly based on precious metals. Consequently, the development of low-cost, highly efficient OER electrocatalysts is of profound significance. This study aims to elucidate the coordination environment around the active metal centers and the electronic structure of metallic species during the synthesis of non-precious multi-nanocrystals and their electrocatalytic processes. We have engineered nanoscale multi-component nanocrystalline alloys FeNiCoMo with crystalline/amorphous structures through a facile synthesis method to enhance OER performance. The anticipated outcomes are expected to augment the foundational knowledge in designing efficient oxygen-generating electrocatalysts and uncover the structural evolution of metal-based materials in the OER. This will likely bolster the advancement of metal-air battery technology, attract increased interest from researchers and industry, and foster a sustainable future.

### Biography



My name is Wu Jintiger, born in 1999. I graduated from East China University of Science and Technology in 2022, earning a Bachelor's degree in Engineering, specializing in Chemical and Fuel Engineering. Presently, I am pursuing a Ph.D. in Chemical Engineering and Technology at Shanghai University, with a research focus on high-entropy catalysts for electrocatalysis. My hobbies encompass swimming, badminton, and table tennis.

# Nitric Oxide-Releasing Tubular Polymersomes toward Advanced Gas Therapeutic Carriers

Zhezhe Li and Hailong Che\*

Department of Chemical Engineering, School of Environmental and Chemical Engineering, Shanghai University, Shanghai, 200444, China  
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**Keywords:** Polymer self-assembly • Polymer vesicles • NO-donors • Anti-tumor

## Abstract:

Polymersomes are nano-assemblies with a double membrane structure. Tubular polymersomes with a high aspect ratio structure are readily endocytosed by cells to achieve enhanced therapeutics, compared to their spherical counterparts. Here we synthesised biodegradable amphiphilic block copolymers containing nitric oxide (NO) donors and constructed tubular NO polymersomes by solution self-assembly technique. We used nuclear magnetic resonance spectroscopy ( $^1\text{H}$  NMR,  $^{19}\text{F}$  NMR) and gel permeation chromatography (GPC) to characterise the amphiphilic block copolymers structure; the prepared polymersomes were confirmed to be tubular in shape and with a uniform particle size distribution by means of transmission electron microscopy (TEM, Cryo-TEM) and dynamic light scattering (DLS). We evaluated the NO release capacity of the tubular polymersomes using UV-visible absorption spectroscopy system, and also investigated their cytotoxicity to tumour cells under dark and light conditions, respectively. It was shown that the tubular polymersomes could release NO gas in a controlled manner under light to exert their biological effects; compared with the spherical polymersomes, the tubular polymersomes released more NO in a dose-dependent manner, and their antiproliferative effects on cancer cells were stronger. In this paper, we propose the use of tubular polymersomes as NO nanocarriers, which can give full play to the characteristics of non-spherical polymersomes assemblies and the advantages of NO gas therapy, and provide a new solution for the construction of smart nanogas therapeutic agents.

## Reference

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# Covalent Triazine Based Frameworks with Donor-Donor- $\pi$ -Acceptor Structures for Dendrite-Free Lithium Metal Batteries

Xiao-Meng Lu and Yong Wang\*

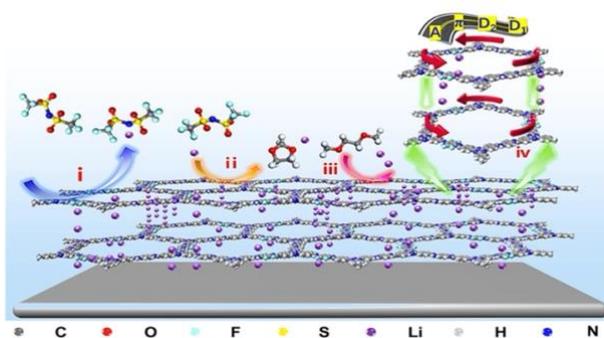
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**Keywords:** covalent triazine framework • donor-donor- $\pi$ -acceptor • interfacial layer • Li metal batteries

## Abstract:

The appearance of disordered lithium dendrites and fragile solid electrolyte interfaces (SEI) significantly hinder the serviceability of lithium metal batteries. Herein, guided by theoretical predictions, a multi-component covalent triazine framework with partially electronegative channels (4C-TA0.5TF0.5-CTF) is incorporated as a protective layer to modulate the interface stability of the lithium metal batteries. Notably, the 4C-TA0.5TF0.5-CTF with optimized electronic structure at the molecular level by fine-tuning the local acceptor-donor functionalities not only enhances the intermolecular interaction thereby providing larger dipole moment and improved crystallinity and mechanical stress, but also facilitates the beneficial effect of lithiophilic sites (C-F bonds, triazine cores, C=N linkages and aromatic rings) to further regulate the migration of Li<sup>+</sup> and achieve a uniform lithium deposition behavior as determined by various in-depth in/ex situ characterizations. Due to the synergistic effect of multi-component organic functionalities, the 4C-TA0.5TF0.5-CTF modified full cells perform significantly better than the common two/three-component 2C-TA-CTF and 3C-TF-CTF electrodes, delivering an excellent capacity of 116.3 mAh g<sup>-1</sup> (capacity retention ratio: 86.8%) after 1000 cycles at 5 C and improved rate capability. This work lays a platform for the prospective molecular design of improved organic framework relative artificial SEI for highly stable lithium metal batteries.



## Reference

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## Biography



Xiao-Meng Lu received her Master's degree from Shanghai University in 2022. Currently, she is pursuing her doctoral degree at Shanghai University under the guidance of Professor Yong Wang. Her research interests are focused on the structural design and interfacial protection for lithium metal batteries.

## Revealing the effect of calcination temperature on the performance of MnO<sub>x</sub>-TiO<sub>2</sub> catalysts for ethanol oxidation at low temperatures

Xueqian Zhang,<sup>1</sup> Shenhua Zhang,<sup>2</sup> Yangjun Wang,<sup>3</sup> Jialiang Feng\*

**Keywords:** transition metal oxides • low-temperature oxidation • ethanol • volatile organic compounds • calcination temperature

### Abstract:

The calcination temperature emerges as a critical modifiable variable influencing catalyst efficacy, given its substantial impact on the crystalline phase development, porosity architecture, and the establishment of surface-active centers. The present work fabricates a series of monolithic MnO<sub>x</sub>-TiO<sub>2</sub>/CHC catalysts subjected to calcination at distinct temperatures 400 °C, 450 °C, 500 °C, 550 °C, 600 °C, and 700 °C (MTC-400, MTC-450, MTC-500, MTC-550, MTC-600, MTC-700), for the purposes of ethanol oxidation catalysis. The removal efficiency of ethanol are in the order MTC-400 ≈ MTC-450 ≈ MTC-500 > MTC-550 > MTC-600 > MTC-700. It revealed the specific influence of calcination temperature on the ultimate composition of the MnO<sub>x</sub>-TiO<sub>2</sub>/CHC catalysts and their catalytic performance in the low-temperature oxidation of ethanol. The results indicated that the excellent activity of the catalysts obtained by calcinating at 500°C was due to the fact that this temperature was more favorable for increasing the content of structural defects on the surface and the better dispersion of active species on the surface. XPS analysis showed that the content of high-valent metal ions (Mn<sup>4+</sup> and Ti<sup>4+</sup>) decreased with the increasing calcination temperature, which inhibited the adsorption of adsorbed oxygen on the catalyst surface and hindered the formation of oxygen vacancies. These findings shed new lights on understanding the effects of low-temperature catalytic combustion of ethanol over transition metal oxide catalysts induced by the calcination temperature.

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## Poster presentation

# Enhancing Peptide Incorporation in Hydrogels for Dense and Sustainable Data Storage

Benxiang Luo,<sup>1</sup> and Xiaoyong Deng\*<sup>1</sup>

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**Keywords:** Peptide encapsulation • Peptide release • Information reading

### Abstract:

Peptide-based information storage technology represents a novel approach to bioinformation storage, facilitating the translation of digital information into peptide sequences for archiving. Compared to traditional bioinformation storage media, such as DNA, peptides present several advantages, including extended storage longevity, enhanced encoding efficiency, and improved stability. However, despite these benefits, the challenge of maintaining the integrity and stability of peptide sequences over extended periods, without information loss, persists as a significant scientific hurdle. One promising strategy to enhance the stability of DNA involves encapsulating it within inorganic matrices or hydrogels, a technique that may be extrapolated to peptide information storage. This study proposes the development of a poly(N-isopropylacrylamide)/chitosan (PNIPAM/CS) semi-interpenetrating network hydrogel, which possesses both thermo-responsive and pH-responsive characteristics. This dual-responsive hydrogel aims to provide an efficient and cost-effective method for peptide preservation. The PNIPAM/CS semi-interpenetrating hydrogel is designed to capture peptides directly from solution through a swelling mechanism. Under acidic conditions (pH = 5), the electrostatic interaction between the negatively charged peptides and the protonated chitosan within the hydrogel enables the concentration of peptides. This concentration is achieved through a series of swelling and deswelling cycles, leading to a high peptide data density of  $1.76 \times 10^{10}$  gigabytes per gram. Upon transitioning the peptide-encapsulated hydrogel to an alkaline environment (pH = 9.5), the chitosan undergoes deprotonation, which disrupts its interaction with the peptides. This change facilitates the release of peptides from the hydrogel, thereby enabling the retrieval of the digital information encoded within the peptides. This process offers a promising avenue for the preservation and recovery of peptide-based information storage systems.

### Biography



Background: B.Sc. in Biological Sciences from Jishou University, China (2015–2019), M.Sc. in Ecology from Jishou University, China (2019–2022), and currently a Ph.D. candidate in Environmental Science and Engineering at Shanghai University (since 2023).

Research interests: Development of technologies utilizing peptides as a medium for information storage. Ecotoxicological research on nanoplastics and heavy metals

### Achievement:

Luo B.X., *et al.* Chronic toxicity effects of sediment-associated polystyrene nanoplastics alone and in combination with cadmium on a keystone benthic species *Bellamya aeruginosa* [J]. **Journal of Hazardous Materials**, 2022, 433: 128800.

Xiang J., Luo B.X. (co-first authors), *et al.* Development of KOH and H<sub>3</sub>PO<sub>4</sub>-modified composite biochar from corn straw and activated sludge for removing methylene blue [J]. **International Journal of Environmental Science and Technology**, 2022: 1–16.

**Excellent Master's Degree Thesis of Hunan Province.** (2024)

# Coordination regulation of solvation structure assisting the wide-temperature sodium-ion batteries.

Xiangwu Chang, Jian Chen, Minghong Wu, Yang Liu, Yun Qiao \*

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**Keywords:** solvation structure • wide temperature electrolyte • sodium-ion batteries

## Abstract:

In the current global context of energy transition and sustainable development, there is a growing emphasis on high-performance and high-security energy storage systems.<sup>1–3</sup> With abundant resources and high cost-effectiveness, sodium-ion batteries (SIBs) are expected to provide strong support for achieving sustainable energy and grid stability.<sup>4–6</sup> Nevertheless, seasonal temperature fluctuations pose another major challenge to the stability and safety of SIB operation. It may not even function properly in extremely cold or hot areas. Electrolyte decomposition on the electrode surface forms an unstable solid-state interface layer, leading to increased consumption of sodium ions at high temperatures.<sup>7,8</sup> Ion transport at the electrolyte and electrolyte-electrode interface layer is critical for the normal operation of the battery at low temperatures ( $<-20\text{ }^{\circ}\text{C}$ ).<sup>9,10</sup> Herein, we conduct an electrolyte by regulating solvent coordination. non-flammable triethyl phosphate (TEP) is used as the main solvent, ensuring the solubility of the salt, and the introduction of methyl propionate (MP), with lower freezing points and low door number, was aimed at enhancing ionic conductivity and reducing solvation energy while promoting more anions to enter the  $\text{Na}^+$  solvation structure to improve the interface. The electrolyte engineering is expected to maintain high safety of sodium batteries while demonstrating good high and low temperature performance.

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## Biography



Xiangwu Chang is currently a PhD candidate at the School of Environmental and Chemical Engineering, Shanghai University. She focuses on the design of wide-temperature electrolytes for sodium-ion batteries.

## Poster presentation

# Controllable synthesis of p-NiO/n-ZnO heterojunctions with preferred orientation of ZnO (100) and (110) planes for enhancing n-butanol sensing performance

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**Keywords:** Gas sensor; NiO/ZnO composite; p-n heterojunction; Crystal planes; n-butanol

## Abstract:

The low responsivity and poor selectivity of ZnO hinder its application in the field of gas sensors. Herein, p-NiO/n-ZnO heterojunctions has been prepared by a simple hydrothermal method followed calcination, in which cone-shaped monocrystalline ZnO nanorods are covered by ultrathin NiO nanosheets. And the NiO/ZnO-2 with 2.06% Ni atomic ratio exhibits a high response ( $R_a/R_g = 140$ ) for 100 ppm n-butanol, and ultra-low detection limit as to 0.2 ppm n-butanol. In particular, the response range of NiO/ZnO-2 to n-butanol can cover 0.2 - 200 ppm. Moreover, NiO/ZnO-2 also appears excellent selectivity and stability. It shows a 6 times higher response to n-butanol than ethanol under the same condition, as well as maintains more than 92% response to n-butanol for 15 days operation. The outstanding gas sensing performance of NiO/ZnO-2 can be attributed to the highly preferred orientation of ZnO (100) and (110) planes in NiO/ZnO-2 at first, which greatly optimizes the conductivity and defects on surface of NiO/ZnO-2. And NiO/ZnO-2 owns more oxygen vacancies on the surface than other samples, which contributes to increase the response sensitivity of gas sensors. Furthermore, the p-n heterojunction formed at the interface between NiO and ZnO play a key role in expand the depletion layer at the interfaces, increasing the amount of adsorbed oxygen, which conduces to heighten the response of NiO/ZnO-2. Our work enhances the gas sensing property of semiconductors by both regulating the orientation of planes and constructing p-n heterojunctions, which gives insight to design high performance gas sensors.

## Biography



I completed my undergraduate studies at Fuzhou University and am currently a first-year master's student in the Environmental Functional Materials Research Group at the School of Environmental and Chemical Engineering, Shanghai University. My research primarily focuses on gas-sensitive materials, with a particular interest in the application of zinc oxide in gas sensing. I am exploring ways to optimize the performance of zinc oxide through the modification with various rare earth metals. In May of this year, I co-authored a paper titled "Controllable Synthesis of p-NiO/n-ZnO Heterojunctions with Preferred Orientation of ZnO (100) and (110) Planes for Enhancing n-Butanol Sensing Performance," published in the journal *Colloids and Surfaces A: Physicochemical and Engineering Aspects*. I sincerely hope to have the opportunity to discuss the research and development of clean energy technologies and new chemical materials with top experts from around the world.

