2025

The 4th CNU-SU Joint Symposium

Chungnam National University

Shizuoka University

August, 1st , A.M. 09:00

Central Library (Lecture Hall, B1) I Poster Session (Seminar Hall, B1)

The Education and Research Group for Convergent Chemical Materials in the 4th Industrial Revolution Era(CCM4)
Chungnam National University

National University Corporation
Shizuoka University

BrainKorea FOUR 21
2020 – 2027

The 4th CNU-SU Joint Symposium

Welcoming Remarks

It is our great pleasure to welcome you to the 4th CNU–SU Joint Symposium, jointly organized by Chungnam National University and Shizuoka University.
Since its inception four years ago, this symposium has grown into a meaningful tradition between our institutions, fostering scientific collaboration, mutual understanding, and lasting friendships. I would especially like to express my sincere appreciation to Professor Nobuyuki Mase, whose outstanding leadership and dedication have been instrumental in sustaining and advancing this event.

We are also excited to introduce a student poster session for the first time this year. This addition marks an important step forward, reflecting the growth and deepening of our joint symposium through the active engagement of the next generation researchers.

Thank you to all participants for your contributions. I hope you enjoy the symposium and take this opportunity to form meaningful and lasting connections.

Sincerely,

Dong-Myung Kim, PhD
Group Leader, CCM4
Department of Chemical Engineering and Applied Chemistry
Chungnam National University

Good morning, everyone.

It is my great pleasure to welcome you all to the 4th CNU–SU Joint Symposium. Seeing so many researchers, colleagues, and students gathered here today fills me with excitement—and, I must admit, a bit of curiosity about what surprises these two days may bring.

This symposium has always been a place where ideas travel freely—sometimes in expected directions, and sometimes in delightfully unpredictable ones. From advanced materials to innovative approaches in chemical and biological sciences, I am certain we will once again be reminded of just how wonderfully broad the world of science can be.

I am especially looking forward to the student poster session. Young researchers have a remarkable way of asking questions and proposing fresh ideas that make us reconsider our own perspectives. And who knows—perhaps the first seeds of the next big collaboration, or even a future breakthrough, will be planted right here in these halls.

I hope these two days will not only deepen the academic partnership between Chungnam National University and Shizuoka University but also strengthen the friendships that make our research journeys so enjoyable.

Thank you for joining us, and I wish you all a stimulating and rewarding symposium.

Just enjoy!!
Sincerely,

Nobuyuki Mase, Ph.D.
Director, Research Institute of Green Science and Technology (RIGST)
Shizuoka University

The Education and Research Group for Convergent Chemical Materials in the 4th Industrial Revolution Era(CCM4)
Chungnam National University

National University Corporation
Shizuoka University

BrainKorea21 FOUR
2020 – 2027

The 4th CNU-SU Joint Symposium

DATE August,1st 2025

VENUE Central Library

CONTENTS

Oral Session

TIME	PRESENTERS	PRESENTATION TITLE
08:30-09:00		Registration
09:00-09:10	Prof. Dong-Myung Kim (CNU)	Welcoming Remarks
Session 1		Chaired by Prof. Jae Bem You
09:10-09:30	Prof. Byeonggwan Kim (CNU)	Stretchable Thermoelectric Fibers for Multisensor in Wearable Electronics
09:30-09:50	Prof. Yuhki Mizushima (SU)	Development of a measurement method for dense foam using an optical fiber probe
09:50-10:10	Prof. Seulki Song (CNU)	Perovskite for Optoelectronic device
		Intermission (10:10 - 10:30)
Session 2		Chaired by Prof. Yuhki Mizushima
10:30-10:50	Prof. Masaki Shintani (SU)	Single-cell Analysis of Original Hosts of Plasmids in Microbial Communities
10:50-11:10	Prof. Jae Bem You (CNU)	Controlling the Crystallization of Organic Compounds in Surface Nanodroplets Under Flow
11:10-11:30	Prof. Jaehoon Choi (SU)	Physiological Characterizations and Biosynthetic Pathways of Fairy Chemicals in Plants
		Photo Time (11:30-11:40) & Lunch (11:40-13:30)
Session 3		Chaired by Prof. Byeonggwan Kim
13:30-13:50	Prof. Kosan Roh (CNU)	Active Learning-Based Optimization of Non-flammable Liquid Electrolytes for High-Performance Li-ion Batteries
13:50-14:10	Prof. Yoshihiko Sano (SU)	A mathematical approach based on the volume-average theory for drip and espresso coffee extraction
14:10-14:30	Prof. Hoon-Hee Ryu (CNU)	Microstructural Optimization of Ni-Rich Layered Cathodes for Durable High-Energy Lithium Batteries
14:30-14:50	Prof. Nobuyuki Mase (SU)	Synthesis of novel plant hormones: Fine bubble and flow technology for fairy chemicals
14:50-15:10	Prof. Jaewon Lee (CNU)	Strategic Design of Molecular Acceptors for Short Wavelength Infrared Photodetection
		Coffee Break (15:10-15:20)
15:20-16:20		Poster Presentation
16:20-16:30	Prof. Nobuyuki Mase (SU)	Closing Remarks & Awards

Stretchable Thermoelectric Fibers for Multisensor in Wearable Electronics

Byeonggwan Kim[1,*]

1. Department of Chemical Engineering and Applied Chemistry, Chungnam National University

*Corresponding author: Prof. Byeonggwan Kim, bg_kim@cnu.ac.kr

Thermoelectric (TE) fibers based on organic-inorganic hybrid composites can be utilized as multi-mode sensors capable of simultaneously detecting thermal and mechanical stimuli, and thus have potential applications in advanced wearable electronics such as health and fitness monitoring (biosensors, activity tracking, remote patient monitoring), connective communication (smartwatch, smart glass, Bluetooth and Wi-Fi), and data processing/analytics (real-time data processing, health algorithms). TE fibers composed of carbon or organic materials can effectively detect thermal changes but have low TE performance, and TE fibers composed of rigid inorganic materials have limited ability to detect mechanical deformation due to their lack of stretchability. In this study, we synthesized copper iodide (CuI), an inorganic TE material, into nanoparticles using a novel solution-based method to develop a stretchable TE fiber-based multisensor. A high-density CuI nanoparticle network embedded in the fiber enables the sensor to achieve both excellent stretchability and superior TE performance. By stacking two fiber sensors coated with a polyurethane dielectric layer, a high-pressure sensing with a precise pressure resolution was achived. In addition, the sensor can simultaneously and independently detect temperature changes, tensile strain, and pressure by measuring various parameters. Its seamless integration into a smart glove demonstrates practical applicability in the field of wearable technology.

References

[1] Yoon K., Lee S., Kwon C., Won C., Cho S., Lee S., Lee M., Lee J., Lee H., Jang K.-I., Kim B., Lee T. Highly Stretchable Thermoelectric Fiber with Embedded Copper(I) Iodide Nanoparticles for a Multimodal Temperature, Strain, and Pressure Sensor in Wearable Electronics. *Adv. Funct. Mater.* **35**, 2407759, (2025).
[2] Kwon C., Lee S., Won C., Lee K. H., Kim B., Cho S., Lee T. Stretchable Ag_2Se Thermoelectric Fabric with Simple and Nonthermal Fabrication for Wearable Electronics. *Small Sci.* **4**, 2400230, (2024).

Development of a measurement method for dense foam using an optical fiber probe

Yuki Mizushima[1,2]

1. Graduate School of Integrated Science and Technology, Shizuoka University
   3-5-1 Johoku, Chuou-ku, Hamamatsu, 432-8561, Japan
2. Research Institute of Green Science and Technology, Shizuoka University
   3-5-1 Johoku, Chuou-ku, Hamamatsu, 432-8561, Japan

mizushima.yuhki@shizuoka.ac.jp

Dense foam emerges in various engineering processes such as refrigeration systems, fire extinguishing, insulation material, detergents, and food. A reliable and accurate measurement technique for the dense foam has been required to improve efficiency and safety in these processes. Currently, the conventional methods for measuring the foam are confined to measuring an average foam-cell size near a glass wall; these techniques cannot measure foam-cell size at optional places. An optical fiber technique was proposed for foam measurement, but its noisy signal was hard to use for practical purposes[1].

We offer a new foam measurement technique using an Optical fiber Probe (OFP)[2]. The OFP is our original measurement system for a gas–liquid two-phase flow. It is an intrusive but real-time measurement; the OFP is inserted in the flow to measure the parameters of droplets/bubbles[3,4]. In addition, the optical device is small and simple; hence, our OFP is manageable in industrial fields. In this study, we conducted two measurements: a flat and thin soap film and dense foam made by soap liquid. Compared the signals obtained by the computational results with the experimental ones, we analyzed the characteristics of the OFP system and considered the performance of the system. In addition, we developed a code to process raw signals from the OFP practically.

References

[1] Besperink, C.G.J., Ronteltap, A.D., Prins, A., Bubble-size Distributions in Foams, *Adv. Colloid Interface Sci.*, **38**, 13-32 (1992).
[2] Mizushima, Y., Saito, S., Development of a simultaneous measurement of film thickness and size of liquid foam by optical fiber probing, *Proc. 12th International Conference on Multiphase Flow 2025*, No. 972 (2025).
[3] Mizushima, Y., Sakamoto, A., Saito, T., Measurement technique of bubble velocity and diameter in a bubble column via single-tip optical-fiber probing with judgment of the pierced position and angle, *Chem. Eng. Sci.*, **100**, 98-104 (2013).
[4] Mizushima, Y., Saito, T., Improving the accuracy of droplet measurement by optical fiber probe using 3D ray-tracing simulation, *J. Chem. Eng. Japan*, **52**(2), 171-178 (2019).

Perovksite for Optoelectronic device

Seulki Song*

Chungnam National University (CNU)

Department of Chemical Engineering and Applied Chemistry Affiliation

Perovskite is attracting attention as a promising material for many optoelectronic devices due to its high light absorption rate, easily tunable band gap, and solution processability. It is applied to solar cells, with perovskite solar cells reporting high efficiencies of over 27%. In addition, it can be applied to sensors and communications by utilizing its ability to absorb light and generate electricity. This presentation will cover perovskite solar cells and their applications in optical communications

References

[1] Heesu K., Byeongil N., Cheong Beom L, Eun Young P.k, Gunoh L., Hyuntae C., Yeji K., Kyeounghak K., Nam Joong J., Kyung Jin L., Seulki S. Nanoscopic Parylene Layer: Enhancing Perovskite Solar Cells Through Parylene-D Passivation *Small Method* 2500395(2025).