# Constructing functional organic interfacial layers with tethered electric double layer on Zn metal anodes for ultra-stable Zn-ion batteries

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**Keywords:** Zinc-ion battery • Zn Anode • Functional organic interfacial layers • Electrolyte design • organic-assist SEI pre-construction

## Abstract:

Rechargeable zinc ion (Zn-ion) batteries have been considered one of the most promising candidates for potential large-scale applications in energy storage owing to their high safety and low cost. However, the use of Zn metal in batteries suffers from many severe issues, including dendrite growth and parasitic reactions, which often lead to short cycle lives. Herein, we propose the construction of functional organic interfacial layers (OIL) on the Zn metal anodes to address these limiting issues. Through a well-designed organic-assist solid electrolyte interfaces (SEI) pre-construction (OAPC) process, we are able to synthesize a densely packed artificial layer featuring the tethered electric double layer from the additive zwitterion imidazolium salt, which can significantly increase the kinetics of  $Zn^{2+}$  transport and facilitate the smooth Zn plating and stripping. Thus, as a result, the Zn metal anode with the functional OIL can significantly improve the cycling capability of the symmetric cell to over 5900 h stable operation. When paired with  $H_2V_3O_8$  cathode, the resulting full cell of aqueous Zn-ion batteries can be continuously cycling over 7000 cycles, marking an important milestone for Zn anode development for potential industrial applications.

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## Biography



I am a master's student at Shanghai University. I have a strong research interest in aqueous zinc-ion batteries, fortunately, I have done in-depth research on the design of anode and electrolyte of aqueous zinc-ion batteries during my master's degree, and have made some progress.

# Discharge Plasma-assisted ball milling is used to convert photovoltaic waste silicon into high-performance lithium-ion battery anode materials

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**Keywords:** • solar energy • lithium ion battery • discharge plasma-assisted ball milling • silicon

## Abstract:

With the rapid growth of solar energy, recycling and reuse of end-of-life solar modules have become a critical issue<sup>[1]</sup>. In light of this, a simple, yet environmentally friendly, ball milling process was used to transform the recycled Si of waste solar cells into a lithium ion battery (LIB) anode material. The recycled silicon of ball milling is further combined with carbon and bismuth metal, and the composite electrode is made by discharge plasma-assisted ball milling (DBDP). Provides a high discharge capacity of 1442 mA hg<sup>-1</sup> after 300 cycles at a current density of 500 mA/g capacity retention of approximately 95% and 525 mA hg<sup>-1</sup> at 1000 cycles at a current density of 7 Ag<sup>-1</sup>, which is also demonstrated in the post-cycling SEM images due to the fast charging effect of bismuth metal and the plasma-assisted ball milling technology that stabilize the material structure and alleviate the high stress generated by silicon<sup>[2]</sup> during cycling during the electrode reaction

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# Artificial Protective Layer Enhancing Stable Dendrite-Free Lithium Metal Batteries Enabled by Metal Organic Framework

Yibo Wu,<sup>1</sup> Yong Wang\*<sup>1,2</sup>

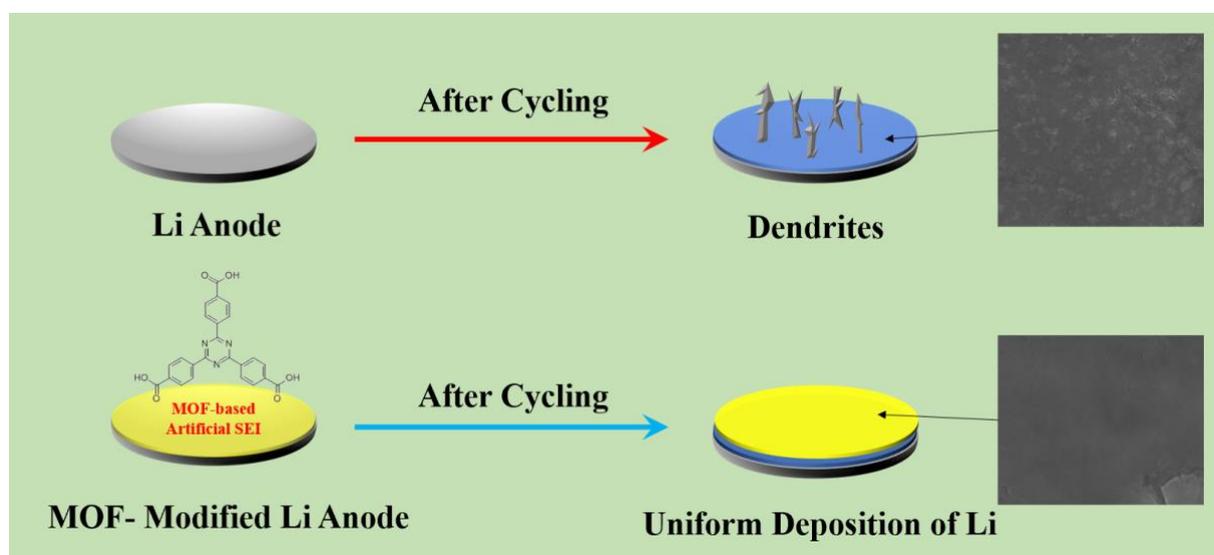
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**Keywords:** lithium metal anode • artificial solid electrolyte interphase • improved Li deposition • dendrite-free • metal organic framework

## Abstract:

Lithium metal has been deemed to have immense potential as an anode for rechargeable batteries due to its extremely high theoretical capacity and low redox potential. However its actual usage in batteries is greatly hindered by the dendrite formation due to the nonuniform deposition of lithium, and the instability of the solid electrolyte interface (SEI) layer. In this work, we use lithium metal organic framework (based on 2,4,6-Tris(4-Carboxyphenyl)-1,3,5-Triazine) as an artificial protective layer on the Li anode. As a porous material, the Li-MOF provides direct and orderly channels for the transport of Li ions. On the other hand, it can coordinate with solvated Li ions, accelerating the desolvation process of Li<sup>+</sup>, facilitating rapid lithium conduction, and effectively suppressing the growth of lithium dendrites. SEM images of lithium coins batteries after cycling confirm outstanding dendrite suppressing ability. The mechanics of the uniform lithium deposition are also evidenced by *in-situ* optical microscopy, *in-situ* and *ex-situ* FTIR. As a result, symmetric Li||Li cells (over 1200 h at 1 mA cm<sup>-2</sup> and 1 mAh cm<sup>-2</sup>) and Li||Cu cells (over 400 cycles at 0.5 mA cm<sup>-2</sup> and 0.5 mAh cm<sup>-2</sup>) demonstrate outstanding long cycle performance.



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## Poster presentation

# Enabling Gradient Structured Solid Electrolyte Interphase by a Hydrated Eutectic Electrolyte for High-Performance Zn Metal Batteries

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**Keywords:** gradient structure hydrated; eutectic electrolyte; SEI; solvation sheath; Zn metal batteries

### Abstract:

Aqueous Zn metal batteries are attracting tremendous interest as promising energy storage systems due to their intrinsic safety and cost-effectiveness. Nevertheless, the reversibility of Zn metal anodes (ZMAs) is hindered by water-induced parasitic reactions and dendrite growth. Herein, a novel hydrated eutectic electrolyte (HEE) consisting of  $Zn(BF_4)_2 \cdot xH_2O$  and sulfolane (SL) is developed to prevent the side reactions and achieve the outstanding cyclability of ZMAs. The strong coordination between  $Zn^{2+}$  and SL triggers the eutectic feature, enabling the low-temperature availability of HEEs. The restriction of  $BF_4^-$  hydrolysis in the eutectic system can realize favorable compatibility between  $Zn(BF_4)_2$ -based electrolyte and ZMAs. Besides, the newly-established solvation structure with the participation of SL,  $H_2O$ , and  $BF_4^-$ , can induce in situ formation of desirable SEI with gradient structure consisting of B, O-rich species, ZnS, and  $ZnF_2$ , to offer satisfactory protection toward ZMAs. Consequently, the HEE allows the Zn||Zn symmetric cell to cycle over 1650 h at  $2\text{ mA cm}^{-2}$  and  $1\text{ mA h cm}^{-2}$ . Moreover, the Zn||NH<sub>4</sub>V<sub>4</sub>O<sub>10</sub> full batteries can deliver a prolonged lifespan for 1000 cycles with a high capacity retention of 83.4%. This work represents a feasible approach toward the elaborate design of advanced electrolyte systems for next-generation batteries.

### Biography



My name is Jiang Chenxu. I graduated from Nanjing Tech University of Technology with a bachelor's degree in light chemical engineering. Now I am a third-year graduate student in the School of Environmental and Chemical Engineering, Shanghai University. My major is New Energy Materials, and my main research direction is the eutectic electrolyte (Aqueous zinc metal battery and Aqueous manganese battery). I'm very interested in rechargeable batteries. Published an article as third author in the journal Small in the first half of 2024. An existing article is collating data for publication before the end of the year.

# Effect of electrical treatment on CFRP recycling by chemical dissolution method

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**Keywords:** CFRP recycling • electrical treatment • chemical dissolution • nitric acid

## Abstract:

Carbon fiber reinforced plastic (CFRP) is a composite material consisting of carbon fibers reinforced with epoxy resin, and it has attractive properties such as high strength and light weight. Because of these characteristics, demand for CFRP has increased in the aircraft and automotive industries. However, the current disposal method for waste CFRP is mainly landfill. Therefore, effective recycling methods are desired from the standpoint of environmental load; many researchers have investigated CFRP recycling technologies such as pyrolysis and chemical dissolution, but there are issues regarding residual strength, environmental risk, and versatility. In order to develop another recycling technology, we investigated resin separation from CFRP using electrical treatment. In this method, the resin can be separated at ambient temperature and pressure by applying a DC voltage of about 15 V to the CFRP. In this study, we investigated the effect of the electrolytic solution to improve recycling efficiency. From a series of experiments and observations, it was found that the use of nitric acid as an electrolyte enables highly efficient recycling due to the combination of electrical treatment and chemical dissolution.

## Reference

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## Biography



I received my bachelor's degree from Kyushu University and am currently studying in the Department of Chemical Engineering of the Graduate School of Engineering, Kyushu University. My research interests include CFRP recycling, especially the electrical treatment for resin separation.

## Poster presentation

# Catalytic conversion of plastic pyrolysis gas into aromatics using zeolite

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**Keywords:** plastic pyrolysis • zeolite catalyst • aromatization

### Abstract:

In recent years, the feedstock recycling of waste plastics has received great attention as an alternative recycling method to energy recovery due to the circular economy. We investigate the conversion of gases generated during the pyrolysis of commodity plastics, such as PE, PP, and PS, into valuables through a catalytic reaction using zeolites. The gases generated during pyrolysis are difficult to utilize as feedstocks directly because the gas contains various compounds, but catalysts can convert them into valuables efficiently. In this study, a conversion process using zeolite catalysts was investigated to recover valuables from the pyrolysis gas of plastics. Using an MFI-type zeolite, which is a well-known catalyst in petrochemical industries, aromatics (benzene, toluene, and xylene) were selectively obtained as valuable products through the catalytic reaction. In addition, the aromatics yield increased with higher carrier gas velocity, suggesting that a shorter contact time with the catalyst may be effective. Furthermore, the use of air as a carrier enables the oxidation and removal of carbon deposited on the catalyst at the same time as pyrolysis, suggesting the possibility of extending the catalyst life.

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Selective phenol recovery by catalytic cracking of thermal decomposition gas from epoxy-based carbon-fiber-reinforced plastic, K. Oshima, H. Fujii, K. Morita, M. Hosaka, T. Muroi, S. Satokawa, *Industrial & Engineering Chemistry Research*, 59(30), 13460-13466 (2020). Catalytic Aromatization of Rapid Pyrolysis Gas of Low-Density Polyethylene Using a Tandem Reactor, K. Oshima, M. Sakamoto, K. Tashiro, M. Kishida, S. Satokawa, *Journal of the Japan Petroleum Institute*, in press.

### Biography



I received my bachelor's degree from Kyushu University and am currently studying in the Department of Chemical Engineering of the Graduate School of Engineering, Kyushu University. My research interests include the catalytic conversion of waste plastics, especially the combination of plastic pyrolysis and its catalytic conversion using zeolite.

## Poster presentation

# Development of Tissue Engineering Scaffolds by Spatial Configuration Control of Wet Electrospun 3D Fibers

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**Keywords:** wet electrospinning • 3-D nanofiber • cell culture scaffolds • tissue engineering

### Abstract:

Three-dimensional (3D) cell culture scaffolds, particularly electrospun nanofibers, closely resemble the extracellular matrix (ECM) and have garnered attention for applications in disease treatment and drug assays. While traditional electrospinning produces 2D membrane-type scaffolds, wet electrospinning using a liquid collector enables the fabrication of 3D fibers that more accurately mimic the ECM's spatial configuration. However, the intricate complexity of human organs, such as the liver, necessitates the further refinement of wet electrospinning techniques to fabricate 3D fiber scaffolds that closely mimic the extracellular matrix (ECM). This study aims to optimize the morphology of 3D PCL/GT (polycaprolactone/gelatin) scaffolds by adjusting the spinning parameters and processing method. PCL and GT were dissolved in hexafluoroisopropanol and electrospun into 100% ethanol, with GT crosslinked using EDC/NHS to prevent dissolution. After replacing the ethanol in the fibers with different concentrations of tert-butanol in a stepwise manner, the fibers were freeze-dried and subsequently stored in a vacuum drying oven (0.1 atm, 50°C). Fibroblast (3T3) cell cultures were seeded onto the scaffolds to assess cell infiltration and biocompatibility through histological analysis. The results demonstrate that the 3D fiber morphology can be effectively preserved through freeze-drying following tert-butanol replacement (Fig.1(a)), suggesting an expanded application of 3D fibers as cell scaffolds. SEM and laser microscopy revealed that the fabricated fibers possess enough large pore sizes for cell arrangement within them (Fig.2(b)), and during cell culture, cells were observed to infiltrate within the scaffold and homogeneously distribute (Fig.3(c)). These findings suggest that 3D fibers produced optimized via wet electrospinning method hold significant promise for applications in tissue engineering.

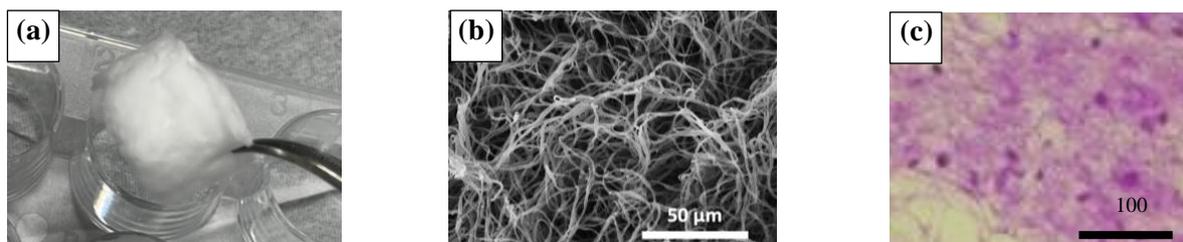


Fig.1 Fiber morphology. (a) Fiber morphology after freeze drying. (b) SEM image of fiber cross section. (c) Morphology of cell distribution in the fiber.

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### Biography



I obtained my Bachelor's degree from both Zhengzhou University (China) and Nagaoka University of Technology (Japan). Subsequently, I graduated early from Kyushu University (Japan) with a Master of Engineering degree. Currently, I am pursuing a PhD in Chemical Engineering at the Faculty of Engineering, Graduate School, Kyushu University. My research focuses on biomaterials, tissue engineering, electrospun nanofibers, and liver regeneration

# Viscosity Reduction of Heavy Oil Using Bi-Metallic Catalyst in Low-Temperature Aquathermolysis Reactions

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**Keywords:** Aquathermolysis • Heavy oil recovery • In-situ upgrading • Catalyst • Hydrogen donor

## Abstract:

This study utilized catalytic aquathermolysis as an in-situ upgrading method to reduce the viscosity of heavy oil by breaking down large and complex hydrocarbon molecules. A nano-sized bi-metallic composite catalyst (Ni/Fe-Si) was synthesized using a chemical reduction process, with hydrophilic and hydrophobic silica nanoparticles as support materials. The catalysts were characterized using BET, XPS, and FE-SEM analyses. The study also investigated the impact of adding a hydrogen donor to improve the aquathermolysis process. Under a specific reaction condition (180 °C, 3 MPa, and 24 hours), a 0.5% loading of the bi-metallic catalyst led to a 50.2% reduction in crude oil viscosity and a 6.79% decrease in sulfur content. When 5% formic acid was introduced, the viscosity and sulfur reductions were even greater, reaching 74.4% and 19.5%, respectively. Additionally, FTIR analysis of the extracted asphaltene revealed the highest molecular cleavage index in the sample with a hydrogen donor+catalyst, following by the sample with catalyst alone and without catalyst, respectively. A similar trend was confirmed by the distillation profiles of the oil phase analyzed by the GC-SimDist technique.

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## Biography



I obtained my B.S. and M.S. degrees from Chulalongkorn University in chemical technology and Petroleum technology. I'm currently Ph.D. candidate in Petrochemical technology, petroleum and petrochemical college, Chulalongkorn University. My research interests are in the areas of enhance oil recovery, aquathermolysis, zeolite, adsorption.

# CHA Zeolite/Cellulose Acetate Mixed Matrix Membranes for CO<sub>2</sub>/CH<sub>4</sub> Separation via Microwave-Assisted Synthesis

Weerawit Luewanichwong<sup>a,b</sup>, Thanakorn Wasanapiarnpong<sup>b,c</sup>, Takeshi Hagio<sup>d,e</sup>, Uthaiporn Suriyaphadilok<sup>a,b</sup>

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**Keywords:** Mixed matrix membrane, CO<sub>2</sub>/CH<sub>4</sub> separation, CHA zeolite, Cellulose acetate, Microwave synthesis

## Abstract:

Separation of CO<sub>2</sub> from fuel components is essential in the purification of natural gas or biogas to improve energy efficiency and reduce the environmental impact. Mixed-matrix membranes (MMMs) have emerged as a promising solution for CO<sub>2</sub>/CH<sub>4</sub> separation due to their potential to enhance gas selectivity and permeability. In this study, MMMs were fabricated by incorporating CHA zeolite into a cellulose acetate (CA) polymer matrix to achieve improved separation performance. The synthesis of CHA zeolite was optimized by adding 1% seed crystals and employing microwave-assisted synthesis, which significantly reduced the synthesis time from 96 hours to 6 hours and increased the product yield by 22.5% compared to the conventional hydrothermal method at 96 hours. Single gas permeation tests revealed that the presence of CHA zeolite in the CA polymer matrix substantially enhanced CO<sub>2</sub> permeability and CO<sub>2</sub>/CH<sub>4</sub> ideal selectivity, with permeability increasing from 0.16 to 0.33 GPU and selectivity from 1 to 60. The CA membrane containing 5 wt% CHA exhibited the highest selectivity of 60 at a feed pressure of 5 bar. These results demonstrated that CHA/CA MMMs offer significant potential for industrial CO<sub>2</sub> removal, making them an effective solution for CH<sub>4</sub> purification in gas separation applications.

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## Biography



I earned my B.Eng. from Thammasat University SIIT and continued with my M.Sc. and Ph.D. studies at the Petroleum and Petrochemical College, Chulalongkorn University. My research focuses on zeolites, CO<sub>2</sub> adsorption, separation, and sequestration.

## Poster presentation

# Molecular Dynamics Simulation of Cationic Surfactant Adsorption for Steel Corrosion Protection in CO<sub>2</sub>-Rich and High-Salinity Conditions

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**Keywords:** Surfactant • Adsorption • Corrosion Inhibitors • Corrosion • Molecular Dynamics Simulations

### Abstract:

CO<sub>2</sub>-induced corrosion is a critical challenge in the production phase of the oil and gas industry, especially in environments involving produced water, such as those found in Carbon Capture, Utilization, and Storage (CCUS) sites, enhanced oil recovery (EOR) operations, and hydrocarbon transportation. Produced water, with high levels of CO<sub>2</sub> and salinity, accelerates the corrosion of steel surfaces, leading to material degradation, operational failures, and costly maintenance. Surfactant-based corrosion inhibitors offer significant advantages over traditional methods by forming stable, dense protective layers on steel surfaces, providing effective corrosion resistance under harsh conditions. This study examines the effectiveness of cationic surfactant-based inhibitors with diverse structural moieties in competing with CO<sub>2</sub> species for adsorption onto steel surfaces. The goal is to establish barriers that prevent corrosive species from interacting with the steel, enhancing corrosion resistance during operations. Molecular dynamics (MD) simulation using the OPLS-AA force field in GROMACS model the competitive adsorption behavior under CO<sub>2</sub>-rich and high-salinity conditions. Key parameters such as molecular orientation, binding energy, surface coverage, and interaction strength are analyzed to determine optimal surfactant characteristics, guiding the development of more efficient inhibitors and improving the durability of steel in these challenging environments.

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### Biography



I hold a Bachelor of Science degree in Petrochemical and Polymer Material Engineering from Silpakorn University and a Master of Science degree in Petroleum and Energy Technology from the Petroleum and Petrochemical College at Chulalongkorn University, Thailand. Currently, I am pursuing a PhD in Petrochemical Technology at the Petroleum and Petrochemical College, Chulalongkorn University. My research focuses on surfactant adsorption, molecular dynamics (MD) simulations, and machine learning.

## Poster presentation

# Extraction, Purification, and Analysis of Carbonic Anhydrase from *Caulerpa lentillifera* (Sea Grapes): Evaluating Its Effectiveness in CO<sub>2</sub> Sequestration

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**Keywords:** Sea Grapes, Carbonic Anhydrase, Carbon Sequestration

## Abstract:

Carbon capture and storage (CCS) is a critical strategy for mitigating climate change and promoting carbon sequestration. While CCS offers a promising solution to the global challenge of reducing atmospheric CO<sub>2</sub> levels, the potential for CO<sub>2</sub> leakage from underground storage sites remains a significant concern. Additionally, the natural formation of carbonates is a slow process, which limits the efficiency of carbon sequestration. Carbonic anhydrase (CA) is proposed to catalyze the hydration of CO<sub>2</sub> into carbonic acid, which then later spontaneously dissociate into bicarbonates, and, finally to carbonate rocks, thereby accelerating the carbon sequestration. In this study, CA was extracted and purified from a novel plant, *Caulerpa lentillifera* (Sea Grapes), for CO<sub>2</sub> conversion into CaCO<sub>3</sub>. The molecular size of purified CA was conducted by SDS-PAGE. Then, purified SDS-PAGE protein bands were identified to determine the amino acid sequence by MALDI-TOF mass spectrometry. The specific activity of purified CA was 0.1967 U/mg. The active pH for CA enzyme was determined to be in the pH ranges of 2 to 12. The effect of temperature was performed at appropriate pH by varying in the range of 25 to 95 °C. In addition, the CO<sub>2</sub> sequestration into calcium carbonate (CaCO<sub>3</sub>) was carried out in the absence and presence of purified CA. It was found that the presence of purified CA could improve the amount of CaCO<sub>3</sub> more than that of the absence of purified CA, approximately 45%. The formed CaCO<sub>3</sub> were further characterized by SEM and XRD.

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## Biography



My name is Kattariya Srasamran. I hold a Bachelor of Engineering in Petrochemicals and Polymeric Materials Technology from Silpakorn University, Thailand, and a Master of Science in Petroleum and Energy Technology from the Petroleum and Petrochemical College at Chulalongkorn University, Thailand. Currently, I am pursuing a Doctor of Philosophy in Petrochemical Technology at the Petroleum and Petrochemical College, Chulalongkorn University. My research interests focus on surfactant encapsulation and biological carbon sequestration.

## Poster presentation

# Coating effect of metal organic complex (Co-DTPMP) layer on enhancing PEC water oxidation performance of BiVO<sub>4</sub> photoanode

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**Keywords:** Photoelectrochemical, Water-splitting, Bismuth vanadate, Metal organic complex, Hydrogen production, Co-catalysis.

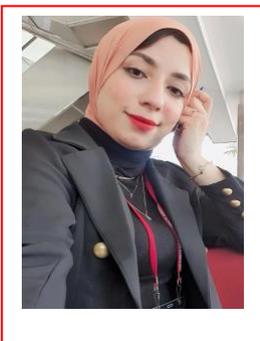
### Abstract:

Photoelectrochemical (PEC) water splitting is a promising method for transforming solar energy into clean and sustainable energy. However, PEC is severely limited, and they cannot achieve the predicted photocurrent density owing to the severe photochemical deterioration of the electrode and the recombination of photo-generated carriers. In this study, BiVO<sub>4</sub>/Co-diethylenetriamine Penta (methylene phosphonic acid) (BVO/Co-DTPMP) co-catalyst was successfully prepared as a nanoporous photoanode. Diethylenetriamine Penta (methylene phosphonic acid) was crosslinked with Co ions and coated on the BiVO<sub>4</sub> surface by successive ionic layer adsorption and reaction (SILAR) to reduce fast recombination, which correlated with the BiVO<sub>4</sub> photoanode. Various characterization and PEC measurements were conducted, revealing that the co-catalyst thin layer enhanced the charge separation and electrons transfer which significantly affected on the PEC performance of BiVO<sub>4</sub>, and the current density by BVO/Co-DTPMP was 4 mA cm<sup>-2</sup> at 1.23 V vs. RHE. Furthermore, the co-catalyst exhibited improved charge transport and long-term stability.

### Reference

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### Biography



I obtained my BS in double major (Zoology/Chemistry) and MS degrees in organic Chemistry major from Faculty of Science, Bani Suif University. I performed as Teaching assistant in the Industrial Faculty in Banisuef University. Currently, I am a PhD student in the School of Chemical Engineering at Yeungnam University, Korea.

## Poster presentation

# Advancing Co-N-C electrocatalyst by enlarged accessible active sites for a highly efficient PEMFC cathode

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**Keywords:** PEMFC • ORR • M-N-C • Electrocatalyst • ZIF

### Abstract:

Transition metal-nitrogen-carbon (M-N-C) catalysts are recognized as alternatives to the expensive platinum (Pt) catalysts for the critical oxygen reduction reaction (ORR) in proton exchange membrane fuel cells (PEMFCs). Among these, Fe-N-C electrocatalysts have demonstrated promising performance in PEMFCs, delivering high power densities. However, they experience degradation due to the Fenton reaction, which damages the membrane. In this study, we explore cobalt-based M-N-C (Co-N-C) catalysts, derived from bimetallic zeolite imidazolate frameworks (BMZIF) as precursors. These catalysts offer greater durability as they are not susceptible to the Fenton reaction, unlike their Fe-N-C counterparts. Despite their robustness, Co-N-C catalysts typically exhibit lower activity, making it crucial to enhance their performance. We focused on improving fuel diffusion and catalyst contact by converting the pore structure to mesoporous carbon. This was achieved by introducing melamine during the thermal decomposition process. We investigated how the pore structure and the density of active sites influence performance. The electrochemical capabilities of the mesoporous Co-N-C (mCo-NC) were assessed through techniques such as linear sweep voltammetry (LSV), cyclic voltammetry (CV), and double-layer capacitance in a half-cell setup, as well as through polarization curves in a single-cell system.

### Reference

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## Methane Pyrolysis using Molten salt

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**Keywords:** CH<sub>4</sub> pyrolysis • Density Functional Theory • Ab initio Molecule Dynamics • graphitic carbon-hydrogen

### Abstract:

In our investigation, molten manganese chloride (MnCl<sub>2</sub>) was utilized as a liquid catalyst for methane pyrolysis (CH<sub>4</sub> → C + 2H<sub>2</sub>). To improve catalytic performance of MnCl<sub>2</sub>, we mixed various monovalent and divalent chloride salts, including KCl, LiCl, NaCl, MgCl<sub>2</sub>, and CaCl<sub>2</sub>. Notably, the addition of KCl enhanced catalytic activity more effectively than the other salts. We confirmed that CH<sub>2</sub> plays a significant role as an intermediate in the reaction. Also, produced solid carbons has a characteristic of fine graphitic carbon compared to the solid carbon from methane pyrolysis in MnCl<sub>2</sub>. We additionally conducted the ab-initio MD and DFT simulations to understand the mechanisms of CH<sub>4</sub> pyrolysis and why the well-developed graphitic carbon was observed from CH<sub>4</sub> pyrolysis in MnCl<sub>2</sub>-KCl. The DFT simulation results show that addition of KCl makes CH<sub>2</sub> formation reaction facile resulting in making CH<sub>2</sub> species dominant. Additional MD simulation provided the potential of gas phase reaction which leads to the higher quality of graphitic carbon. We will discuss about the graphitic carbon formation mechanisms through both surface and gas-phase reactions in further discussions.