Single-cell analysis of original hosts of plasmids in microbial communities

Masaki Shintani[1,2]*

1. Shizuoka University, Japan
2. Japan Collection of Microorganisms, RIKEN BioResource Research Center, Japan

*Corresponding author: shintani.masaki@shizuoka.ac.jp

PromA is a broad-host-range plasmid group proposed in 2009[1)] that is widely distributed across various natural environments[2)]. Most PromA plasmids have been obtained via exogenous plasmid capture methods[3)], and thus their original hosts remain unidentified. In addition, PromA plasmids typically carry no accessory genes that alter host phenotypesm and their transmission pathways and their ecological roles remain poorly understood. The objective of this study is to identify the original hosts of the PromA plasmids to better understand their ecological behavior. Here, we depeloped a culture-independent single-cell method by combining droplet digital PCR (ddPCR) with 30 μm diameter water-in-oil droplets with a targeted single-cell dispensing system (utilizing On-chip® Droplet Selector; On-chip Biotechnologies). Each droplet contained a single microbial cell of extracted from lake sediment. Multiplex ddPCR was performed using specific primers and green-fluorescent probe targeting the replication initiation protein gene (*repA*) of PromA plasmids, as well as primers for partial amplification of the 16S rRNA gene (V3-V4 region). A total of 2,296,472 droplets were analyzed, of which 68,890 were estimatind to contain microbial cells. Among them, 548 droplets showed green fluorescence, indicating that the presence of PromA plasmid-harboring cells. Of these, 373 droplets were indivisually sorted, and partial 16S rRNA gene sequences were successfully obtained from 42 samples. As a result, bacteria belongin to 17 genera were identified as potential hosts of PromA plasmids. Seven of these were previously known hosts[4)], while three candidates showed less than 90% sequence identity in the V3-V4 region of the 16S rRNA gene with sequences in public database (NCBI and SILVA).

References

[1] van der Auwera, G. A., Król, J. E., Suzuki, H., Foster, B., Van Houdt, R., Brown, C. J., Mergeay, M., & Top, E. M. Plasmids captured in *Cupriavidus metallidurans* CH34: defining the PromA family of broad-host-range plasmids. *Antonie van Leeuwenhoek* **96**, 193–204 (2009). [2] Hayakawa, M., Tokuda, M., Kaneko, K., Nakamichi, K., Yamamoto, Y., Kamijo, T., Umeki, H., Chiba, R., Yamada, R., Mori, M., Yanagiya, K., Moriuchi, R., Yuki, M., Dohra, H., Futamata, H., Ohkuma, M., Kimbara, K., & Shintani, M. Hitherto-unnoticed self-transmissible plasmids widely distributed among different environments in Japan. *Appl. Environ. Microbiol.* **88**, e01114-22 (2022). [3] Yanagiya, K., Maejima, Y., Nakata, H., Tokuda, M., Moriuchi, R., Dohra, H., Inoue, K., Ohkuma, M., Kimbara, K., & Shintani, M. Novel self-transmissible and broad-host-range plasmids exogenously captured from anaerobic granules or cow manure. *Front. Microbiol.* **9**, 2602 (2018). [4] Tokuda, M., Yuki, M., Ohkuma, M., Kimbara, K., Suzuki, H., & Shintani, M. Transconjugant range of PromA plasmids in microbial communities is predicted by sequence similarity with the bacterial host chromosome. *Microb. Genom.* 9, mgen001043 (2023).

Controlling the crystallization of organic compounds in surface nanodroplets under flow

Jae Bem You*

Department of Chemical Engineering and Applied Chemistry,

Chungnam National University

*Email: jb.you@cnu.ac.kr

Droplets act as excellent platforms to perform various unit operations including mixing, chemical reaction, extraction, and others. Among all, liquid-liquid extraction of chemicals using droplets from an immiscible solvent is particularly interesting owing to the fast mass transfer enabled by the high surface area-to-volume ratio of the droplets. A notable application of exploiting enhanced liquid-liquid extraction using droplets is in analytical chemistry wherein the droplets act as platform to preconcentrate traces of chemicals from surrounding fluids that enabling highly sensitive detection. Recently, it came to our attention that due to the finite solubility of the droplets in the solvent, coupled with their low volume, the preconcentrated chemicals can eventually be supersaturated. Then, given the correct type of chemicals, it is possible to induce and control the formation of organic crystals within the dissolving droplets. Herein using surface nanodroplets – with volumes in femtoliter scale – we show crystallization of organic compounds from an unsaturated solution. Using trimesic acid (TMA) as model compound, we demonstrate that when exposed to a flowing stream of aqueous solution containing TMA, the surface nanodroplets readily extract the TMA molecules increasing their concentration inside. At the same time, due to finite solubility, surface nanodroplets slowly dissolve in the aqueous solution driving supersaturation and finally crystallization of TMA. We show that crystallization can be controlled by independently tuning the droplet size, the flow velocity of aqueous solution, and the initial concentration of TMA. We believe the technique shown here can be widely applicable to various areas including crystallization of pharmaceutical compounds, formation of metal-organic frameworks, among others.

Physiological Characterizations and Biosynthetic Pathways of Fairy Chemicals in Plants

Jae-Hoon Choi*

1. Laboratory of Biological Chemistry, Faculty of Global Interdisciplinary Science and Innovation, Shizuoka University, 836 Ohya, Suruga-ku, Shizuoka 422-8529, Japan

2. Laboratory of Biological Chemistry, Research Institute of Green Science and Technology

3. Laboratory of Biological Chemistry, Research Institute for Mushroom Science

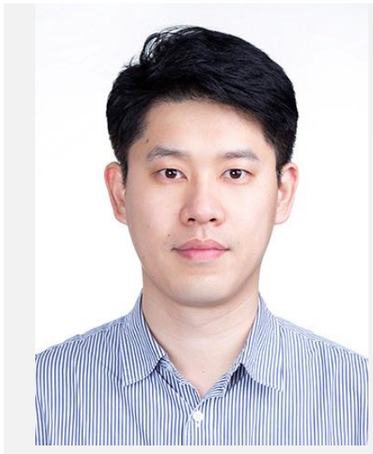
*Corresponding author: Prof. J.-H. Choi, choi.jaehoon@shizuoka.ac.jp

"Fairy rings" is a phenomenon of plants with excessive growth or death in the form of a ring. 2-Azahypoxanthine (AHX) and imidazole-4-carboxamide (ICA) were isolated as the fairy ring-inducing substances, and 2-aza-8-oxohypoxanthine (AOH) was obtained as a metabolite of AHX in rice.1-3 All the three compounds named fairy chemicals (FCs) regulated the growth of various plants and conferred stress tolerance to the plants. Moreover, FCs have been proven to be present endogenously in all the plants tested, suggesting the possibility that FCs are a novel family of plant hormone.3 It was revealed that FCs are biosynthesized from 5-aminoimidazole-4-carboxamide (AICA), a common member of the purine metabolism. Further metabolism of AICA in organisms had been unclear, indicating a novel purine metabolism on which FCs are biosynthesized. In this study, we conducted the following three studies using rice and Arabidopsis: 1) RNA-Seq analysis was performed when the production of FCs was increased by treatment with AICA, and candidate genes involved in FCs biosynthesis were identified by the analysis: 2) Metabolism of AHX to AOH is similar to that of xanthine to uric acid catalyzed by XDH; metabolic and gene expression studies using xdh1 and xdh2 mutants showed that xdh1 mutant contribute to oxidation at C-8 of AHX structure: 3) We isolated insensitive mutants to AICA and FCs from Arabidopsis mutants obtained by ethyl methyl sulfonate treatment and succeeded in obtaining some mutants that showed differences in the metabolism of FCs among them.

References

[1] Choi, J-H., et al., ChemBioChem, 11, 1373－1377, 2010
[2] Choi, J-H., et al., J. Agric. Food Chem., 58, 9956－9959, 2010
[3] Choi, J-H., et al., Angew. Chem. Int. Ed., 53, 1552－1555, 2014.

Active Learning-Based Optimization of Non-flammable Liquid Electrolytes for High-Performance Li-ion Batteries



Kosan Roh[1,*], Jaehyun Park[1], Taekeon Oh[1], Kihun An[1], Dung Tien Tuan Vu[1], Pius Appiah[1], Sangbaek Park[1], Woo-Jin Song[1], Seung-Wan Song[1]

1. Department of Chemical Engineering and Applied Chemistry, Chungnam National University

*Corresponding author: Prof. Kosan Roh, ksroh@cnu.ac.kr

The growing demand for lithium-ion batteries (LIBs) with high energy density and safety has become critical as the secondary battery market expands. However, optimizing the composition of battery materials (e.g., electrolytes) through iterative experiments is time-consuming and resource-intensive, primarily due to the lengthy cycle testing process. To address this challenge, a multi-objective constrained batch Bayesian optimization is developed for the highly efficient design of experiments targeting non-flammable liquid electrolytes for high-performance, safe LIBs. We introduce new performance metrics that reliably predict long-term cyclability using short-cycle data. Our probabilistic approach enables the design of efficient experiments—requiring only a few battery cycle tests—while optimizing battery performance and ensuring non-flammability. Using this method, we identified a new composition that improves retention by 6% at the 200th cycle compared to a heuristically optimized composition, achieving this with only 3% of the effort needed for a full factorial design.

A mathematical approach based on the volume-average theory for drip and espresso coffee extraction

Yoshihiko SANO[1]* and Fujio KUWAHARA[1]

1. Department of Mechanical Engineering, Shizuoka University,
3-5-1 Johoku, Naka-ku, Hamamatsu, 432-8561, Japan

*Corresponding author: Prof. Yoshihiko SANO, sano.yoshihiko@shizuoka.ac.jp

Coffee is loved all over the world, as evidenced by data showing that 500 million cups of Italian espresso coffee are drunk every day (Illy and Navarini, 2011). Coffee extraction is the complex mass transfer process that takes place between hot water and ground coffee beans when the water passes through a bed of coffee grounds. If a concentration equilibrium is not reached between the ground coffee beans and the coffee solution during coffee extraction, the taste (i.e. concentrations of the compounds contained in the coffee) would be varied by extraction conditions. Indeed, even when using the same type of bean, the taste of a drip coffee is quite different from that of an espresso coffee. In this study, a general set of macroscopic governing equations for coffee extraction, treating the coffee bed as a porous medium, were derived using the volume averaging theory (proposed by Vafai and Tien, 1981). Moreover, an appropriate dimensionless parameter, termed the “café number,” that controls mass transfer in the coffee extraction processes was proposed by normalizing the ordinary differential equations. Analytical formulas for the extraction of drip coffee and espresso coffee were derived to establish a prediction tool for coffee extraction. In this presentation, I will present the formulation of coffee extraction, citing parts of the presenter's paper (Y. Sano et al, 2019).