### Reference

1. Methane pyrolysis and carbon formation mechanisms in molten manganese chloride mixtures, D Bae, Y Kim, EH Ko, SJ Han, JW Lee, M Kim, D Kang, Applied Energy 336 (2023), 120810

### Biography



I obtained my BS degrees from Yeungnam University. I am currently studying for master's program at Yeungnam University, majoring in chemical engineering. My current research area is methane decomposition and conversion. I published 5 papers (35 citations and h-index 3). My research interests are in the area of catalyst development by using computational chemistry and machine learning.

# Investigation of the Zn/Co ratio impact on water electrolysis activity using bimetallic selenides derived from zeolitic imidazolate frameworks

Hyeonwook Son, Jinhyuk Baek, Yunji, Jeong, Moonsu Kim, and Gibaek Lee\*

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**Keywords:** water splitting • ZIF • active site • OER • agglomeration

## Abstract:

Precious metal-based electrocatalysts for water electrolysis face significant challenges, including high costs and poor stability during catalytic processes. This necessitates a shift towards transition metal-based electrocatalysts. In this study, we propose a bimetallic electrocatalyst, ZnSe@CoSe<sub>2</sub>, synthesized via a calcination process from zeolitic imidazolate frameworks (ZIFs). CoSe<sub>2</sub>, derived from ZIFs, features a high specific surface area and a porous structure, enhancing the exposure of active sites and facilitating the transfer of ions and electrons. However, during calcination, Co tends to agglomerate, leading to a reduction in surface area and active sites. To counteract this, Zn is incorporated into the ZIF structure. Although Zn and ZnSe are inactive in water electrolysis, it is crucial to investigate the synergistic effects of the Zn/Co ratio. Our findings demonstrate that an optimally determined Zn/Co ratio significantly enhances electrochemical performance and stability, as evidenced by improvements in oxygen evolution reaction (OER) and hydrogen evolution reaction (HER) activities, as well as in the electrochemical surface area (ECSA). Additionally, we examine the physical and chemical characteristics to better understand the roles of Zn and Co. This study suggests that innovative electrocatalyst designs based on the Zn/Co ratio could provide new approaches in the field of water electrolysis.

## Reference

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# A LiF-rich solid electrolyte interphase formation by fluorinated carbon host for anode-free lithium metal batteries

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**Keywords:** lithium metal • SEI layer • LiF • carbon host • anode free

## Abstract:

As the demand for high-energy-density Li-ion batteries grows with the advancement of portable electronics and electric vehicles, the direct use of lithium metal is being intensively evaluated again. Lithium metal offers the highest specific capacity ( $3860 \text{ mAh g}^{-1}$ ) and the lowest reduction potential ( $-3.04 \text{ V vs. SHE}$ ), promising enhanced power and energy density. However, challenges such as dendrite formation and dead lithium during cycling can still lead to battery failure and safety concerns. To address these issues, state-of-the-art host material coating methods have emerged as promising solutions. These methods prevent volume expansion from lithium metal plating/stripping, promoting uniform nucleation due to the lithiophilicity and large surface area of the materials.

In this study, we introduce a fluorine-nitrogen co-doped carbon-based host material prepared using zeolitic imidazolate frameworks (ZIFs). Heating ZIF-8 produces nitrogen-doped carbon that is rich in Zn metal ions and has high lithiophilicity, which helps overcome the lithium nucleation barrier. The resulting amorphous carbon, with its large pore volume and surface area, serves as an effective host for lithium storage by facilitating uniform Li-ion flux. Doping with fluorine increases the ratio of LiF in the SEI layer, leading to the formation of a robust SEI layer that suppresses dendrite growth and extends battery cycle life. The stability of the fluorine-doped carbon host material and the formation of the SEI layer were confirmed through TEM, XPS, and XRD analysis. Half-cell tests were conducted to measure reversible reactions and nucleation overpotential. Additionally, symmetric cell tests and an anode-free full cell were performed, demonstrating improved dcycle stability even under poor conditions with an N/P ratio of 1.

## Reference

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## Poster presentation

# Synergistic Effect of 3D/2D Vanadium Diselenide/Tungsten Diselenide Hybrid Materials: Electrochemical Detection of 5-Nitroquinoline Hazardous to the Aquatic Environment

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**Keywords:** Multidimensional • 2D-Nanoflakelets • 3D-Microspheres • 5-Nitroquinoline.

### Abstract:

The development of multidimensional structured electrode materials with simple synthetic methods and their electrochemical sensing ability against environmental pollution is still a challenge. In this article, we propose a hybrid formed using multidimensional (3D/2D) vanadium diselenide microspheres and tungsten diselenide nanosheets ( $VSe_2/WSe_2$ ) for the electrochemical detection of 5-nitroquinoline (5-NQ), a highly toxic and hazardous substance that is polluting aquatic life due to increasing industrial activities. The 3D/2D  $VSe_2/WSe_2$  hybrids were prepared by a simple solvothermal method and their morphological and structural analysis was confirmed by various spectroscopy and analytical techniques. The proposed 3D/2D architecture showed a strong synergistic effect between the two components as well as high electrical conductivity. As a result, an increased peak current for the reduction and detection of 5-NQ was achieved compared to other modified and unmodified disposable screen-printed electrodes (SPE), such as bare SPE,  $VSe_2/SPE$ , and  $WSe_2/SPE$ . Under the optimized electrochemical conditions,  $VSe_2/WSe_2/SPE$  showed large linear response ranges (0.012–1053, 1183–3474  $\mu M$ ), a low detection limit (0.002  $\mu M$ ), good sensitivity along with good selectivity, and repeatability for the detection of 5-NQ. With this prominent electrochemical behavior, the  $VSe_2/WSe_2$  electrode has clear potential to produce high-performance sensor devices.

### Reference

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### Biography



I received my BS & MS degrees in Electronic Science from Savitribai Phule University, India. Currently, I am a PhD student at School of Chemical Engineering, Yeungnam University, Republic of Korea, I published 9 papers (48 citations and h-index 4). My research interests are in the areas of nanomaterial synthesis for electrochemical sensor applications.

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## Poster presentation

# Synergistic Design of Processable Nb<sub>2</sub>O<sub>5</sub>-TiO<sub>2</sub> Bilayer Nanoarchitectonics: Enhancing Coloration Efficiency and Dual-band Electrochromic Energy Storage Stability

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**Keywords:** Dual-band electrochromism; Energy storage; Bilayer thin film; Nb<sub>2</sub>O<sub>5</sub>-TiO<sub>2</sub>; Hydrothermal.

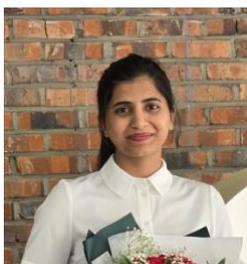
## Abstract:

This paper presents a novel proof of concept for a dual-band electrochromic (EC) device designed to selectively regulate solar light transmission in both the visible and near-infrared regions. EC materials based on ion insertion/extraction mechanisms also present the possibility for energy storage, widening its functionality to the supercapacitor platform. The bi-functional performance of controlling radiation in two spectral bands while storing energy was achieved by utilizing two abundant metal oxides. A Nb<sub>2</sub>O<sub>5</sub>-TiO<sub>2</sub> bilayer structure was synthesized on fluorine-doped tin oxide (FTO) glass using a one-step hydrothermal method. The annealing temperature of TiO<sub>2</sub> was found to significantly impact the crystallinity and surface morphology, which in turn affects the dual-band EC energy storage performance. The optimized NT-500 sample demonstrated enhanced electron-charge transport, resulting in superior electrochemical performance. The film achieved large optical modulations of 80.4% at 600 nm and 89.8% in the near-infrared region (800 nm), along with an areal capacitance of 88.1 mF/cm<sup>2</sup> and excellent cycling stability, maintaining performance over 18,000 seconds of continuous EC cycles. This paper presents a prototype bi-functional device based on NT-500, which showed independent control and modulation of visible and near-infrared transmittance. Notably, the device retained excellent energy storage performance alongside its advanced optical functionalities. The bilayer structure leverages the electrochemical strengths of both materials, offering a promising advancement in the field of EC-energy storage systems.

## Reference

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## Biography



I obtained my BS and MS degrees from Nanoscience and Nanotechnology at Shivaji University, India and PhD degree in Chemical Engineering, Yeungnam University, Republic of Korea. Currently I am a postdoc fellow in Chemical Engineering, Yeungnam University Republic of Korea. My research focus on the synthesis, optimization of performance metrics and characterizations of nanostructured metal oxides for electrochromic energy storage applications.

## Poster presentation

# Simplifying nitridation of Li metal anode by direct Lewis acid-base reaction

Seokjun Kim, Taehyung Kim, and Seho Sun\*

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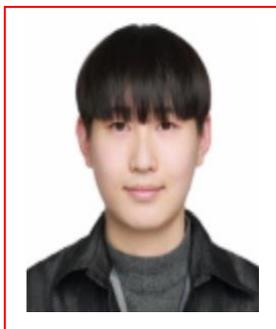
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**Keywords:** Li metal anode, Protective layer, Solid electrolyte interfaces, Simple process

### Abstract:

Metallic lithium (Li) has garnered significant attention due to its high theoretical specific capacity (3860 mAh g<sup>-1</sup>), low weight (0.53 g cm<sup>-3</sup>), and lowest electrochemical potential (-3.04 V vs. standard hydrogen electrode). However, commercialization has been hindered by challenges such as lithium dendrite formation, side reactions, and unstable interfacial reactions with electrolytes. To address these issues, research has focused on controlling interfacial layers, such as solid electrolyte interfaces (SEI) or protective coatings, to safeguard the Li metal. Here, we suggest a simple process to enhance the stability of lithium metal anodes by applying a Li<sub>3</sub>N (lithium nitride) coating. First, Thin native oxide layer and impurities on the Li metal are removed through chemical polishing. Then, the purified Li metal is immersed in xylene diamine to form the Li<sub>3</sub>N protective layer. The application of the Li<sub>3</sub>N protective layer creates a stable interface on the lithium metal, which suppresses dendrite growth during charge/discharge cycles and exhibits low interfacial resistance. The Li anode with the Li<sub>3</sub>N protective layer demonstrates superior cycle life compared to bare samples in both Li||Li symmetric and Li||NCM full cells. To conclude, this simple process for applying a Li<sub>3</sub>N protective coating has the potential to facilitate the commercialization of lithium metal anodes by significantly improving its stability and performance.

### Biography



Seokjun Kim is an Graduate students in the School of Chemical Engineering at Yeungnam University in Korea. He got his Bachelor's Degree in the School of chemical engineering at Yeungnam University.

## Poster presentation

# Enabling uniform microstructure of dry electrode via pre-kneading process

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**Keywords:** Lithium-ion batteries • Dry process • Electrode engineering • Pre-kneading process

### Abstract:

Lithium-ion batteries are crucial as energy storage devices in modern technology. With the increasing demand for these batteries, it is essential to enhance the efficiency of the manufacturing process and to develop batteries that are high in energy density, cost-effective, and environmentally friendly. Traditionally, slurry-based wet processes have been used to manufacture lithium-ion battery electrodes. However, these processes require a significant amount of solvent, leading to environmental pollution and high energy consumption associated with solvent use. Consequently, dry processing, which does not use solvents, is gaining attention for its potential to improve process efficiency and reduce environmental impact. Despite these advantages, dry processing faces challenges such as lower energy density and weaker inter-particle bonding compared to conventional wet processes, making it insufficient for practical use. To address these issues, we introduce a pre-kneading process that produces electrodes with higher energy density and stronger inter-particle bonding. This process enhances fibrillation between the active material and the binder, resulting in a more uniform electrode microstructure and increased energy density. Our research suggests that the pre-kneading process could be a practical method for the commercialization of dry processing in the future.

### Biography



Taehyeong Kim is an Graduate students in the School of Chemical Engineering at Yeungnam University in Korea. He got his Bachelor's Degree in the School of Chemical Engineering at Yeungnam University.

## Poster presentation

# Determining the difference in conversion of CO by comparing the Gibbs free energy of CO to methanol in Cu, In/Cu, and In<sub>2</sub>O<sub>3</sub> surface with DFT

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**Keywords:** CO conversion, methanation, CO to methanol, DFT

### Abstract:

CO<sub>2</sub> is a major greenhouse gas contributing to global warming. To mitigate CO<sub>2</sub> emissions, research efforts have focused on its conversion into methanol, which serves as a crucial chemical intermediate and platform molecule for synthesizing valuable commodities such as formaldehyde and acetic acid. Methanol production from CO<sub>2</sub> offers both environmental and economic benefits. In this study, we conducted a DFT investigation to elucidate the mechanism behind the enhanced CO conversion observed when indium is introduced in the CO<sub>2</sub>-to-methanol reaction. Specifically, we compared the Gibbs free energy profiles for CO<sub>2</sub>-to-methanol and methanation on Cu, In/Cu, and In<sub>2</sub>O<sub>3</sub> surfaces. The hydrogenation of CO\* proceeds via two distinct pathways to produce CH<sub>3</sub>OH\*: the CHO-based pathway (CO\* → CHO\* → CH<sub>2</sub>O\* → CH<sub>3</sub>O\* → CH<sub>3</sub>OH\*) and the COH-based pathway (CO\* → COH\* → CHOH\* → CH<sub>2</sub>OH\* → CH<sub>3</sub>OH\*). Our findings reveal that CO is converted voluntarily into COH\* or CHO\* on the In<sub>2</sub>O<sub>3</sub> surface, whereas on Cu and In/Cu surfaces, this conversion is not voluntary. In particular, the Cu surface facilitates side reactions leading to CH<sub>x</sub> formation due to the involuntary conversion of CO to COH\* and CHO\*. On the In<sub>2</sub>O<sub>3</sub> surface, the thermodynamically preferred CHO-based hydrogenation pathway to CH<sub>3</sub>OH\* effectively suppresses the side reaction of CH<sub>x</sub> formation from CHO\*, thereby favoring methanol production. Consequently, the presence of the In<sub>2</sub>O<sub>3</sub> phase enhances CO conversion and improves coking resistance.

### Reference

1. Methanol synthesis from CO<sub>2</sub>: A mechanistic overview, Noerma J. Azhari, Denanti Erika, St Mardiana, Grandprix T.M. Kadja, Results in Engineering 16 (2022) 100711

### Biography



I am senior majoring in Chemical Engineering at Yeungnam University, where I have been an undergraduate researcher for the past two years under the guidance of Professor Minkyu Kim. My research focuses on catalyst development using DFT (Density Functional Theory), with current projects on ammonia decomposition and the conversion of CO<sub>2</sub> to BTX. I have also authored a paper on ozone decomposition, titled Synergistic effects of copper and oxygen vacancies in enhancing the efficacy of partially crystalline CuMn<sub>x</sub>O<sub>y</sub> catalyst for ozone decomposition.

# Halogenated Heterocyclic Scaffolds as Antimicrobial Agents against Uropathogenic *E. coli*

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**Keywords:** Antibiotics; Biofilm; Multidrug resistance; Halogenated hydrocarbons; UPEC; Virulence

## Abstract:

Uropathogenic *Escherichia coli* (UPEC) is a urinary tract pathogen responsible for most nosocomial urinary tract infections and can cause severe conditions such as acute cystitis of the bladder or pyelonephritis. Halogenated compounds demonstrated the ability to enhance antimicrobial efficacy, pharmacological profile as well as circumvent resistance mechanisms. Therefore, halogenated heterocycles were evaluated for their antibiofilm, antimicrobial, and antivirulence potentials against UPEC by studying two prominent pharmacological scaffold classes: indoles and chromones. Three derivatives from each class were identified as hits: 6-bromo-3-formylchromone, 6-chloro-3-formylchromone, and 3-formyl-6-isopropylchromone among the chromones, and 4-chloroindole, 5-chloroindole, and 5-chloro-2-methylindole among the indoles. These three chloroindoles exhibited MICs of 75 µg/ml and inhibited biofilm formation by an average of 67% at 20 µg/ml, while the chromones had MICs against UPEC of 20, 20, and 50 µg/ml, respectively, and inhibited biofilm formation by 72 to 96% at 20 µg/ml. Both sets of derivatives inhibited UPEC-associated virulence factors, including hemolysis, motility, curli and siderophore production, indole production, quiescent colony formation, and cell surface hydrophobicity. Gene expression analysis indicated that these derivatives downregulated virulence genes associated with toxins, biofilm production, and stress regulation. 3D-QSAR analysis showed that substitutions at the third and sixth positions of the chromone and the fourth and fifth positions of the indole scaffold favor antimicrobial activity against UPEC. Furthermore, ADME profiles and *C. elegans* cytotoxicity assays indicated that these chromone and indole derivatives are potent, safe drug candidates.

## References:

1. Boya BR, Lee J-H and Lee J. Antimicrobial and Antibiofilm Activities of Chromone Derivatives against Uropathogenic *Escherichia coli*. *Microbiological Research*. 278:127537 (2024)
2. Faleye, OS<sup>§</sup>, Boya BR<sup>§</sup>, Lee, J-H, Choi I, & Lee J. Halogenated Antimicrobial Agents to Combat Drug-Resistant Pathogens. *Pharmacological Reviews*, 76(1), 90-141 (2024).
3. Boya BR, Lee J-H and Lee J. Antibiofilm and Antimicrobial Activities of Chloroindoles against Uropathogenic *Escherichia coli*. *Frontiers in Microbiology* 13: 872943 (2022)

## Biography



Mr. Bharath Reddy Boya obtained his B. Tech degree in bioinformatics from Prist University, India. He completed his M.Sc. in Chemical Engineering from Yeungnam University and is currently a chemical engineering Ph.D. scholar at Prof. Jintae Lee's lab, at Yeungnam University. His research interests include antimicrobial and antibiofilm agents, microbial pathogenesis, microbial phylogenetics, nosocomial urinary tract infections, and *in silico* drug discovery. He has published 5 research articles in SCI-international journals discovering various halogenated scaffolds as antibiofilm agents for pathogenic microbes.

## Antimicrobial activities of flavonoids against *Vibrio* species

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**Keywords:** antibacterial, antibiofilm, flavonoids, *Vibrio parahaemolyticus*

### Abstract:

*Vibrio parahaemolyticus* is a significant foodborne pathogen associated with raw or undercooked seafood. The pathogen's ability to form biofilms poses serious threats to both food safety and economic value. Therefore, we explored the antimicrobial properties of some flavonoids against *Vibrio* and other common food pathogens. Our research identified three flavonoid derivatives—6-aminoflavone (6-AF), 3,2-dihydroxyflavone (3,2-DHF), and 2,2-dihydroxy-4-methoxybenzophenone (DHMB)—as effective biofilm inhibitors. Specifically, 3,2-DHF and DHMB showed minimum inhibitory concentrations (MICs) of 20 µg/mL and 50 µg/mL, respectively, against *Vibrio*. They were also effective in disrupting mature biofilms and reducing virulence factors such as motility, iron acquisition, and hemolysin production at sub-MIC levels. The flavonoids achieved these effects by interfering with metabolic activities, cell division, membrane permeability, and gene expression profiles. Additionally, 6-AF and 3,2-DHF proved non-toxic in the *C. elegans* model and demonstrated potentials to protect shrimps from biodeterioration. Moreover, these flavonoids exhibited broad-spectrum biofilm inhibitory effects against mixed-species biofilms including *Vibrio* and *Staphylococcus aureus*. Overall, our study highlights flavonoid derivatives as promising food-compatible agents that could effectively protect seafood from the threats posed by *V. parahaemolyticus* and other foodborne pathogens.

### Reference

1. Faleye, O. S., Lee, J. H., & Lee, J. (2023). Selected flavonoids exhibit antibiofilm and antibacterial effects against *Vibrio* by disrupting membrane integrity, virulence and metabolic activities. *Biofilm*, 6, 100165.

### Biography



The researcher bagged his Masters degree (Medical Microbiology) from the Federal University of Technology, Akure, Nigeria and currently pursuing a Ph.D program in Chemical Engineering at Yeungnam University, Gyeongsan, Korea. Recipient of Ekiti State Government Scholarship for undergraduate studies and under the University scholarship for PhD. My research interests bother on biotechnology viz-a-viz biofilm formation and microbial virulence control, natural product derivatives, toxicity and *in-silico* studies. Author's recent publication was accepted in *Pharmacological Reviews* (IF: 21).

# Antimicrobial Potentials of Iodinated Amino Acid against *Staphylococcus aureus*

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**Keywords:** Biofilm, Virulence, *Staphylococcus aureus*, MRSA

## Abstract:

*Staphylococcus aureus* represents a major health threat to humans due to its ability to form biofilms and release virulence factors. The growing prevalence of antibiotic-resistant strains complicates treatment efforts, highlighting the critical need for new antimicrobial controls. Our study focused on the effectiveness of halogenated phenylalanine derivatives in inhibiting *S. aureus* biofilm formation and some virulence factors. Among the tested halogenated compounds, Fmoc-4-iodo-phenylalanine was most effective at preventing *S. aureus* biofilm formation. The compound's superior antibiofilm activity was further confirmed through various microscopic techniques. Additionally, it significantly reduced virulence factors such as cell surface hydrophobicity, hemolysin and slime production at concentrations below the minimum inhibitory concentration (sub-MIC). It also prevented biofilm development in strains of methicillin-resistant *S. aureus* (MRSA) and *Staphylococcus epidermidis*, but showed no activity against the Gram-negative bacteria and fungi tested. Furthermore, Fmoc-Iodo-Phe downregulated the expression of critical biofilm and virulence genes, *agrA* and *RNAIII*, with these findings supported by molecular docking studies. Notably, it demonstrated non-toxic effects in the *C. elegans* model and met drug likeliness criteria based on ADMET predictions, suggesting good bioavailability. These results present Fmoc-Iodo-Phe as a potential candidate for new antimicrobial development strategies against *S. aureus* infections.

## References

1. Antibiofilm and Antivirulence Potentials of Iodinated Fmoc-phenylalanine against *Staphylococcus aureus* **O. O Faleye**, J. H Lee, Y. G Kim, O. S Faleye, J. Lee, 2024. (Submitted to Microbial Pathogenesis-under review).

## Biography



I hold a B.Sc degree in Microbiology from the University of Ado-Ekiti, Nigeria, and possess years of industrial experience in pharmaceuticals. Currently I am pursuing my master's degree in Chemical Engineering at Yeungnam University Korea under the supervision of Professor Jintae Lee. My research focuses on antibiotics, antimicrobial agents, biofilm formation and virulence factors, with a passion for exploring novel solutions in these areas.

## Poster presentation

# Antibacterial Efficacy of Halogenated Phenol

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**Keywords:** Triiodophenol • Antibacterial • Biofilm • *Staphylococcus aureus*

### Abstract:

Antimicrobial resistance is a critical global public health issue, compromising the efficacy of treatments for infectious diseases and leading to a significant rise in healthcare expenditures. Among Gram-positive bacteria, *Staphylococcus aureus* stands out for its ability to develop resistance to multiple antibiotics, posing substantial challenges in both food and healthcare settings. Biofilm formation by *S. aureus* has largely contributed to its resistance and pathogenicity, further complicated by the production of virulence factors. This study evaluated the effects of 126 halogenated compounds on *S. aureus* biofilm formation, with five halogenated phenols showing the high potency. Among them, 2,4,6-triiodophenol (2,4,6-TIP) emerged as the most effective, demonstrating significant biofilm inhibitory effects on *S. aureus* at a minimum inhibitory concentration of 5 µg/mL. Additionally, 2,4,6-TIP effectively inhibited the biofilms of methicillin-resistant *S. aureus* MW2 and Gram-negative bacteria, including *Vibrio parahaemolyticus*, uropathogenic *Escherichia coli*, and the fungal specie *Candida albicans*. It also prevented polymicrobial biofilms with *S. aureus* and *C. albicans*. Moreover, 2,4,6-TIP exhibited potential to control *S. aureus* virulence factors by inhibiting hemolysis and protease activity. Transcriptomic analysis revealed that 2,4,6-TIP notably repressed the gene expression of RNAPIII, associated with biofilm and virulence production in *S. aureus*. Furthermore, in silico analysis and plant and nematode assays showed that 2,4,6-TIP exhibited reduced toxicity compared to phenol. These findings unveiled the strong antimicrobial potential of 2,4,6-TIP and suggest a broad-spectrum capacity to target the virulence characteristics of medically important pathogens. They also highlight that strategic positional halogenation may play a critical role in enhancing the activity of phenolic compounds while alleviating their toxicity profiles.

### Reference

1. Antimicrobial and antibiofilm activities of halogenated phenols against *Staphylococcus aureus* and other microbes, OR Olalekan, JH Lee, YG Kim J Lee, (Under revision for Chemospher)

### Biography



I hold a BS degree in Biochemistry from Lagos State University, Lagos, Nigeria, and have a professional experience in pharmaceutical industry having worked with Vitabiotics Nigeria in different roles. Currently, I am an MS/PhD Graduate student in Biotechnology Lab under Professor Jintae Lee in the School of Chemical Engineering at Yeungnam University, Korea. My first paper which focuses on broad-spectrum application of halogenated phenol is under review. My research interests include antibiotics, antimicrobial resistance, toxicology and bioremediation.

## Poster presentation

# Antibiofilm Characteristic of Crocetin against *Staphylococcus aureus*

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**Keywords:** Antibiofilm • Crocetin • Fibrils • *Staphylococcus aureus* • *Staphylococcus epidermidis*

### Abstract:

*Staphylococcus aureus* and *Staphylococcus epidermidis* are significant health threats due to their propensity to form biofilms, which shield them from antibiotics and the immune system. To address this, we investigated the effects of carotenoids, particularly crocetin and crocin, on four Staphylococcal strains. Crocetin was found to be the most effective, significantly reducing biofilm formation in strains like *S. aureus* ATCC 6538 at 50 µg/mL, and also inhibiting biofilm formation in MSSA 25923, *S. epidermidis*, and methicillin-resistant *S. aureus* MW2. However, crocetin showed minimal antibiofilm activity against Gram-negative bacteria and the fungal strain *Candida albicans*. Additionally, it reduced fibril formation, a key component in *S. epidermidis* biofilms. ADME analysis revealed crocetin's low toxicity, and when combined with tobramycin, it displayed synergistic antibiofilm effects. Its efficacy is likely due to its polyene chain with carboxylic acid groups, suggesting that apocarotenoids like crocetin could be promising candidates for controlling biofilm formation by *S. aureus* and *S. epidermidis*.

### Reference

1. Antibiofilm activity of carotenoid crocetin against Staphylococcal strains, S Paramanya, JH Lee, J Lee, *Frontiers in Cellular and Infection Microbiology* 14 (2024): 1404960.

### Biography



I have completed a Bachelor of Science in Chemistry and a Master of Science in Analytical Chemistry from Ramnarain Ruia Autonomous College, Mumbai, India. I have gained professional experience as a lab trainee at a healthcare company in India. Currently, I am pursuing a PhD in Chemical Engineering under the supervision of Professor Jintae Lee in the School of Chemical Engineering at Yeungnam University, Korea. My primary research paper explores the potential of carotenoid crocetin in controlling biofilm formation. My research interests encompass antibiotics, antimicrobial resistance, toxicology, and bioremediation.

## Poster presentation

# Phthalimide derivatives as antifungal agents

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**Keywords:** antifungal • antibiofilm • phthalimides • *Candida* strains

### Abstract:

This study explores the antifungal, antibiofilm, and antihyphal properties of six *N*-substituted phthalimides against *Candida* species, which causes common fungal infections. Among these compounds, *N*-butylphthalimide was effective against various *Candida* species, including those that are both resistant and sensitive to fluconazole, at a low concentration (100 µg/ml) and was also effective against other types of bacteria. The biofilm formation (which make infections harder to treat) was inhibited at even lower concentrations (10-50 µg/ml). It also disrupted the formation of fungal structures like hyphae, which *Candida* uses to invade and spread in the body, and altered the appearance of the fungal colonies in a dose-dependent manner. Through qRT-PCR analysis, the compound was found to observe reduced in the activity of key genes responsible for forming biofilms and hyphae, such as *ALS3*, *ECE1*, and *HWPI*. Overall, the study suggests that this compound could be a good alternative to current antifungal treatments, showing strong effects against various *Candida* species.

### Reference

1. Antifungal, anti-biofilm, and anti-hyphal properties of *N*-substituted phthalimide derivatives against *Candida* species, S Shaik, JH Lee, YG Kim, J Lee, *Frontiers in Cellular and Infection Microbiology*, 14, 1414618 (2024).

### Biography



I obtained my BS and MS degrees from JSS college of Pharmacy, Ooty, India. Currently, I am PhD graduate student in Biotechnology lab under Professor Jintae Lee in the School of Chemical Engineering at Yeungnam university. My research interests are in the areas of herbo nanotechnology, antibiotics, and antimicrobial resistance.