References

[1] Ernesto Illy, Luciano Navarini, Neglected food bubbles; The espresso coffee foam. *Food Biophys*. 6, 335-348, (2011).
[2] Vafai, K., and Tien, C. L., Boundary and inertia effects on flow and heat transfer in porous media. *Int. J. Heat Mass Transfer*. 24, 195-203, (1981).
[3] Y. Sano, S. Kubota, A. Kawarazaki, K. Kawamura, H. Kashiwai and F. Kuwahara, Mathematical model for coffee extraction based on the volume averaging theory, *Journal of Food Engineering*. 263, 1-12, (2019).

Microstructural Optimization of Ni-Rich Layered Cathodes for Durable High-Energy Lithium Batteries

Hoon-Hee Ryu[*]

Department of Chemical Engineering and Applied Chemistry, Chungnam National University, Daejeon, 34134, South Korea
E-mail: hryu@cnu.ac.kr

Among battery components, cathode chemistry is considered a defining feature because it primarily determines both battery cost and performance. Leveraging the advantageous intersection of $Li[Ni_{1-x-y}Co_xMn_y]O_2$ (NCM) and $Li[Ni_{1-x-y}Co_xAl_y]O_2$ (NCA) cathodes, $Li[Ni_{1-x-y-z}Co_xMn_yAl_z]O_2$ (NCMA) cathode chemistry is one of the practical directions for improving the durability of Ni-rich cathode materials. However, as the Ni content of commercial cathodes approaches over 90%, the simply composition-engineered NCMA cathode lacks chemical and mechanical stabilities to suppress the surface degradation and the development of permanent microcracking due to the high population of the highly reactive Ni^{4+} species.

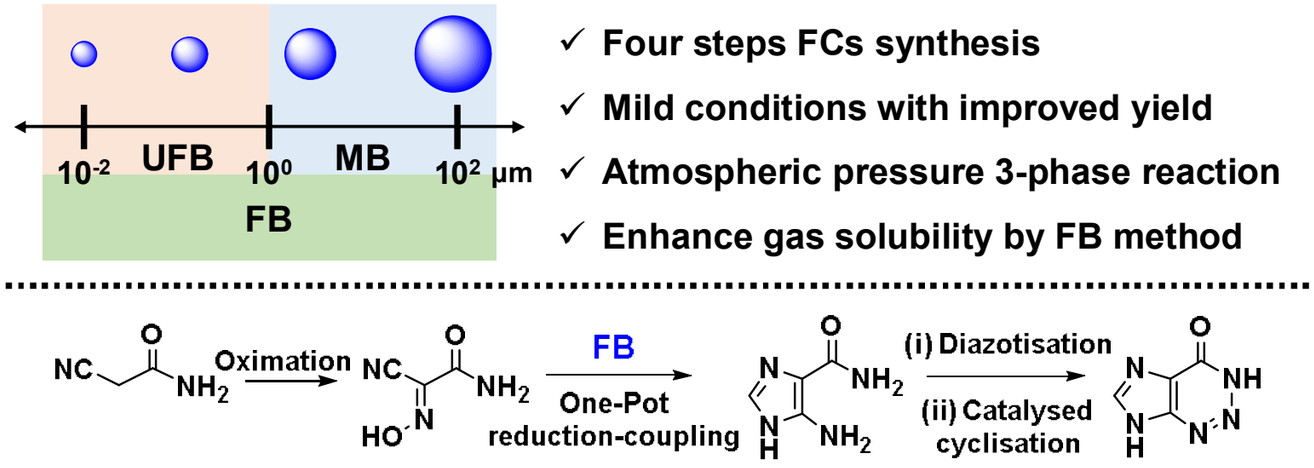
To suppress the development of microcracks on cathode materials, Ni-rich cathode materials should guarantee mechanical stability even in highly charged states. Although the mechanical stress arising from the anisotropic lattice volume change is inevitable, the stress-induced microcracking can be alleviated through the microstructure engineering of cathode materials. One of the most practical approach to suppress the damages from microcracking is tailoring primary particles of cathode materials to have an elongated shape with nanoscale size. In this presentation, Ni-rich layered cathodes through precision microstsructural control are presented.

Synthesis of novel plant hormones: Fine bubble and flow technology for fairy chemicals

Nobuyuki MASE

Research Institute of Green Science and Technology, Shizuoka University,
3-5-1 Johoku, Chuo-ku, Hamamatsu, Shizuoka 432-8561, Japan
mase.nobuyuki@shizuoka.ac.jp

Fairy chemicals (FCs), such as 2-azahypoxanthine (AHX), represent a potential new class of plant hormones, naturally occurring in plants and produced via a novel purine metabolic pathway. FCs contribute to plant resilience against various stresses and regulate plant growth. Despite their biological significance, efficient and sustainable synthetic routes remain limited. In this study, we developed a four-step method for synthesizing AHX from 2-cyanoacetamide, employing fine bubble and flow chemistry to enhance efficiency. Initially, oxime was synthesized from 2-cyanoacetamide via an oximation reaction. A cascade-type, one-pot selective Pt/C-catalyzed reduction of oxime, followed by a coupling reaction with formamidine acetate, afforded the intermediate 5-amino-1H-imidazole-4-carboxamide (AICA). Fine bubble technology significantly improved the conversion efficiency of oxime to AICA, achieving a 69% yield. Subsequently, 4-diazo-4H-imidazole-5-carboxamide (DICA) was synthesized from AICA via a diazotization reaction. Notably, we successfully obtained stable solid-state DICA, overcoming previous reports of instability. Finally, intramolecular cyclization of DICA, catalyzed by $PhI(OAc)_2$ (0.5 mol%) in water, yielded AHX with an overall yield of 47%. This study uses modern fine bubble and flow technologies to establish an efficient and scalable synthetic route for FCs. The process improves yield and selectivity and enhances environmental sustainability. These findings provide a foundation for further research on FCs and their agricultural applications, paving the way for future studies on their physiological roles and potential benefits in plant science.



References

[1] "Fine bubble technology for the green synthesis of fairy chemicals" Manna, A. K.; Doi, M.; Matsuo, K.; Sakurai, H.; Subrahmanyam, C.; Sato, K.; Narumi, T.; Mase, N., *Org. Biomol. Chem.* **2024**, *22* (17), 3396-3404. https://doi.org/10.1039/d4ob00237g; Featured as a Front Cover article.

Strategic Design of Molecular Acceptors for Short Wavelength Infrared Photodetection

Junhwan Lee, Hajeong Kim, Mengqiang, Alam Shabaz, Jaewon Lee*

Department of Chemical Engineering and Applied Chemistry

Chungnam National University

*Corresponding author: Prof. Jaewon Lee, jaewonlee@cnu.ac.kr

Organic semiconductors have recently emerged as promising materials for photodetection beyond the visible spectrum, offering unique advantages such as mechanical flexibility, tunable absorption profiles, and low-cost fabrication. In this work, we report the molecular design and synthesis of ultra-narrow bandgap organic semiconductors tailored for short-wave infrared (SWIR) photodetector applications. The fabricated SWIR organic photodetectors (OPDs) exhibit photoresponses in the 1000–1500 nm range. In addition to the material-level advances, we demonstrate the practical utility of these OPDs in two critical application domains: (1) **SWIR imaging**, where we obtain high-contrast images of concealed objects through non-visible barriers, and (2) **optical communication**, where our device enables real-time signal transmission using IR light.

The 4th CNU-SU Joint Symposium

DATE August, 1st 2025

VENUE Central Library

CONTENTS

Poster Session

No.	PRESENTERS	PRESENTATION TITLE
P-1-1	Yoshihito Hashino (SU)	Directed evolution of a crystalline chitin-binding domain into a PET-bin ding protein
P-1-2	Futa Morii (SU)	Search for metabolites of fairy chemicals in Cordyceps militaris
P-1-3	Saki Uchida (SU)	Studies on biosynthesis of fairy chemicals in rice
P-1-4	Yukino Yajima (SU)	Studies on the metabolism of AICA, a biosynthetic precursor of fairy chemicals, in rice
P-1-5	Akitsugu Yamada (SU)	Accuracy of the fiber-optic local void fraction estimation in vertical up ward gas–liquid two-phase flow
P-1-6	Rin Yamazaki (SU)	Identification and characterization of plasmids carrying carbapenem-resistance genes across clinical and environmental settings in the Philippines
P-2-1	Junhwan Lee (CNU)	Designing SWIR-Absorbing Non-Fullerene Acceptors for Organic Photodet ectors
P-2-2	Nguyen Bao Han (CNU)	Flame-Retardant Electrolyte Design for High-Nickel Cathode
P-2-3	Dan Ah Kim (CNU)	Formation of metal-organic cocrystal via DES-based surface nanodroplets
P-2-4	Yeonguk Kim (CNU)	Early-Stage Economic and Environmental Assessment for Emerging Chemi cal Technologies: Back-casting Approach
P-2-5	Jae Seong Kim (CNU)	Label-free bacterial enumeration in microfluidic droplets for single cell anti microbial susceptibility testing and its application to clinical samples
P-2-6	Jihyun Kim (CNU)	Enhanced Thermoelectric Performance via Synergistic Ionic Transport in M ixed Ionic–Electronic Conductive Films
P-2-7	Hajeong Kim (CNU)	SWIR Organic Photodetectors Utilizing IndanoneDerived Non-Fullerene Acc eptors with Malononitrile
P-2-8	Dong-Yeon Song (CNU)	Reprogramming the Genetic Code through Structure-Guided tRNA Rec ognition in a Cell-Free Protein Synthesis System
P-2-9	Hyeonho Song (CNU)	Effect of Chlorinated Feedstock on the catalytic performance of Pt/Zeolite during hydroisomerization
P-2-10	Gunoh Lee (CNU)	Performance Enhancement of Triboelectric Nanogenerators via Functionali zed Parylene Thin Films
P-2-11	Meng Qiang Li (CNU)	π-Bridge Engineering of Nonfullerene Acceptors for High-Performance Nea r-Infrared Organic Photodiodes Beyond 1200 nm
P-2-12	Eun Ju Lee Haneul Choi (CNU)	Prediction of Biological Activities for Small Molecules via Conjoint Mole cular Fingerprints and Deep Learning
P-2-13	In Woo Lee (CNU)	Improved electrochemical properties of activated carbon/nickel fluorid e electrode for hybrid supercapacitor
P-2-14	Jaeyu Lee (CNU)	3D micropatterning process using thermochromic polymer microfiber
P-2-15	Eungyeol Lim (CNU)	Molecular Interaction Tuning of Zwitterions for Rational Interface Passi vation in Perovskite Solar Cells