## Poster presentation

# Multi-halogenated Pyrimidines as Antibiofilm and Antimicrobial Agents Against *Staphylococcus aureus*.

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**Keywords:** Antibiofilm; Antimicrobial; Halogenated Pyrimidines; *Staphylococcus aureus*

### Abstract:

*Staphylococcus aureus* poses significant challenges in both healthcare and community settings due to its ability to form biofilms, which enhance resistance to antibiotics and immune responses. Recent studies have shown promising potential for halogenated compounds in inhibiting biofilm formation and antimicrobial resistance. This study investigated the potential of halogenated pyrimidine derivatives to inhibit biofilm formation and reduce virulence factors in *S. aureus*. Among the 31 multi-halogenated compounds tested, 2,4-dichloro-5-fluoropyrimidine (24DC5FP), 2,4-dichloro-5-bromo-7H-pyrrolo[2,3-d]pyrimidine (24DC5BPP), and 2,4-dichloro-5-iodo-7H-pyrrolo[2,3-d]pyrimidine (24DC5IPP) were identified as potent inhibitors of biofilm formation. 24DC5BPP and 24DC5IPP partially reduced cell growth, while 24DC5FP inhibited both planktonic cell growth and alpha-hemolysin production. The antibacterial activity of these compounds was confirmed, with minimum inhibitory concentrations (MICs) ranging from 50 to 100 µg/mL. These findings suggest that halogenated pyrimidines, particularly 24DC5FP, have strong potential as novel antibiofilm and antimicrobial agents that target both biofilm formation and virulence in *S. aureus*, offering a promising alternative for addressing biofilm-associated infections.

### Biography



I obtained my Bachelor's degree in Chemical Engineering from Yeungnam University in 2024 and am currently pursuing a Master's degree in Chemical Engineering at Yeungnam University under the supervision of Professor Jintae Lee. My research interests focus on the development of antimicrobial and antibiofilm agents, microbial pathogenesis, and the inhibition of *Staphylococcus aureus* biofilms. I am currently investigating the antibiofilm effects of halogenated pyrimidine derivatives, and I am scheduled to present my research findings at the 2024 8th SKY Symposium.

# Antibiofilm activities of halogenated pyrimidines against enterohemorrhagic *Escherichia coli*

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**Keywords:** Antibiofilm • Antimicrobials • *Escherichia coli* • Halogenated pyrimidines

## Abstract

Enterohemorrhagic *Escherichia coli* (EHEC) is a significant public health concern due to its ability to form biofilms, enhancing its resistance to antimicrobials and contributing to its persistence in food processing environments. Traditional antibiotics often fail to target these biofilms effectively, leading to increased bacterial resistance. This study aims to explore the efficacy of novel antibiofilm agents, specifically halogenated pyrimidine derivatives, against EHEC. We screened pyrimidine and 31 halogenated pyrimidine derivatives for their antimicrobial and antibiofilm activities against EHEC using biofilm quantification assays, SEM analysis, motility, and curli production assessments. Our findings reveal that certain halogenated pyrimidine derivatives, notably 2-amino-5-bromopyrimidine (2A5BP), 2-amino-4-chloropyrrolo[2,3-d]pyrimidine (2A4CPP), and 2,4-dichloro-5-iodo-7H-pyrrolo[2,3-d]pyrimidine (2,4DC5IPP), exhibited significant inhibitory effects on EHEC biofilm formation without affecting bacterial growth, suggesting a targeted antibiofilm action. These compounds effectively reduced curli production and EHEC motility, essential factors for biofilm integrity and development. Additionally, *in silico* ADME-Tox profiles indicated that these compounds exhibit favorable drug-like properties and lower toxicity compared to traditional pyrimidine. The study highlights the potential of halogenated pyrimidine derivatives as effective antibiofilm agents against EHEC, offering a promising strategy for enhancing food safety and controlling EHEC infections. The distinct mechanisms of action of these compounds, particularly in inhibiting biofilm formation and virulence factors without promoting bacterial resistance, underscore their therapeutic potential.

## Reference

1. Inhibitory effects of bromoindoles on *Escherichia coli* O157: H7 biofilms, Jeon, H., Boya, B. R., Kim, G., Lee, J. H., & Lee, J. (2024), *Biotechnology and Bioprocess Engineering*, 1-10.

## Biography



Hyejin Jeon is currently pursuing her Master's in Chemical Engineering at Yeungnam University under the supervision of Professor Jintae Lee. She earned her Bachelor's degree from the School of Chemical Engineering at Yeungnam University in August 2023. Her research focuses on discovering novel substances to inhibit biofilm formation, particularly targeting *Escherichia coli* O157: H7 (EHEC). In 2024, she published her paper, "Inhibitory effects of bromoindoles on *Escherichia coli* O157: H7 biofilms," in the BBE journal. Her research interests include antibiotics, antimicrobial resistance and cosmetics.

# Analysis of Separation Mechanism on Photovoltaic Module with Sacrificial Layer

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**Keywords:** Silicon solar cell, Photovoltaic, Solar module, Separation, TCO corrosion

## **Abstract:**

Silicon photovoltaic modules are already widely installed and used worldwide, and the installation volume is increasing, but at the same time, the amount of end-of-life modules is also increasing. These end-of-life modules are difficult to remove the encapsulant used to bond the components of the module, and typically, the method of incineration is used to remove the encapsulant. In addition, methods such as using a heated cutter, chemical solvents etc., have been studied. The glass of the module occupies a large part of the volume and weight of the module and is strongly bonded to the encapsulant. If the glass can be easily removed from the encapsulant, it will be of great help in recovering the remaining materials. In this study, a structure in which a TCO is added to the photovoltaic module structure was proposed, inspired by the corrosion phenomenon of TCOs studied earlier. The TCO located between the glass and the encapsulant was artificially corroded to confirm that the glass is separated from the module structure.

# Enhanced Oxygen Evolution Reaction Performance Using a CNSe/FeOOH Bilayer Electrocatalyst

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**Keywords:** Transition metals, selenides, oxyhydroxides, oxygen evolution reaction, synergic effects.

## Abstract

The rapid development of bilayer electrocatalysts has gathered significant attention for water splitting applications due to their enhanced redox reactions, greater electrical conductivity, synergistic effects, and increased electroactive sites, all of which can greatly boost electrochemical performance. In this study, cobalt nickel selenide (CoNi<sub>2</sub>Se<sub>4</sub>, or CNSe) thin film nanosheets were combined with iron oxyhydroxide (FeOOH) thin film nanosheets on a nickel foam (Ni-foam) substrate using an electrodeposition method. This CNSe/FeOOH bilayer thin film catalyst demonstrated a low overpotential of 222 mV at a current density of 10 mA cm<sup>-2</sup> and a small Tafel slope of 43 mV dec<sup>-1</sup>. Additionally, it maintained a stable potential for over 120 hours during a chronopotentiometry test at a constant current density of 10 mA cm<sup>2</sup>. The superior performance is attributed to its unique structural characteristics, high double-layer capacitance, and rapid charge transfer. This research offers a novel approach to creating high-performance oxygen evolution reaction (OER) materials through a straightforward electrochemical deposition process.

## Poster presentation

# Unveiling the Potential of High-Temperature Chemical Vapour Deposition Growth of Boron Carbide: Investigating Physicochemical, Mechanical and Electrical Properties

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**Keywords:** Chemical vapour deposition; Boron carbide; Mechanical properties; Electrical properties.

## Abstract:

Chemical vapor deposition (CVD) is a widely employed industrial method known for its precision and reliability, particularly in the synthesis of hard ceramic materials. In this investigation, a gas mixture of  $\text{BCl}_3\text{-CH}_4\text{-H}_2$  was employed to deposit boron carbide ( $\text{B}_4\text{C}$ ) onto graphite substrates, aiming to understand the influence of substrate temperature on the material's properties. X-ray diffraction (XRD) and micro-Raman spectroscopy were utilized to examine the phase composition and vibrational properties of the deposited  $\text{B}_4\text{C}$ . FE-SEM images revealed a transition in morphology from murataite to triangular flakes with increasing substrate temperature, along with noticeable grain expansion. EDS analysis showed a rise in boron concentration and a corresponding decrease in carbon as the temperature increased. These temperature-dependent changes significantly affected the deposition rate and the mechanical and electrical characteristics of  $\text{B}_4\text{C}$ . At  $1200^\circ\text{C}$ , the deposition rate was  $1476 \mu\text{m/hr}$ , with the material displaying a hardness of 3166 HV and an electrical conductivity of  $18.358 \Omega^{-1}\text{cm}^{-1}$ . This study highlights the importance of controlling substrate temperature during CVD for optimizing the properties of  $\text{B}_4\text{C}$  in industrial settings.

## Reference:

1. Ahir, Namita A., et al. "Unveiling the potential of high-temperature chemical vapour deposition growth of boron carbide: Investigating physicochemical, mechanical and electrical properties." *Ceramics International* (2024).

## Biography:



I obtained my BS and MS degrees from Shivaji University, Kolhapur, India. Currently, I am a PhD student in the School of Chemical Engineering at Yeungnam University, South Korea, with a research focus on the deposition and optimization of boron carbide using the CVD method. I published 10 papers until the data (having 85 citations and h-index 6). My research interests span a diverse range of advanced materials and technologies, including the deposition and optimization of ceramic materials, the development and improvement of memory devices, the fabrication and application of nanofibers, and innovations in energy storage devices.

# Optimizing Isopropyl Alcohol – Water Separation: Modeling of Cyclic Heterogeneous Azeotropic Distillation

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**Keywords:** Isopropyl alcohol separation, cyclic distillation, heterogeneous azeotropic distillation, cyclohexane entrainer, energy efficiency

## Abstract:

Isopropyl alcohol is a widely used solvent in the chemical industry, where achieving high purity is crucial for its various applications. However, separating isopropyl alcohol from water is challenging due to the azeotropic behavior of the mixture. Conventional heterogeneous azeotropic distillation, which employs cyclohexane as an entrainer, typically involves columns with numerous trays, resulting in high energy demands and increased equipment costs. This study explores cyclic distillation with cyclohexane as an entrainer as a more efficient alternative for separation. By comparing cyclic distillation with conventional heterogeneous azeotropic methods, the proposed approach shows a significant reduction in both the number of trays and energy consumption. Simulations conducted using Aspen Custom Modeler V14 with the NRTL property package offer detailed insights into mass and energy balances, including dynamic vapor flow rates across trays. The results indicate that the cyclic distillation configuration achieves isopropyl alcohol purity exceeding 99.99% while lowering energy usage compared to the conventional method. This innovative process offers a more efficient and cost-effective solution for high-purity isopropyl alcohol-water separation.

# Simulating Cyclic Dividing-wall Column for Enhanced Separation Efficiency in Alcohol Separation

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**Keywords:** Cyclic distillation, dividing-wall column, alcohol mixture, Aspen Custom Modeler (ACM).

## Abstract:

In chemical engineering, distillation is a fundamental method for separating complex mixtures. One promising but underexplored technique is the combination of dividing-wall column (DWC) with cyclic distillation. This study aims to investigate the integration of cyclic distillation with DWC technology for separating the ethanol – propanol – butanol mixture, a topic that has not been widely studied. Using Aspen Custom Modeler V.14 with the Peng-Robinson property package, simulations will be conducted to evaluate the effectiveness of this novel approach. The focus will be on analyzing the potential for energy savings and improved efficiency through this combined method. By conducting a detailed analysis, this study will explore the untapped synergies between cyclic distillation and DWC, potentially leading to more sustainable and resource-efficient distillation processes.

# Fabrication of Pepstatin A labeled Solid Lipid Nanoparticles for theranostic applications in Adenocarcinoma

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**Keywords:** Theranostic • adenocarcinoma • Solid Lipid Nanoparticles

## Abstract:

Lung cancer ranks as the second most common cancer globally and the leading cause of cancer-related mortality. Extensive research is underway to develop effective theranostic platforms for oncology management including the use of Solid Lipid Nanoparticles (SLNPs). This study focuses on the use of SLNPs for the treatment of lung adenocarcinoma. In this work, the highly expressed diagnostic marker for adenocarcinoma, Napsin A, is being targeted for their downregulation using the protease inhibitor Pepstatin A. to impart synergistic effect of downregulation of Napsin A and chemotherapy, Doxorubicin is loaded inside the SLNPs internal architect. The overall system will be physicochemically evaluated for their size, charge, surface roughness, and porosity. Further, the drug loaded ability of SLNPs along with their drug release behaviour will be evaluated. Additionally, to test the target specificity of the SLNPs based drug delivery system, in vitro assessment will be conducted on A549 adenocarcinomic human alveolar basal epithelial cells. In order to demonstrate the imaging ability, the designed system is further supplemented by tagging Tc based radionucleotide to its surface to get PET imaging facilities. The properties of TC 99 tagged pepstatin A decorated SLNPs include biodegradability, controlled drug release, and targeted delivery, makes them a promising approach for enhancing lung cancer treatment.

## Biography



Yumi Son is a graduate student the Department of Chemical Engineering at Yeungnam University in Korea. She received her bachelor's degree from the Department of Chemical Engineering at Yeungnam

# Synergistic insights into the electrocatalytic mechanisms of ZIF-derived $\text{Co}_3\text{S}_4$ on 1T- $\text{WS}_2/\text{WO}_3$ Bifunctional Catalyst for overall water splitting

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**Keywords:** Hydrogen energy, water splitting, mixed matrix, transition metal dichalcogenides, electrocatalyst

## Abstract:

An intelligent strategy for producing massive amounts of hydrogen fuel by electrochemical water splitting is to design highly efficient and reasonably priced bifunctional electrocatalysts for the hydrogen evolution reaction (HER) and the oxygen evolution reaction (OER). A new and very effective ZIF-derived  $\text{Co}_3\text{S}_4$  on  $\text{WS}_2\text{-WO}_3$  electrocatalyst for general water splitting reactions is shown here. As an essential source of sulfur, thioacetamide (TAA) and its  $\text{NH}_4^+$  ions served as an intercalating agent to enlarge the layers of 1T  $\text{WS}_2$ . The uniform integration and adjustable characteristics of nano-sized  $\text{Co}_3\text{S}_4$  on  $\text{WS}_2\text{-WO}_3$  enable high electrocatalytic performances. With an overpotential of only 73 mV and excellent OER efficiency at  $10 \text{ mA cm}^{-2}$ , the electrocatalyst demonstrated impressive HER performance. In order to understand the performance, the active site of the electrocatalyst is examined and its surface reconstruction is examined in both HER and OER. The long-term CV (2000 cycles) and chronopotentiometry (24 hours) results support the electrocatalysts stability. The  $\text{WS}_2\text{-WO}_3/\text{Co}_3\text{S}_4$  electrocatalyst in an asymmetric device demonstrated a respectable two-electrode total water splitting performance, paving the way for further advancements in the design and optimization of electrocatalysts for the conversion of renewable energy sources.