The 4th CNU-SU Joint Symposium

DATE August,1st 2025

VENUE Central Library

CONTENTS

Poster Session

No.	PRESENTERS	PRESENTATION TITLE
P-2-16	Geurin Kim (CNU)	Morphology-Driven Degradation and Stress-Relief Design in Ni-Rich Cathodes: Single-Crystal vs. Refined Polycrystal
P-2-17	Kanghyun Jo (CNU)	Doping Control of Mixed-Wall Carbon Nanotubes for Enhanced Thermoelectric Performance
P-2-18	Eunseon Chae (CNU)	Electrodeposited Co(OH)2 nanoflakes on O2 plasma-modified activated carbon for high performance supercapacitors
P-2-19	Seoyeong Cheon (CNU)	Preparatin of SiOx-void@C with a controlled SiOx composition via NF3 fluorination as a lithium-ion batteries anode material
P-2-20	Hyunsuk Choi (CNU)	Encapsulation Characteristics of Diverse Biomolecules in Membrane-Less Vesicle-Like Condensates Formed by Coacervate Rearrangement
P-2-21	Jaemin Han (CNU)	Biochemical Characterization of csTyr, an Organic Solvent–Tolerant Tyrosinase, for Enhanced Catechol Biosynthesis
P-2-22	Jueun Hwang (CNU)	Enhanced OER Performance of Zn-NiFe LDH Electrode Synthesized using One-pot precipitation in Alkaline water electrolysis

Directed evolution of a crystalline chitin-binding domain into a PET-binding protein

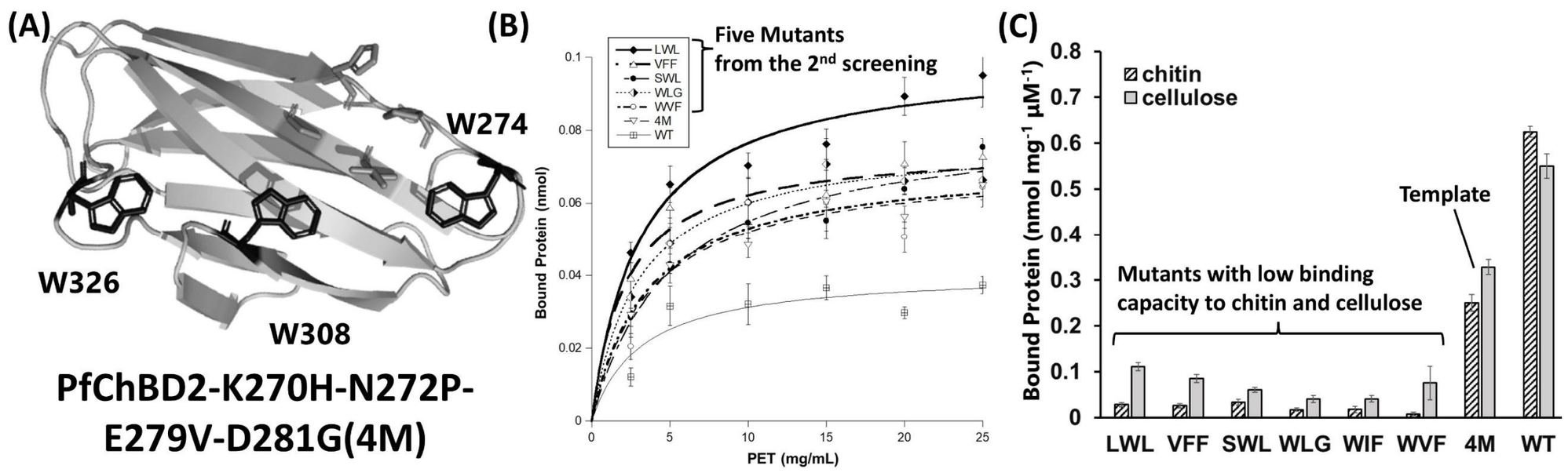
Yoshihito Hashino[1], Akihiko Nakamura[2*]

1. Department of Bioscience, Graduate School of Science and Technology, Shizuoka University

2. Research Institute of Green Science and Technology, Shizuoka University

*Corresponding author: Prof. Akihiko Nakamura, aki-naka@shizuoka.ac.jp

In recent years, plastic pollution on Earth has become a serious issue. Reducing the amount of plastic present in, and leaking into, the environment is crucial. Therefore, we aimed to develop a Polyethylene terephthalate (PET)-binding protein that can be used as a tool to specifically stain and detect only PET, and as a substrate-binding domain for PET-degrading enzymes. In this study, we developed an amorphous PET binding protein by phage display, using a chitin-binding domain from an archaeon *Pyrococcus furiosus* (PfChBD2) as a template. An M13 phage library displaying PfChBD2 mutants on the gIII protein were prepared by a saturation mutagenesis on the residues constructing chitin-binding surface (Fig. A). A single round of incubation, washing, elution and amplification against PET-film was repeated three times during the screening. In the first screening, three PfChBD2 mutant were obtained. One of them, which was PfChBD2-K270H-N272P-E279V-D281G (4M), showed solubility and higher affinity for PET than WT, but chitin binding capacity remained. In the second screening, three tryptophans of 4M were further mutated, and five mutants were obtained. They indicate binding affinity for PET was conserved or improved, and almost lost native-substrates binding ability (Fig. B, C). Therefore, we succeeded in evolving PfChBD2 into a PET-binding domain.



Search for metabolites of fairy chemicals in *Cordyceps militaris*

Futa MORII[1], Jae-Hoon CHOI[1-4*], Hirokazu KAWAGISHI[4,5*]
1. Grad. Sch. of Inte. Sci. and Tech., Shizuoka Univ.
2. Fac. Glob Int. Sci. Inno., Shizuoka Univ.
3. Res. Inst. Green Sci., Shizuoka. Univ.
4. Res. Inst, Mushroom Sci. Tech., Shizuoka Univ.
5. Fac. Agric., Shizuoka Univ.

*Corresponding author: Prof. Jae-Hoon CHOI, choi.jaehoon@shizuoka.ac.jp, Prof. Hirokazu KAWAGISHI, kawagishi.hirokazu@shizuoka.ac.jp

2-azahypoxanthine (AHX) and imidazole-4-carboxamide (ICA) were isolated from a fungus *Lepista sordida* that cause "fairy rings," a phenomenon in which turfgrass exhibits a ring-like pattern of growth or death[1,2]. AHX is metabolized to 2-aza-8-oxohypoxanthine (AOH) in plants[3]. The three compounds, AHX, AOH, and ICA, are collectively known as "fairy chemicals (FCs)" (Fig. 1). FCs are endogenous in many plants and mushrooms and have growth-regulating activity against all tested plants and mushrooms. Based on these findings, it has been hypothesized that FCs are a novel family of plant and mushroom hormones[4,5]. To evaluate this hypothesis, it is essential to study the detailed metabolic pathways and mechanisms of action of FCs. In rice, AHX is metabolized to AOH and then to glucose glycosides[6]. In contrast, little is known about how AHX is metabolized in fungi, except for in *L. sordida* from which AHX was originally isolated.

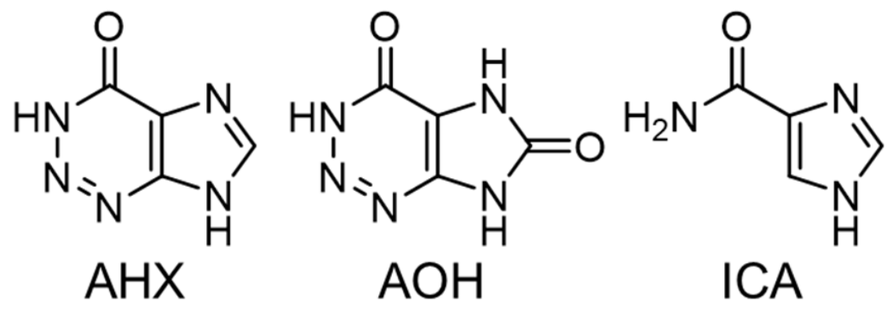


Fig. 1 The structures of FCs

In this study, we investigated the metabolism of AHX and AOH in *Cordyceps militaris*, an entomopathogenic fungus known to produce a variety of bioactive compounds.

[Methods and Results]

The mycelia of *C. militaris* were cultured in media supplemented with AHX or AOH, and the resulting culture filtrates were analyzed by UPLC, which revealed that AHX was converted to AOH and subsequently to unknown metabolites. To elucidate the structures of the metabolites, a large-scale culture of the fungus was performed and four compounds were isolated and structurally determined (Fig. 2). Furthermore, AOH and these metabolites were also detected by LC-MS/MS in the intact culture filtrate, indicating their endogenous production. Various bioassays are currently being conducted on these compounds.

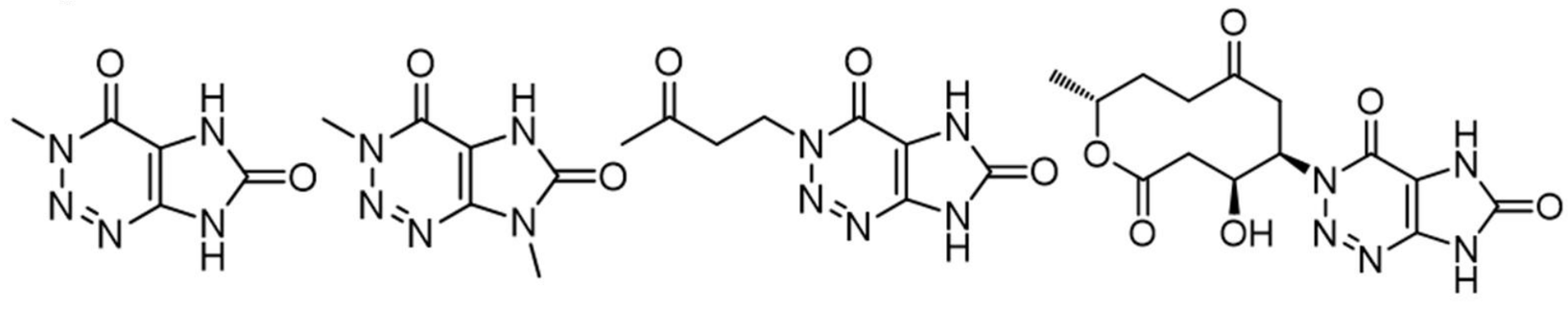
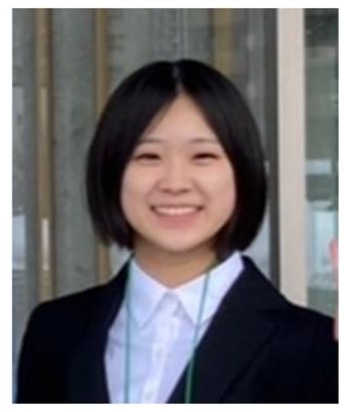


Fig. 2 The structures of novel AOH metabolites

References

1. J. H. Choi, *et al*., *ChemBioChem* **11**, 1373–1377 (2010)
2. J. H. Choi. *et al., J. Agric. Food. Chem.* **58**, 9956–9959 (2010)
3. J. H. Choi *et al., Angew. Chem. Int. Ed.* **53**, 1552–1555 (2014)
4. H. Kawagishi, *Biosci. Biotechnol. Biochem*. **82**, 752–758 (2018)
5. H. Kawagishi, *Proc. Jpn. Acad., Ser. B* **95**, 29–38 (2019)
6. J. H. Choi, *et al., Org. Lett.* **20,** 312–314 (2018)

Studies on biosynthesis of fairy chemicals in rice

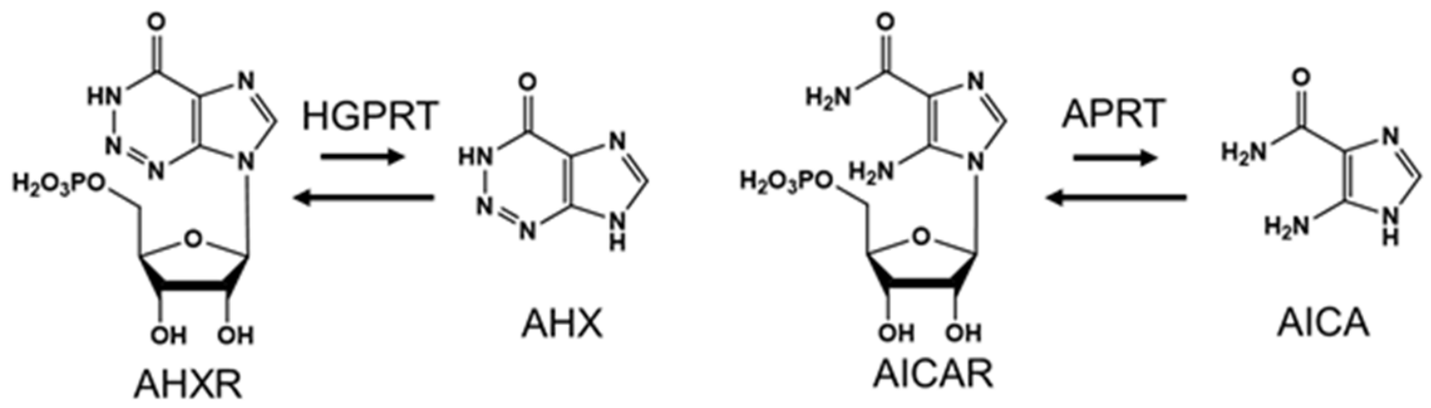


Saki UCHIDA[1] , Jae-Hoon CHOI[1-4*], and Hirokazu KAWAGISHI[4, 5*]
1. Grad. Sch. Inte. Sci. and Tech., Shizuoka Univ.
2. Fac. Glob. Int. Sci. Inno., Shizuoka Univ.
3 Res. Inst. Green Sci. Tech., Shizuoka Univ.
4. Res. Inst. Mushroom Schi. Tech., Shizuoka Univ.
5. Fac. Agr., Shizuoka Univ.
*Corresponding authors: Prof. Jae-Hoon CHOI, choi.jaehoon@shizuoka.ac.jp, Prof. Hirokazu KAWAGISHI, kawagishi.hirokazu@shizuoka.ac.jp

"Fairy rings" is a phenomenon where mushrooms appear after turfgrass grows or dies in a ring shape. We discovered 2-azahypoxanthine (AHX), imidazole-4-carboxamide (ICA), and 2-aza-8-oxohypoxanthine (AOH) as the principles that cause fairy rings, and named fairy chemicals (FCs)[1-3]. FCs are biosynthesized from 5-aminoimidazole-4-carboxanmide (AICA)[3]. The elimination and addition of phosphate groups of FCs ribonucleotides and AICA ribonucleotide are catalyzed by hypoxanthine-guanine phosphoribosyltransferase (HGPRT) and adenine phosphoribosyltransferase (APRT). However, the elimination reaction is much weaker than the addition reaction. Therefore, we hypothesized that there might be other enzyme(s) that catalyzes the elimination from AHX ribonucleotide (AHXR) and AICA ribonucleotide (AICAR). Our purpose in this study was to search for enzyme(s) other than HGPRT and APRT.

The crude enzyme solution extracted from cultured rice cells was fractionationated by ultrafiltration and ion-exchange chromatography. Enzyme activiy of the obtained fractions was measured using AHXR as a substrate and a fraction showed higher activity than the other fractions. Further fractionation of the fraction is now in progress.

References



[1] J. H. Choi, *et al*., *ChemBioChem* **11**, 1373–1377 (2010)
[2] J. H. Choi *et al., Angew. Chem. Int. Ed.* **53**, 1552–1555 (2014)
[3] Kawagishi, H., *Proc Japan Acad. Ser B*, **95**, 29-38 (2019)
[4] Ito, A. *et al*, *J Nat. Prod.* **83**, 2469-2476 (2020)

Studies on the metabolism of AICA, a biosynthetic precursor of fairy chemicals, in rice

Yukino YAJIMA[1)], Jae-Hoon CHOI[1-4)]*, Hirokazu KAWAGISHI [1,4)]*

1) Fac. Agr., Shizuoka Univ.

2) Fac. Glob Int. Sci. Inno., Shizuoka Univ.

3) Res. Inst. Green Sci., Shizuoka. Univ.

4) Res. Inst, Mushroom Sci. Tech., Shizuoka Univ.

*Corresponding authors: Prof. Jae-Hoon CHOI, choi.jaehoon@shizuoka.ac.jp, Prof. Hirokazu KAWAGISHI, kawagishi.hirokazu@shizuoka.ac.jp

The rings, ribbons, or arcs of stimulated plant growth and/or of the fruiting bodies of the larger fungi that often occur in floors of woodlands and agricultural or amenity grassland in most parts of the world are commonly called “fairy rings”. We have discovered 2-azahypoxanthine (AHX), imidazole-4-carboxamide (ICA), and 2-aza-8-oxohypoxanthine (AOH) that induce the phenomenon and refer to these compounds as fairy chemicals (FCs). [1-4] FCs regulate plant growth, resulting in the increase of crop yields. They have been suggested as a new family of plant hormones[4,5], although their detailed biosynthetic pathways and mechanisms of action have not yet been fully understood. The biosynthesis is presumed to originate from 5-aminoimidazole-4-carboxamide (AICA), a purine-related intermediate. However, most AICA is converted into non-FCs in rice when the plant was treated with AICA externally. In this study, we aimed to elucidate the AICA metabolic pathway and to identify compounds involved in it. We obtained a fraction with AICA-converting activity from cultured rice cells by successive chromatography and identified it as ascorbate peroxidase 1 or 2 (APX1 or 2) by MASCOT search.

Subsequent application of ascorbic acid to rice seedlings resulted in a significant increase in the accumulation of AOH in the shoot. These findings suggest that the APX-mediated oxidation of AICA may be competitively suppressed by the acid. Additionally, we are currently exploring metabolites other than FCs that are derived from AICA.

References

1. J. H. Choi, et al., *ChemBioChem* 11, 1373–1377 (2010)
2. J. H. Choi et al., *Angew. Chem. Int. Ed.* 53, 1552–1555 (2014)
3. J. H. Choi, et al., *J Agric Food Chem.* 58, 9956–9959, (2010)
4. H. Kawagishi, *Biosci. Biotechnol. Biochem.* 82, 752–758 (2018)
5. H. Kawagishi, *Proc. Jpn. Acad., Ser.* B 95, 29–38 (2019)

Accuracy of the fiber-optic local void fraction estimation in vertical upward gas–liquid two-phase flow

Akitsugu Yamada[1], Yuki Mizushima[1,2,*]

1. Graduate School of Integrated Science and Technology, Shizuoka University
   3-5-1 Johoku, Chuou-ku, Hamamatsu, 432-8561, Japan

2. Research Institute of Green Science and Technology, Shizuoka University
   3-5-1 Johoku, Chuou-ku, Hamamatsu, 432-8561, Japan

*Corresponding author: Prof. Yuki Mizushima, mizushima.yuhki@shizuoka.ac.jp

Gas–liquid two-phase flow is closely related to the operational safety of industrial equipment. For instance, in nuclear power plants, an increase in local void fraction can reduce the cooling performance of the reactor core[1], potentially leading to serious and catastrophic accidents. Therefore, the development of a real-time and high-accuracy measurement technique for local void fraction is of critical importance for the risk mitigation. Although previous studies have employed visualization technique[2], wire-mesh sensor[3], and X-ray imaging[4] to measure void fractions, these methods have inherent limitations in terms of pressure resistance, heat tolerance, chemical durability, and ease of installation in practical systems.

In this study, we focus on the optical fiber probe (OFP) method[5], which offers superior environmental resistance along with high spatial and temporal resolution. The measurement accuracy of the OFP method was validated through comparison with the conventional differential pressure method. Experiments were conducted using upward gas–liquid two-phase flow in a vertical acrylic pipe. The local void fractions obtained via the OFP method showed agreement with those from the differential pressure method within around ±15%. Furthermore, a difference was found in the time required for estimating local void fraction depending on the flow pattern.

References

[1] Issiki, N., et al., Developments in Thermal and Hydraulic Design of Reactors, (I), *J. At. Energy Soc. Jpn.*, **9**, 159-169 (1967).
[2] Higuchi, M., et al., Visualization of bubbly flow within a large diameter pipe and the fluctuation of local void fraction, *Journal of the Visualization Society of Japan*, **29**, 7-8 (2009) (*japanese*).
[3] Furuichi, H., et al., Measurement of void fraction and velocity distributions in a large diameter chimney at BWR nominal pressure and temperature, *Nucl. Eng. Des*, **424**, 113-147 (2024).
[4] Arai, T., et al., Research and development for understanding two-phase flow behavior inside a fuel bundle (10) Void redistribution behavior around spacers with swirl vanes in a rod bundle, *proc. 2024 Annual Meeting of Atomic Energy Society of Japan*, 2E19 (2022) (*japanese*).
[5] Mizushima, Y., et al., Measurement technique of bubble velocity and diameter in a bubble column via single-tip optical-fiber probing with judgment of the pierced position and angle, *Chem. Eng. Sci.*, **100**, 98-104 (2013).