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## Biography



I obtained my BS and MS degrees from Mahatma Gandhi University, Kerala, India. Currently, I am a PhD student in the School of Chemical Engineering at Yeungnam University, Korea. I published one paper as a first author and 3 paper as a co author. My research interests are in the areas of Water splitting, Bio sensor and Super capacitor applications

## Poster presentation

# Multifaceted Binary Nanohybrids Integrated PLA Composite Films for Active Food Packaging Applications

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**Keywords:** PLA • Hexagonal Boron Nitride • ZnO • Active food packaging • Strawberry packaging

### Abstract:

PLA has significant promise as a sustainable alternative to petroleum-based polymers, particularly in addressing the critical issue of environmental sustainability. Despite this potential, PLA's functional properties are currently limited, and it lacks inherent bioactivity, which restricts its use in active food packaging. This research tackles these limitations by enhancing PLA's functionality through the incorporation of hexagonal boron nitride-ZnO (hBN-ZnO) binary inorganic nanofillers. By optimizing PLA with various hBN ratios, it was determined that the PLA-hBN1.5 film achieved the best overall performance. This film demonstrated excellent formation, the highest tensile strength (62.14 MPa, an increase of 19.75%), the lowest water vapor permeability (WVP) ( $1.23 \pm 0.03 \times 10^{-11} \text{ g}\cdot\text{m}^{-1}\cdot\text{s}^{-1}\cdot\text{Pa}^{-1}$ , a decrease of 32.04%), and improved UV-blocking and thermal resistance properties. To further enhance bioactivity, an hBN-ZnO composite was synthesized through a hydrothermal process and integrated into the optimal PLA-hBN1.5 films, replacing the pure hBN. Including ZnO significantly improved the film's antibacterial, antibiofilm, and antioxidant properties while maintaining its mechanical strength and water vapor barrier capabilities. Comparative packaging studies with fresh strawberries revealed that the PLA-hBN-ZnO composite film outperformed traditional polyethylene (PE) and unmodified PLA films, highlighting its potential as a superior option for sustainable and active food packaging.

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### Biography



I obtained my BS and MS degrees from Mahatma Gandhi University, Kerala, India. Currently, I am a PhD student in the School of Chemical Engineering at Yeungnam University, Korea. I have published 4 papers. My research interests include active food packaging, biopolymers, biocomposites, antimicrobial activity, and green chemistry.

# N-doped Carbon encapsulated Cobalt Vanadium Oxide Nanosheets as a Highly Efficient Bifunctional Electrocatalyst for Overall Water Splitting

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**Keywords:** Oxygen evolution reaction • Hydrogen evolution reaction • Water splitting • Bifunctional electrocatalyst

## Abstract:

The increasing demand for hydrogen energy can be met via the production of hydrogen by various methods. A significant advancement toward achieving the carbon neutrality goals is hydrogen production using electrochemical water electrolysis. Usually, the platinum group metals/compounds (namely, IrO<sub>2</sub>, RuO<sub>2</sub>, and Pt/C) served as effective electrocatalysts for oxygen evolution reaction (OER) and hydrogen evolution reaction (HER). However, high cost, natural scarcity, and undesirable surface corrosion are the major drawbacks to make their industrial applications viable. In this work, a series of low-cost and high-performance cobalt vanadium oxide electrocatalysts for overall water splitting are synthesized by incorporating cobalt on the crystallographically altered vanadium oxides encapsulated in activated carbon (CoV<sub>x</sub>O<sub>y</sub>/C). The structurally interconnected Co with V<sub>x</sub>O<sub>y</sub> gives high OER performance benefits due to the presence of multiple valence states of vanadium and generation of synergy, which promotes metallic behavior and enhanced active site. The carbon enhances the conductivity and electrochemical surface area, accelerating electron transfer and diffusion of ions to give a faster reaction. The CoV<sub>x</sub>O<sub>y</sub>/C gives a reasonable OER activity ( $\eta_{10} = 314$  mV) and excellent HER performance ( $\eta_{10} = 81$  mV) in an alkaline medium of 1M KOH electrolytic solution. The catalyst showcases a high electrochemical surface area ( $C_{dl} = 1.92$  mF), which results in faster electron transfer to facilitate the overall water splitting.

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## Biography



I obtained my BS degree from Aligarh Muslim University (AMU) and MS degree from Indian Institute of Technology (IIT), Roorkee, India. Currently, I am a PhD student in the School of Chemical Engineering at Yeungnam University, Korea. I published 3 papers. My research interests are Catalysis & Reaction Engineering, Nanomaterials, Electrocatalysts, and Electrochemical Water Splitting.

# N-doped Holey CNT Ni-MOF Hybrid as a Bifunctional Electrocatalyst for Overall Water Splitting

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**Keywords:** Hydrogen evolution reaction • Oxygen evolution reaction • Overall water splitting • Bifunctional electrocatalyst • TOF

## Abstract:

This study presents the development of a high-performance electrocatalyst for overall water splitting by integrating functional components into a hybrid heterostructure. The hybrid consists of a 1D N-doped holey carbon nanotube (NHCNT) network and 2D Ni-MOF nanosheets, forming a highly stable, interconnected electronic nanoarchitecture. The tubular structure of the NHCNT facilitates enhanced electron transport and the presence of holes in the nanotubes promotes ion diffusion, significantly boosting the reaction rate. The combination of the 1D/2D NHCNT/Ni-MOF-4 structure delivers outstanding oxygen evolution reaction (OER) performance ( $\eta_{10} = 207.8$  mV, Tafel slope =  $58.7$  mV  $\text{dec}^{-1}$ ) and reasonable hydrogen evolution reaction (HER) activity ( $\eta_{10} = 159.8$  mV, Tafel slope =  $114.2$  mV  $\text{dec}^{-1}$ ) with stable and consistent performance in 1M KOH solution. The catalyst showcases a highly interconnected network that incorporates  $\text{Ni}^{2+}$  and  $\text{Ni}^{3+}$  species, contributing to its high specific surface area ( $235.53$   $\text{m}^2$   $\text{g}^{-1}$ ), electrochemical surface area ( $796.2$   $\text{cm}^2$ ), mass activity ( $4.76$   $\text{mA mg}^{-1}$ ), and turnover frequency ( $3.99 \times 10^{-2}$   $\text{s}^{-1}$ ). The synergy between the NHCNT and Ni-MOF-4 results in exceptional electrocatalytic performance, with the hybrid achieving a low cell voltage of 1.77 V at  $10$   $\text{mA cm}^{-2}$  for overall water splitting.

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## Biography



I obtained my BS and MS degrees from Shivaji University, Kolhapur, India. Currently, I am a PhD student in the School of Chemical Engineering at Yeungnam University, Korea. I published more than 12 papers. My research interests are Electrocatalysts, Oxygen evolution reactions, Hydrogen evolution reactions, Supercapacitors, and Dye degradation.

## Poster presentation

# Engineering heterojunction of multi-morphologies and bifunctional hybrid rGO-V<sub>2</sub>O<sub>5</sub> embedded CeO<sub>2</sub> nanostructures for robust visible-light-driven dye degradation and supercapacitor

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**Keywords:** V<sub>2</sub>O<sub>5</sub> Nanoflower; CeO<sub>2</sub> nanorods; photocatalyst; dye degradation; environmental remediation; supercapacitor

### Abstract:

Photocatalytic degradation of organic pollutants using improved semiconductor materials is a promising method for pollutant-free water systems. We synthesize a ternary nanostructured heterojunction photocatalyst from reduced graphene oxide (rGO), vanadium pentoxide (V<sub>2</sub>O<sub>5</sub>), and cerium dioxide (CeO<sub>2</sub>) using a simple hydrothermal technique. This composite design of V<sub>2</sub>O<sub>5</sub> nanoflowers, rGO sheets, and CeO<sub>2</sub> nanorods has unique microstructural morphologies that improve surface characteristics, provide numerous active sites, and efficiently transfer charge carriers, increasing dye degradation efficiency. Different catalyst compositions (binary and ternary), dosages (40, 50, and 60 mg), and pH levels (4, 6, and 8) were tested for rGO-V<sub>2</sub>O<sub>5</sub>-CeO<sub>2</sub> (rG-V-C) photocatalyst. Under visible-light irradiation, the best rG-V-C-1 catalyst degraded 94.15% RhB in 90 minutes. Under visible light, scavenger experiments revealed that RhB degradation is primarily driven by the production of superoxide radicals (O<sub>2</sub><sup>•-</sup>) and hydroxyl radicals (OH<sup>•</sup>). rG-V-C catalyst was stable and reusable. The synergy between rGO, V<sub>2</sub>O<sub>5</sub>, and CeO<sub>2</sub> reduces photogenerated electron-hole recombination and improves charge separation and transfer, making the rG-V-C composite a potent photocatalyst. Furthermore, the rG-V-C composite showed efficient supercapacitor performances due to the existence of a synergetic effect via effective interaction between each compound in the composite structure. The specific capacitance and energy density of the rG-V-C electrode were obtained at 462 at 1 A g<sup>-1</sup> and 64.16 Wh/kg, respectively in a 1M LiClO<sub>4</sub>-PC

### Biography



I obtained my BS and MS degrees from Shivaji university Kolhapur, India. Currently, I am a PhD student in the School of Chemical Engineering at Yeungnam University, Korea. I published more than 8 papers. My research interests are in the areas of Photo and Sonocatalytic dye degradation and supercapacitor.

# Synthesis and Characterization of Polyimides with Different Main Chain Lengths according to Chain Length of Ethylene Oxide

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**Keywords:** polyimide • ethylene oxide • chain length

## Abstract:

Aromatic polyimides (PIs) have been widely used in the electronic device industry due to their excellent thermal properties, such as heat resistance, high thermal degradation temperature and high glass transition temperature, as well as their electrical and mechanical properties.<sup>1-5</sup> Moreover, ethylene oxide moieties attracted attention, because of transport ability of lithium ion for solid polymer electrolytes (SPE), and the strong affinity of CO<sub>2</sub> towards the oxygen for gas separation membranes. In this study, series of PIs were prepared using newly synthesized diamine containing different chain length of ethylene oxide segments with 6FDA. The chemical structures of the synthesized monomers were characterized by NMR. The chemical structures and thermal properties of the synthesized PIs were determined using spectroscopic methods including NMR, FTIR, DSC, and TGA.

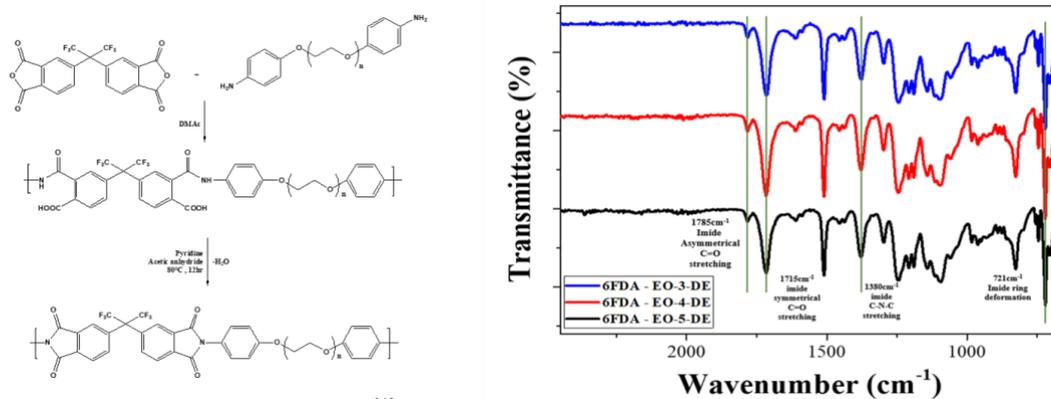


Figure 1: Chemical Structure of PIs used in this study.

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# Characterization of Strict Chain Copolyimide Synthesized Applying Monomer Including Benzoxazole

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**Keywords:** polyimide • benzoxazole • rigid backbone

## Abstract:

Of the many polymeric materials available, aromatic polyimides (PIs) have been used widely in the electronic device, semiconductor devices, and printed circuitry boards industries owing to their high glass transition temperature, dimensional stability and heat resistance, as well as their excellent mechanical, adhesion and dielectric properties.<sup>1-3</sup> Moreover, PIs having rigid-rod backbones attracted much attention because rigidity of polymer chains would impart high tensile modulus and low CTE to the resultant PI. Incorporating heterocyclic units into the PI main chain is another effective way to improve thermal and mechanical properties of PIs.<sup>4,5</sup> In this study, series of PIs were prepared using newly synthesized diamine containing benzoxazole moiety with various dianhydrides. The chemical structures of the synthesized monomers were characterized by NMR. The chemical structures and thermal properties of the synthesized PIs were determined using spectroscopic methods including NMR, FTIR, DSC, and TGA.

## Reference

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## Poster presentation

# Utilizing an organic dye with a simple wet chemical coating of fluorine-TiO<sub>2</sub>/WO<sub>3</sub> as an innovative photo-anode to improve the performance of photoelectrochemical cells

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**Keywords:** WO<sub>3</sub> Photo anode • Photoelectrochemical cells • Fluorine-TiO<sub>2</sub> • Organic dye

### Abstract:

A high-performing photo-electrochemical (PEC) anode must exhibit strong light-harvesting capabilities, efficient charge transport, and effective electron-hole pair separation. In this study, we present a novel WO<sub>3</sub>/fluorine-TiO<sub>2</sub>/organic dye photo-anode developed through a combination of facile wet chemical coating and the incorporation of an organic dye. This newly fabricated photo-anode achieved a high PEC performance with a photocurrent density of 1.54 mAcm<sup>-2</sup>, measured in phosphate buffer at 1.23V versus an Ag/AgCl reference electrode under simulated AM1.5 light conditions. This represents a 111% and 41% improvement over WO<sub>3</sub> alone and WO<sub>3</sub>/fluorine-TiO<sub>2</sub>, respectively. The significant enhancement is attributed to the high surface area and electron trapping sites provided by fluorine-TiO<sub>2</sub>, which improves charge transport and separation, alongside the improved light-harvesting efficiency due to the organic dye.