Identification and characterization of plasmids carrying carbapenem-resistance genes across clinical and environmental settings in the Philippines

Rin Yamazaki[1], Maho Tokuda[2,3], Yuka Sato[1], Shunta Tsuruga[1], Isana Nogami[1], Zoe K Mallonga[4], Kazuhide Kimbara[1,2], Masato Suzuki[5], Masaki Shintani[1,3,6,7,*]

1. Graduate School of Integrated Science and Technology, Shizuoka University, Japan
2. Faculty of Science, Tokyo Metropolitan University, Japan
3. Faculty of Engineering, Shizuoka University, Japan
4. Division of Natural Sciences and Mathematics, University of the Philippines, Tacloban College, Philippines
5. AMR Research Center, NIID, JIHS, Japan
6. Japan Collection of Microorganisms, RIKEN BioResource Research Center, Japan
7. Research Institute of Green Science and Technology, Shizuoka University, Japan

*Corresponding author: Prof. Masaki Shintani, shintani.masaki@shizuoka.ac.jp

Plasmids can serve as vehicles of antimicrobial resistance genes (ARGs), which are often carried by the mobile genetic elements including transposons. Especially, the spread of carbapenem resistant bacteria poses a serious threat to global health, as carbapenems represent the last resort in the treatment of infections. To address this issue, it is essential to monitor plasmids conferring carbapenem resistance and elucidate their behavior in the environment. The problem is especially prevalent in regions with inappropriate antimicrobial usage and poor sanitation[1)].

In this study, we aimed to identify and characterize plasmids carrying carbapenem resistance genes in the Philippines. Microbial samples were collected from hospital wastewater treatment facilities and upstream/downstream sections of the river into which the wastewater is discharged, in Tacloban City, Philippines. Carbapenem-resistant bacteria were isolated from them. Additionally, exogenous plasmid capture was performed using *Metapseudomonas resinovorans* CA10dm4RGFP as a recipient. The complete nucleotide sequences of meropenem-resistant isolates and transconjugants were determined with both long-read and short-read sequencing.

A total of eight meropenem-resistant bacteria were isolated from hospital wastewater and six from river, and three complete genome sequences were determined. Among these, *Acinetobacter towneri* harbored a plasmid with the co-occurrence of $bla_{\text{NDM-1}}$ and *tet*(X7), conferring resistance to carbapenems and tigecycline[2)]. Another isolate, *Pseudomonas inefficax*, harbored a plasmid carrying $bla_{\text{VIM-2}}$, within a class 1 integron, which was also embedded in a Tn3-family transposon.

Furthermore, we obtained nine transferable plasmids from hospital and four from river by exogenous plasmid capture. Among these, plasmids classified under the IncC/P-3 group were commonly identified at hospital and river samples. In addition, they carried $bla_{\text{NDM-1}}$, which was flanked by IS*Aba125* or IS*110* family insertion sequence.

In conclusion, we identified plasmids carrying carbapenem-resistance genes not only from hospital wastewater but also from river in the Philippines. Currently, we are analyzing carbapenem-resistant bacteria from river water.

References

1) Hounmanou *et al*., 2025. Mitigating antimicrobial resistance through effective hospital wastewater management in low- and middle-income countries. *Front Public Health*, 12:1525873.

2) Mallonga et al., 2025. Emergence of *Acinetobacter towneri* harbouring a novel plasmid with $bla_{\text{NDM-1}}$ and *tet*(X7) from hospital wastewater in the Philippines. *J Glob Antimicrob Resist*, S2213-7165(25)00024-4.

Designing SWIR-Absorbing Non-Fullerene Acceptors for Organic Photodetectors

Junhwan Lee [1], Minyoung Jeong [2], Kilwon Cho[*2], Jaewon Lee[*1]

1. Department of Chemical Engineering and Applied Chemistry, College of Engineering, Chungnam National University,99. Daehak-ro(st), Yuseon-gu, Daegeon 34134, Republic of Korea

2. Center for Advanced Soft Electronics, Department of Chemical Engineering, Pohang University of Science and Technology, Pohang 37673, Republic of Korea

*Corresponding author: Prof. Jaewon Lee, jaewonlee@cnu.ac.kr

Prof. Kilwon Cho, kwcho@postech.ac.kr

SWIR organic photodetectors (OPDs) have become a central focus in diverse technological fields, including image sensing, medical imaging, and optical communications. As their absorption spectrum extends deeper into the long-wavelength region, these devices continue to find new potential applications. Nevertheless, there remains a scarcity of non-fullerene acceptors (NFAs) exhibiting photoresponsive properties beyond 1000 nm. In our quest to improve molecular charge transfer dynamics, we have initiated the creation of a series of materials based on the acceptor-donor-acceptor-donor-acceptor (A-D-A-D-A) framework. This approach involves modifying the functional groups of the core acceptor, resulting in materials characterized by bandgaps (Eg) below 1.0 eV.

Flame-Retardant Electrolyte Design for High-Nickel Cathode

Nguyen Bao Han,[a,§] Dongmyeong Kim,[b,§] Yen Hai Thi Tran,[a]

Chunjoong Kim,[b*] Seung-Wan Song [a*]

[a] *Dept. of Chemical Engineering & Applied Chemistry, Chungnam National University*

[b] *Dept. of Materials Science & Engineering, Chungnam National University*

[§] *These authors equally contributed to this work*

Developing a lithium-ion battery (LIB) that is safe, affordable, long-lasting, and has a higher energy density than state-of-the-art ones has been pursued to increase the market acceptability of electric vehicles. Because of the high specific capacity and moderate cost of low-Co cathode active materials, high-Ni $LiNi_xCo_yMn_zO2$ (NCM; $x \geq 0.9$) compounds are one of the most promising active materials for high energy density LIBs. However, the detrimental cathode-electrolyte instability, continual irreversible phase transition and metal-dissolution lead to the poor cycle and rate performance in the high-Ni cathode. Furthermore, the high flammability of traditional organic liquid electrolyte for high-Ni LIBs is a cause of the risk of thermal runaway and battery fire. To ensure the safety and performance, we conducted electrolyte engineering to achieve a flame-retarding liquid electrolyte formulation suited for a graphite//high-Ni LIB. Fundamental understanding of well-working mechanisms behind the interfaces of cathode-electrolyte and anode-electrolyte will be discussed in this presentation.

Formation of metal-organic cocrystal via DES-based surface nanodroplets

Dan Ah Kim, Ji Woo Seo, Jae Bem You*

Department of Chemical Engineering, Chungnam National University

*Email: jb.you@cnu.ac.kr

Cocrystal is a material in which two or more types of molecules form a crystal together to form a single complex crystal structure. In particular, since each molecular species that makes up the produced cocrystal has a specific stoichiometric ratio, it contributes to changes in physical properties such as the melting point of the cocrystal or in the shape of the crystal depending on the substance used. Recently, we have shown the formation of metal-organic cocrystals through liquid-liquid extraction using surface nanodroplets with a femtoliter volume grown from the substrate surface.[1] The surface nanodroplets were composed of Deep Eutectic Solvent (DES), which are substances composed of hydrogen bond donors (HBDs) and hydrogen bond acceptors (HBAs). When HBD and HBA are mixed at a certain ratio, they have the same eutectic point and form a solvent. Among the various DESs, a carboxylic acid-based DES was used to form the cocrystals through metal-ligand bonding during the extraction process from inorganic aqueous solutions. Herein, we demonstrate the changes in cocrystals formed according to the components of DES-based surface nanodroplets. The type of carboxylic acids(different number of carbon atoms or the molecular structure) affects the shape of the cocrystals formed and the amount of metal ions composing the crystals. It is expected that the technology presented in this study can be applied to various fields which require delicate synthesis of materials such as semiconductors and catalyst engineering by controlling the properties.

Keywords: cocrystal, crystallization, surface nanodroplets, deep eutectic solvents

Reference

1. E. Lim, B. Kim, M. S. Oh, J. B. You, *J. Colloid Interface Sci.*, 643, 82-91 (2023).

Early-Stage Economic and Environmental Assessment for Emerging Chemical Technologies: Back-casting Approach

Yeonguk Kim[1], Kosa Roh[1,*]

1. Department of Chemical Engineering and Applied Chemistry, Chungnam National University, Daejeon 34134, Republic of Korea

*Corresponding author: Prof. Kosan Roh, ksroh@cnu.ac.kr

The emergence of alternative chemical technologies has made their reliable economic and environmental assessments indispensable for guiding future research and development. However, these assessments are inherently challenging due to the lack of comprehensive understanding and technical knowledge of such technologies, particularly at low technology readiness levels (TRLs). This knowledge gap complicates accurate predictions of their real-world performance, economics, and potential environmental impacts. To address these challenges, we adopt a back-casting approach to demonstrate a TRL-based early-stage evaluation procedure, as previously proposed by Roh et al1). (2020, Green Chem. 22, 3842). In this work, we apply this framework to methanol production based on the reforming of natural gas, which is a mature chemical technology, to explore its suitability for evaluating emerging chemical technologies. The target technology is assumed to be at three stages of maturity: theoretical, intermediate, and engineering stages. We analyze economic and environmental indicators of the technology using the available information at each stage and then see how similar the indicators calculated at the theoretical and intermediate stages are compared to those at the engineering stage. The analysis shows that the performance indicators are lowest at the theoretical stage due to relying solely on reaction stoichiometry. In the case of the intermediate stage, despite considering various factors, it yields slightly higher performance indicators than the engineering stage due to the lack of process optimization. The outcomes of this study enable a proactive assessment of emerging chemical technologies, providing insights into their feasibility at various stages of development.

References

[1] Alayoglu, S., Nilekar, A. U., Mavrikakis, M. & Eichhorn, B. Ru–Pt core–shell nanoparticles for preferential oxidation of carbon monoxide in hydrogen. *Nat. Mater.* **7**, 333-338, (2008).