### Biography



Donghwan Kim got his BS degree in Chemical Engineering from Yeongnam University. He is currently pursuing a master's degree under Professor Jaehong Kim in Yeongnam University. His research interest is mainly focused on the areas of organic functional materials, photo-electrochemical cells for hydrogen energy and secondary battery, and Hole transport material in Perovskite Solar Cell

# The role of dye anchor counter electrode on solid state-DSSC to achieve enhanced efficiency: a mechanistic approach

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**Keywords:** Sensitizer, Dye anchor counter electrode, solid-state dye-sensitized solar cells, Light-harvesting capability, efficiency, photocurrent

## Abstract:

A key limitation of dye-sensitized solar cells (DSSCs) is their restricted absorption spectrum, which impedes the attainment of optimal efficiency. In this study, we present the newly developed DACE (Dual Active Component Electrode) technique to achieve panchromatic absorption in solid-state DSSCs. TVP208 and DPP13 dyes were synthesized and systematically investigated for their application in DACE-based DSSCs, with their performance compared to conventional solid-state DSSC devices. The TVP208 and DPP13 dyes exhibited complementary absorption profiles, a critical requirement for achieving panchromatic absorption in DACE-based systems. The solid-state DSSC device incorporating a TVP208-sensitized working electrode and a DPP13-based DACE electrode (SS-Device2) demonstrated an enhanced efficiency of 5.08%. The superior efficiency of DACE-based solid-state DSSC devices compared to traditional counterparts can be attributed to the improved light-harvesting capabilities facilitated by the DACE electrode. The enhanced IPCE in DACE-based devices further underscores the significant role of the DACE electrode in augmenting overall device performance.

## Biography



OhJoon Kwon received his BS degree in Energy Chemical Engineering from the School of Chemical Engineering at Yeungnam University. He is currently pursuing an MS degree in the same department. His research interests primarily focus on organic functional materials, photo-electrochemical cells for hydrogen energy, and secondary batteries. He has made significant contributions to these research fields and industries.

## Poster presentation

# Improved dye-sensitized photoelectrochemical water oxidation through the introduction of hydroxamic acid group in dye structure

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**Keywords:** Dye-sensitized photoelectrochemical cell, Carboxylic Acid, Hydroxamic Acid, Anchoring, LSV (Linear Sweep Voltammetry)

### Abstract:

Hydroxamic acid-based (BTPA-HA) and cyanoacetic acid-based (BTPA-CN) dyes were synthesized and applied to dye-sensitized photoelectrochemical (DS-PEC) water oxidation. Among the two, the BTPA-HA dye exhibited superior DS-PEC performance compared to BTPA-CA. The improvement in DS-PEC efficiency is attributed to the stable bidentate keto anchoring mode provided by the hydroxamic acid group, which facilitates efficient electron injection. Additionally, BTPA-HA demonstrated greater stability across various pH conditions than BTPA-CA, highlighting the advantages of hydroxamic acid anchoring groups over cyanoacetic acid in this context.

### Biography



Kim Seo-Young received her bachelor's degree from Yeungnam University. She is currently pursuing a master's degree at Yeungnam University. Her research interest is mainly focused on the areas of organic functional materials, photo-electrochemical cells for hydrogen energy and secondary battery. She made significant contributions to these research fields and industries.

# Solution-based synthesis and analysis of WO<sub>3</sub> film as an effective photo-anode for photoelectrochemical cells

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**Keywords:** WO<sub>3</sub> photo-anode • wet chemical synthesis • photo-electrochemical cells • PECs

## Abstract:

This research focusses on facile, single step, cost-effective approach for synthesizing WO<sub>3</sub> nanostructure as a photo-anode for photoelectrochemical cells. Advanced characterization techniques, including X-ray diffraction (XRD), scanning electron microscopy (SEM), diffuse reflectance spectroscopy (DRS), and Linear sweep voltammetry (LSV) have been utilized to systematically investigate the influence of reaction time on structure, morphology, optical, and photo-electrochemical properties of the WO<sub>3</sub> films, respectively. The results reveal that the reaction time is a remarkable parameter that significantly control over the morphology, optical characteristics, and photo-electrochemical performance of the WO<sub>3</sub> films. Notably, the solar water splitting system has achieved a photo-current density of 2.08 mA/cm<sup>2</sup> with the 2-hour photoanode, representing an enhancement of approximately 58% compared to the lowest systems with 4-hour photoanode. The improvement could be attributed to the suitable deposition amount of WO<sub>3</sub> on fluorine-doped tin oxide - FTO glass, which facilitates efficient charge transfer, charge separation, and increases the number of active reaction sites on the photo-anode.

## Biography



Yujeong Hwang got his B.S degrees from Yeungnam University and she is currently a M.S. student in Chemical Engineering from Yeungnam University in Korea. Her research interestes are maily focussed on the areas of organic functional materials, photoelectrochemical cells for hydrogen energy, and perovskite solar cells.

# Designing Cost-Effective Alloy Catalysts for NH<sub>3</sub> Decomposition : Reducing Ruthenium Dependence Through DFT Calculations

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**Keywords:** Ammonia decomposition, Hydrogen carrier, Bimetallic catalyst

## Abstract:

Hydrogen is gaining significant attention as an environmentally friendly energy source capable of accelerating the transition to a decarbonized era. However, storing and transporting large volumes of hydrogen in its gaseous state is impractical, leading to the proposal of ammonia as a viable hydrogen carrier. Among various catalysts tested, ruthenium (Ru) has demonstrated the highest performance in experimental studies. However, the high cost of Ru presents a major economic barrier to commercialization. To address this, we employed DFT calculations to design alloy catalysts with the goal of reducing Ru content or replacing it with low-cost, high-performance alternatives. Despite outstanding catalytic properties of Ru, identifying an alloy catalyst that matches or surpasses its performance remains a significant challenge. Our research is focused on discovering catalysts that maintain high efficiency while offering cost benefits.

## Reference

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## Biography



I am a fourth-years undergraduate in ths School of Chemical Engineering at Yeungnam University. My major is Chemical Engineering Systems. I am affiliated to laboratoty and My academic adviser is Professor Minkyu Kim from Yeungnam university. Our laboratory mainly research on catalysts. My research interests are in the areas of catalysts, Ammonia decomposition and Chemical Looping Cumbustion.

# Red Mud as a Low-Cost Catalyst for Sulfur Removal and COS Decomposition: A Theoretical and Experimental Study

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**Keywords:** red mud • desulfurization • Fe<sub>2</sub>O<sub>3</sub> • dopant effect • dft

## Abstract:

The growing use of fossil fuels has driven industrial development, but it has also intensified global warming and climate change through increased CO<sub>2</sub> emissions. Reducing these emissions and identifying alternative energy sources, such as hydrogen, have become critical priorities. Hydrogen, which produces no CO<sub>2</sub> emissions and offers a high calorific value, is both economically and environmentally advantageous. One promising method is the production of blue hydrogen, generated from natural gas or coal with carbon capture and storage (CCS). However, impurities in the syngas from coal gasification must be removed to prevent equipment damage and maintain fuel cell performance. This study evaluated red mud as a sulfur absorbent for COS(g) desulfurization by both theoretically and experimentally, demonstrating its ability to decompose COS(g) into CO(g) due to the synergistic effects between main component of Fe<sub>2</sub>O<sub>3</sub> and other elements. These findings confirm red mud potential as a low-cost sulfur absorbent and COS decomposition catalyst.

## Reference

Synergistic Desulfurization Performance of Industrial Waste Red Mud : A Comprehensive Experimental and Computation Study for COS Removal and CO(g) Production, Seongjun Lee, Ji Eun Lee, Seung Jong Lee, Jin Wook Lee, Yongseung Yun, No-Kuk Park, Dohyng Kand, Minkyu Kim, Applied Surface Science 649(2024)

## Biography



My name is Ga-yeong Kim, and I am a third-year student majoring in Chemical Engineering at Yeungnam University. I am studying computational chemistry under Professor Min-kyu Kim. My research focuses on catalyst development using DFT(Density Functional Theory), and I am currently working on Red mud as a Low-Cost Catalyst for Sulfur Removal and COS decomposition.

# Rotating packed beds for CO<sub>2</sub> Capture: Efficiency Improvements and Cost Reduction Strategies

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**Keywords:** Rotating packed bed, process intensification, CO<sub>2</sub> capture

## **Abstract:**

The use of conventional absorption columns for CO<sub>2</sub> capture presents challenges due to their large size and high cost. However, the emergence of Rotating Packed Beds (RPBs) offers a compact and efficient alternative for process intensification. To capture CO<sub>2</sub> efficiently, high concentrations of Monoethanolamine (MEA) are required, but this results in high viscosity. Consequently, using conventional absorption columns can increase mass transfer resistance. In contrast, RPBs provide excellent mass transfer performance due to centrifugal force, enabling CO<sub>2</sub> capture with high-concentration MEA. This study explores the application of RPB absorbers, which contribute to enhanced post-combustion CO<sub>2</sub> capture by reducing volume and improving mass transfer compared to traditional packed beds. RPB modeling has been successfully implemented using Aspen Custom Modeler (ACM) V14, and thermodynamic properties are calculated using the ENRTL-RK property method. Monoethanolamine (MEA), a solvent widely used in CO<sub>2</sub> capture, was selected. The two-film theory was integrated into the RPB modeling framework. Results indicate that RPB adoption leads to a reduction in volume requirements by over 9 times compared to traditional packed beds, a decrease in energy consumption by more than 3 times, and CO<sub>2</sub> capture levels exceeding 90%. Additionally, sensitivity analysis was conducted on various input variables, including RPB rotational speeds, lean amine ratios, and stripper reboiler duties, revealing their complex interplay and impact on process efficiency. This research highlights the potential of RPBs to enhance efficiency and reduce costs in acid gas enrichment processes.

## Poster presentation

# Development of a Movable Rotating Packed Bed System for Efficient VOCs Removal in Shipboard Operations

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**Keywords:** Rotating Packed Beds, Movable RPB, VOCs removal

### Abstract:

VOCs are emitted from the main engine, auxiliary engine, and boiler of ships, posing a threat to the environment and human health, making their removal essential. However, the amount of VOCs emitted from ships is relatively small compared to other pollutants like CO<sub>2</sub>, NO<sub>x</sub>, and SO<sub>x</sub>, which makes installing large absorption and stripping towers for VOC removal highly inefficient. Therefore, this study aims to model a movable Rotating Packed Bed (RPB) for the removal of VOCs collected from ships while docked at the port. The movable nature of the RPB system enables easy installation and operation during docking. This means ships do not need to carry bulky and permanent VOC removal systems but can instead connect to the RPB unit when needed. The RPB offers excellent mass transfer performance due to its high rotational speed, which increases the contact between gas and liquid phases. And enables a significant reduction in required volume compared to traditional absorption columns. Thus, the RPB is modeled with constraints of 5 meters in height and 5 meters in width to ensure it remains movable. Additionally, different VOCs have different mass transfer characteristics. Hence, different mass transfer correlations are applied to calculate the mass transfer coefficients for various VOCs. The system can be fine-tuned for optimal performance depending on the VOCs being emitted. The results show that the RPB effectively removes VOCs while meeting the volume constraints. This study highlights the potential of the RPB to reduce both costs and operational complexity by efficiently removing the small amounts of VOCs emitted from ships.

### Biography



Uidong Jin, Master student in Chemical Engineering, School of Chemical Engineering, Yeungnam University. Main research interests: Development of a Movable Rotating Packed Bed System for Efficient VOCs Removal in Shipboard Operations.

## A Customized Core/Shell Architecture: Co<sub>0.85</sub>Se Nanowires Encased in NiCo-LDH for Enhanced Battery-Type Supercapacitor Performance

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**Keywords:** Co<sub>0.85</sub>Se nanowires, NiCo-LDH, Core/shell, Hydrothermal, Battery-type, Energy density.

**Abstract:**

This paper reports the successful creation of a new core/shell structure consisting of cobalt selenide nanowires (Co<sub>0.85</sub>Se) coated with nickel-cobalt layered double hydroxide (NiCo-LDH). The synthesis followed a three-step process: first, cobalt carbonate hydroxide hydrate (CCHH) nanowires were grown on a nickel foam (NF) substrate using a hydrothermal technique. These nanowires were then converted into Co<sub>0.85</sub>Se nanowires through selenization, and NiCo-LDH nanosheets were deposited via electrodeposition to form the outer shell. The resulting Co<sub>0.85</sub>Se@NiCo-LDH material displayed excellent electrochemical properties, with a high specific capacity of 1314 C g<sup>-1</sup> at 1.0 A g<sup>-1</sup>, good rate capability, retaining 61.5% at 20 A g<sup>-1</sup>, and strong cycling stability, maintaining 89.2% capacity after 10,000 cycles.

Additionally, a hybrid supercapacitor was developed using Co<sub>0.85</sub>Se@NiCo-LDH as the positive electrode and activated carbon as the negative electrode. The device achieved an energy density of 72.2 Wh kg<sup>-1</sup> and a power density of 849.9 W kg<sup>-1</sup>, with 88.2% capacity retention after 10,000 cycles. These findings demonstrate the potential of core/shell structures for producing high-performance supercapacitors with improved kinetics and long-term stability.

## Poster presentation

# Microwave-assisted Ultrafast Synthesis of Reduced Graphene Oxide/Mn<sub>3</sub>O<sub>4</sub> Nanocomposites Hydrogels for Bone Tissue Engineering Applications

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**Keywords:** Microwave • manganese oxide • bone tissue engineering • hydrogels

### Abstract:

The development of functional materials with the potential for bone tissue regeneration along with rapid synthesis and cost-effective approach has been challenging. In this regard, hydrogels have been explored as a potent candidate to behave as a 3D scaffold for bone repair. However, poor mechanical attributes impeded their clinical translation. Enthralling demonstration of the potential of carbon-based nanocomposites in bone tissue engineering has been constantly encouraging the fabrication of advanced nanocomposites. Here, we investigated the fabrication of reduced graphene/manganese (II, III) oxide (RGO/Mn<sub>3</sub>O<sub>4</sub>) nanocomposites by taking advantage of the microwave-assisted synthesis approach for cost effective, and ultrafast synthesis. Mn<sub>3</sub>O<sub>4</sub> nanoparticles with uniform distribution in RGO sheets and ~1.7 nm size was fabricated using the approach. Further, fine-tuning of the structural interaction and mechanical behavior of the GelMA-based hydrogels upon reinforcement with RGO/Mn<sub>3</sub>O<sub>4</sub> nanocomposites was investigated as a function of different concentrations of the nanocomposites where upto 50% increment in the compressive stress was observed compared to native GelMA hydrogel. The ability of these hydrogels was further investigated for their osteogenic behaviour on MC3T3-E1 preosteoblast cells where constant cell proliferation for up to 10 days was witnessed for the hybrid hydrogel with the highest concentration of the nanofillers.

### Biography



Ritu Singhmar is a Ph.D. scholar at Biomaterials Lab, School of Chemical Engineering, Yeungnam University, South Korea. She obtained her master of science (M.Sc.) degree in Chemistry from the Indian Institute of Technology Mandi, India. Her M.Sc. thesis focused on synthesizing functionalized nanoparticles for cancer theranostics. Currently, Ritu is working on hydrogels for bone tissue engineering applications.