Label-free bacterial enumeration in microfluidic droplets for single cell antimicrobial susceptibility testing and its application to clinical samples

Jae Seong Kim[1], and Chang-Soo Lee[1,*]

1. Department of Chemical Engineering and Applied Chemistry, Chungnam National University

*Corresponding author: Prof. Chang-Soo Lee, rhadum@cnu.ac.kr

Bacterial communities exhibit significant heterogeneity, resulting in the emergence of specialized phenotypes that can withstand antibiotic exposure. Unfortunately, the existence of subpopulations resistant to antibiotics often goes unnoticed during treatment initiation. Thus, it is crucial to consider the concept of single-cell antibiotic susceptibility testing (AST) to tackle bacterial infections.

We present a droplet-based microfluidic approach for phenotypic antimicrobial susceptibility testing (AST) by determining minimum inhibitory concentration (MIC). Droplets are produced from the microfluidic device, where concentration gradient of antibiotic solution is formed and loaded into droplets with bacteria samples. We analyzed the susceptibility of bacteria under different antibiotic conditions at the single-cell level by enumeration of bacteria in droplets without additional labelling process through automated image analysis. Several clinical isolates of *staphylococcus aureus* are tested to demonstrate the clinical applicability of our microfluidic system. MIC values of commonly used antibiotics are obtained within 3 hours, which showed categorical agreement with reference MICs determined by conventional broth microdilution method. In addition, monitoring of single cells encapsulated in individual droplets revealed a distribution of resistant levels within population of identical cells, which may account for the existence of phenotypic heterogeneity in isogenic population. Due to the capability of absolute bacteria quantification, we believe that our method has the potential to be used in clinically relevant applications offering the information of MICs and heterogeneities for personalized treatment guidelines.

References

[1] Kim, J. S., Kim, J., Kim, J. S., Kim, W., & Lee, C. S. Label-free single-cell antimicrobial susceptibility testing in droplets with concentration gradient generation. *Lab Chip*, **24**, 5274-5289 (2024).

Enhanced Thermoelectric Performance via Synergistic Ionic Transport in Mixed Ionic–Electronic Conductive Films

Jihyun Kim[1], Kanghyun Jo[1], Byeonggwan Kim[1,*]

1. Department of Chemical Engineering and Applied Chemistry, Chungnam National University, 99 Daehak-ro, Yuseong-gu, Daejeon, South Korea

*Corresponding author: Prof. Byeonggwan Kim, bg_kim@cnu.ac.kr

Mixed ionic-electronic conductors have attracted significant attention due to the synergy of high conductivity and sustained power output via electron transport, coupled with outstanding thermovoltage through ion diffusion. Herein, the polymer matrix poly(3,4-ethylenedioxythiophene):poly(styrene sulfonate) (PEDOT:PSS) combined with hard lewis acid to form thermoelectric-ionic conductors. The coordination characteristics of tetravalent cations facilitated proton transport based on the Grotthuss mechanism, while the interactions between the inorganic salt and the conductive polymer formed ionic pathways that enabled enhanced cation diffusion. Spectroscopic characterization confirmed that the introduction of Lewis acid salts induced the oxidation of PEDOT, leading to an increased formation of polarons and bipolarons, as well as enhanced structural stability. Thermoelectric performances of tetravalent-cation-doped proton transport conductor (TPC) films were optimized by precisely controlling the relative humidity (RH) and the aggregation of inorganic salts. Among these, the TPC3 film exhibited remarkable Seebeck coefficient of 23.6 mV K^{-1} and a ionic conductivity of 378.6 mS cm^{-1} under conditions of 90% RH and room temperature. Taking advantage of high performace and excellent voltage stability, TPC3 based ionic thermoelectric supercapacitor and flexible module-type thermoelectric harvester with ten legs were fabricated. This suggests a promising direction for efficient and synergistic thermoelectric energy harvesting even under low-grade thermal conditions.

References

[1] Cho C., Kim B., Park S., Kim E. Bisulfate transport in hydrogels for self-healable and transparent thermoelectric harvesting films. *Energy Environ. Sci.* **15**, 2049, (2022).
[2] Kim B., Na J., Lim H., Kim Y., Kim J., Kim E. Robust high thermoelectric harvesting under a self-humidifying bilayer of metal organic framework and hydrogel layer. *Adv. Funct. Mater.* **31**, 2105297, (2021).

SWIR Organic Photodetectors Utilizing IndanoneDerived Non-Fullerene Acceptors with Malononitrile

Hajeong Kim [1], Minyoung Jeong [2], Kilwon Cho[*2], Jaewon Lee[*1]

1. Department of Chemical Engineering and Applied Chemistry, College of Engineering, Chungnam National University,99. Daehak-ro(st), Yuseon-gu, Daegeon 34134, Republic of Korea

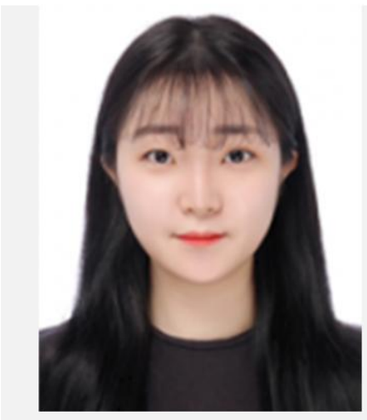
2. Center for Advanced Soft Electronics, Department of Chemical Engineering, Pohang University of Science and Technology, Pohang 37673, Republic of Korea

*Corresponding author: Prof. Jaewon Lee, jaewonlee@cnu.ac.kr

Prof. Kilwon Cho, kwcho@postech.ac.kr

Photodetectors are devices that transduce light into electrical signals and find applications across various fields requiring light-sensing technology, such as medical imaging, environmental monitoring, and camera systems. Active layers based on inorganic semiconductors still face drawbacks, including high fabrication costs, bulkiness, and pronounced dark-current issues. This has spurred ongoing efforts to employ organic semiconductors as viable alternatives. In this work, we concentrate on the synthesis of non-fullerene acceptors (NFAs) for organic photodetectors, which afford extended absorption and superior thermal robustness. One of the synthesized compounds exhibits a narrow bandgap of 0.85 eV, underscoring its strong promise for SWIR detection.

Reprogramming the Genetic Code through Structure-Guided tRNA Recognition in a Cell-Free Protein Synthesis System



Dong-Yeon Song[1], Dong-Myung Kim[1,*]

1. Department of Chemical Engineering and Applied Chemistry, Chungnam National University

*Corresponding author: Fax: +82-42-822-6637 E-mail address: dmkim@cnu.ac.kr

Aminoacyl-tRNA synthetases (aaRSs) usually recognize amino acids via tRNA anticodons. However, group III aaRSs instead recognize structural elements like the T-loop. Leveraging this, we reassigned the tryptophan codon by altering the anticodons of these tRNAs in a cell-free protein synthesis system. We hypothesized that their aaRSs would still charge the modified tRNAs, allowing the incorporation of alanine, serine, or leucine at tryptophan positions. To test this, we used a tryptophan-free system and superfolder GFP (sfGFP) as a model protein. Fluorescence intensity indicated successful incorporation of the reassigned amino acids. Notably, incorporation efficiency varied among tRNA species, even for the same amino acid, suggesting that additional factors influence charging and incorporation. This study demonstrates the potential of using tRNA structural recognition for codon reassignment and offers insights into optimizing tRNA engineering for synthetic biology applications.

References

[1] S. Cusack, Aminoacyl-tRNA synthetases, Curr. Opin. Struct. Biol. 7, 881-889(1997).

[2] R. B. Ganesh and S. J. Maerkl, Biochemistry of Aminoacyl tRNA Synthetase and tRNAs and Their Engineering for Cell-Free and Synthetic Cell Applications, Front. Bioeng. Biotechnol. 10, 918653(2022).

Effect of Chlorinated Feedstock on the catalytic performance of Pt/Zeolite during hydroisomerization

Hyeonho Song, Sungtak Kim*

Department of Chemical Engineering and Applied Chemistry, Chungnam National University, Daejeon, Korea

*Corresponding author: Prof. Sungtak Kim, sunnykim@cnu.ac.kr

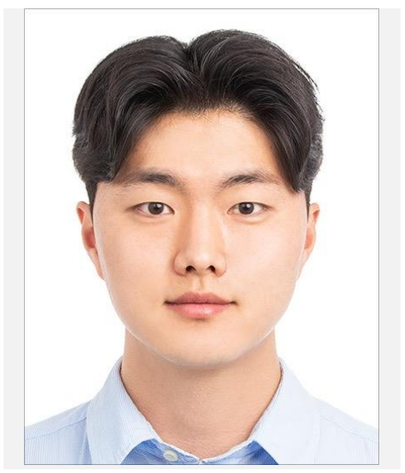
The presence of chlorine-containing compounds in waste plastic pyrolysis oil poses a critical challenge to hydroprocessing, particularly in hydroisomerization reactions over noble metal-supported zeolites. This study investigates the influence of chlorine on hydroisomerization performance using a 0.5 wt% Pt/Zeolite Y(30) catalyst. To simulate chlorinated pyrolysis oil, a model feedstock was prepared by blending hexadecane with chlorohexadecane to achieve a chlorine concentration of 2000 ppm. Two sets of experiments were conducted: one using pure hexadecane and the other using the chlorinated feedstock.

The hydroisomerization reactions were carried out in a fixed-bed reactor at temperatures ranging from 250 ℃ to 270 ℃, a pressure of 20 bar, a H_2-to-hydrocarbon molar ratio of 10, and a weight hourly space velocity (WHSV) of 5 h^{-1}. Reaction products were analyzed by gas chromatography with flame ionization detection (GC-FID) to assess catalytic activity and selectivity.

Post-reaction characterization was performed using ammonia temperature-programmed desorption (NH_3-TPD), pyridine-adsorbed infrared spectroscopy (Py-IR), temperature-programmed oxidation (TPO), and CO chemisorption. The results indicated that chlorine exposure led to a significant reduction in Brønsted acid sites and overall acid site concentration, as well as a notable increase in coke formation, particularly on the external surface of the catalyst. Additionally, a decrease in Pt dispersion and CO uptake suggested that chlorine negatively affected the metallic function of the catalyst.

These findings provide insights into the dual deactivation mechanisms—acidity loss and metal deactivation—induced by chlorine and emphasize the importance of chlorine-tolerant catalyst development for the efficient recycling of chlorinated waste plastics.

Performance Enhancement of Triboelectric Nanogenerators via Functionalized Parylene Thin Films



Gunoh Lee[1], Minsoo P. Kim[2,3], Hyunhyub Ko[3,*], Kyung Jin Lee[1,*]

1. Department of Chemical Engineering and Applied Chemistry, College of Engineering, Chungnam National University, Daejeon, Republic of Korea

2. Department of Chemical Engineering, Sunchon National University, Suncheon, Republic of Korea

3. School of Energy and Chemical Engineering, Ulsan National Institute of Science and Technology (UNIST), Ulsan, Republic of Korea

*Corresponding author: Prof. Kyung Jin Lee, kjlee@cnu.ac.kr, Prof. Hyunhyub Ko, hyunhko@unist.ac.kr

The growing demand for self-powered intelligent systems such as wearable, implantable, and sensor devices emphasizes the need for compact, energy-autonomous solutions like triboelectric nanogenerators (TENGs). Flexible and stretchable devices increasingly rely on organic materials due to their mechanical advantages over inorganics. Among various performance-determining factors, the dielectric permittivity of the polymer is particularly crucial.

In this study, we designed a bilayer polymer system composed of PDMS embedded with multi-walled carbon nanotubes (MWCNTs) and a surface-coated parylene-based dielectric layer. To enhance the interfacial polarization effect—which significantly influences the overall dielectric response—we functionalized parylene via simple organic reactions during the dimer synthesis step. Dipolar functional groups such as hydroxyl and amino moieties were introduced into the [2.2]paracyclophane precursor to yield high-permittivity parylene derivatives.

The resulting functionalized parylene films were deposited using a chemical vapor deposition (CVD) process, ensuring uniform, pinhole-free coatings. When layered on MWCNT-dispersed PDMS, the bilayer architecture promoted strong interfacial polarization, effectively enhancing the system's dielectric constant.

TENGs fabricated with this bilayer structure demonstrated a significant improvement in output power, with values ranging from 30 to over 5,000 times higher than those reported for conventional parylene (2.2–18 mW/cm²) or PDMS-based (0.0013–2.5 mW/cm²) triboelectric devices. This work presents a straightforward yet effective strategy to improve TENG performance by molecularly engineering the dielectric interface through functionalized parylene coatings.

References

[1] Kim, M. P., Lee, G., Noh, B., Kim, J., Kwak, M. S., Lee, K. J., Ko, H. Enhancing energy harvesting performance of bilayered parylene triboelectric nanogenerators through interfacial polarization. *Nano Energy*. **119**, 109087, (2024).

π-Bridge Engineering of Nonfullerene Acceptors for High-Performance Near-Infrared Organic Photodiodes Beyond 1200 nm

Meng Qiang Li [1], Minyoung Jeong [2], Kilwon Cho[*2], Jaewon Lee[*1]

1. Department of Chemical Engineering and Applied Chemistry, College of Engineering, Chungnam National University,99. Daehak-ro(st), Yuseon-gu, Daegeon 34134, Republic of Korea

2. Center for Advanced Soft Electronics, Department of Chemical Engineering, Pohang University of Science and Technology, Pohang 37673, Republic of Korea

*Corresponding author: Prof. Jaewon Lee, jaewonlee@cnu.ac.kr

Prof. Kilwon Cho, kwcho@postech.ac.kr

Organic photodiodes (OPDs) sensitive to the near-infrared (NIR-II) region (>1000 nm) are promising for biomedical sensors and optical communication but suffer from limited responsivity and high dark current. Here, we systematically engineered π-bridge units of nonfullerene acceptors (NFAs) to enhance intramolecular charge transfer (ICT) and extend absorption beyond 1200 nm. Three novel NFAs—FCTT2-F, FCTCN-F, and FCCN2-F—were synthesized by replacing the thienothiophene (TT) π-bridge with cyano thiophene (TCN). Density functional theory (DFT) calculations and optical analysis showed the optical bandgap reduced from 1.12 to 1.05 eV, improving NIR absorption. Grazing-incidence X-ray scattering (GIWAXS) and atomic force microscopy (AFM) revealed suppressed molecular aggregation, leading to efficient charge dissociation. The optimized FCCN2-F OPD achieved a high detectivity (3.43×10^{11} Jones), fast response (58.6 kHz), and low dark current at 1050 nm under –2 V bias. Practical demonstrations in photoplethysmography (PPG) and optical wireless communication validated the device's excellent sensitivity and real-time performance, highlighting π-bridge engineering as a powerful approach for advanced NIR-II OPDs.

Prediction of Biological Activities for Small Molecules via Conjoint Molecular Fingerprints and Deep Learning

Eun Ju Lee†[1], Haneul Choi†[1], Hae-Min Park[1,*]

1. Department of Chemical Engineering and Applied Chemistry, Chungnam National University, Daejeon, Korea

† These authors contributed equally to this work

*Corresponding author: Prof. 박해민, haemin.park@cnu.ac.kr

Predicting the bioactivity of compounds that can exert various biological effects in vivo is a critical task in drug discovery and related fields. To fulfill this need, a growing body of machine learning research has aimed at making accurate predictions. In this study, we developed a model, which harnesses conjoint molecular fingerprints and deep learning methods, to enable more accurate prediction of biological activities for small molecules. The predictive performance was assessed on a test dataset of 450 small molecules with hemolytic toxicity by using machine learning and deep learning methods, which include k-nearest neighbors (KNN), support vector machine (SVM), random forest (RF), gradient boosting machine (GBM), and deep neural network (DNN). The results showed that the DNN algorithm trained with the conjoint fingerprint - a combination of extended connectivity fingerprint, up to four bonds (ECFP4) and MinHash fingerprint, up to six bonds (MHFP6), achieved the highest performance in terms of precision, recall, accuracy, and model robustness. We applied the model to predicting sedative-hypnotic activity for small molecules, observing an F1 score of 0.939 ± 0.008, Mattews correlation coefficient (MCC) of 0.801 ± 0.026, and the area under the receiver operating characteristic curve (AUC) of 0.973 ± 0.005 at a 95% confidence level. Despite relying on compound structure for classification, our method has demonstrated strong performance across diverse small molecule datasets with various bioactivities. These results suggest the possibility of saving time and resources while discovering the activity of new substances within the biosimulation process.

References

[1] Zheng, S., Wang, Y., Liu, H., Chang, W., Xu, Y., & Lin, F. (2019). Prediction of hemolytic toxicity for saponins by machine-learning methods. *Chemical Research in Toxicology*, *32*(6), 1014-1026.

Improved electrochemical properties of activated carbon/nickel fluoride electrode for hybrid supercapacitor

In Woo Lee[1], Seongjae Myeong[1], Seoyoung Cheon[1], Eunseon Chae[1], and Young-Seak Lee[1,2,*]

1. Department of Chemical Engineering and Applied Chemistry, Chungnam National University, Daejeon, 34134, Republic of Korea

2. Institute of Carbon Fusion Technology (InCFT), Chungnam National University, Daejeon, 34134, Republic of Korea

*Corresponding author: Prof. Young-Seak Lee, youngslee@cnu.ac.kr

Supercapacitors (SCs) are increasingly recognized as promising electrochemical energy storage devices, especially in applications that involve intermittent renewable energy sources such as solar or wind power. In this work, we present a simple and efficient approach to synthesize nickel fluoride-doped activated carbon ($AC@NiF_2$) by combining nickel impregnation with thermal fluorination using nitrogen trifluoride (NF_3) gas. The high reactivity of NF_3 enables rapid formation of NiF_2 on the surface of activated carbon. During electrochemical cycling, NiF_2 undergoes reversible redox reactions that lead to the formation of nickel oxyfluorides and induce mixed-valence states in the nickel component. These characteristics substantially enhance the electrochemical performance of the electrode. When used as a positive electrode in a three-electrode system, the $AC@NiF_2$ material demonstrated a high specific capacitance of 357.1 F/g at a current density of 1 A/g, indicating excellent charge storage capability. Furthermore, a hybrid supercapacitor (HSC) was constructed using $AC@NiF_2$ as the positive electrode and pristine activated carbon as the negative electrode. This device achieved a specific capacitance of 87.1 F/g at 1 A/g, along with an impressive energy density of 33.9 Wh/kg and a power density of 2000 W/kg at a working voltage of 1.5 V. These findings highlight the advantages of transition metal fluoride-carbon composites for supercapacitor applications. This study provides a promising

pathway toward the development of advanced electrode materials for next-generation energy storage and conversion systems.

References

[1] Oh, Ji., Lim, E., Chun, J., Jo, C., Nickel fluoride (NiF_2)/porous carbon nanocomposite synthesized via ammonium fluoride (NH_4F) treatment for lithium-ion battery cathode applications. *J. Power Sources.* **521**, 230935 (2022).

3D micropatterning process using thermochromic polymer microfiber

Jaeyu Lee[1], Kyung Jin Lee[1,*]

1. Department of Chemical Engineering and Applied Chemistry, College of Engineering, Chungnam National University, 99 Daehak-ro, Yuseong-gu, Daejeon, 34134, Republic of Korea

*Corresponding author: Prof. Kyung Jin Lee, kjlee@cnu.ac.kr

Thermochromism is currently commercialized phenomenon in various fields which can make response to heat such as cup, heat sensor, smart window, etc. Here, we manufacture 3D thermochromic micropatterns and structures using polymer microfiber via charge reversal electro-jet writing method with conventional 3D printer. Thermochromic pigments of various colors are dispersed homogenously in polymer microfiber and their representative colors are displayed successfully in the polymer 3D structure, changing color state reversibly at a quick response depending on the temperature. By simply mixing two color pigments with different thermochromic temperature ranges or fabricating bicompartmental microfiber structure, multiple color phases including combined color state can be shown in a single structure through temperature change. Not only color variations, 3D printing process using the 3D printer also enables various kinds of visible expressions in 3D patterns by diverse patterning methods. Desired specific letter or symbol can be hidden or emphasized in a ordinary pattern using same color pigments which have different thermochromic temperature ranges, and polymer types are not limited to manufacture thermochromic 3D structure maintaining the characteristic properties of each polymer. Furthermore, Joule heating can also cause color changing reaction by indirect heat using conductive metal wire connected with 1.5 V battery. These 3D thermochromic polymer micropatterns can be applied to anti-counterfeiting, wearable heat sensing patch, and other diverse areas.

References

[1] Jaeyu Lee, Kyung Jin Lee, 3D micropatterning with thermochromic polymer microfiber. *Adv. Mater. Technol.* **10**, 2401344, (2025).

Molecular Interaction Tuning of Zwitterions for Rational Interface Passivation in Perovskite Solar Cells

Eungyeol Lim, Seulki Song*

1. Department of Chemical Engineering and Applied Chemistry, Chungcam National University(CNU)

*Corresponding author: Prof. Seulki Song, sksong@cnu.ac.kr

Enhancing the efficiency and stability of perovskite solar cells (PSCs) requires effective passivation of perovskite crystals. Zwitterions, characterized by their dual positive and negative charges within a single molecule, have shown promise as passivating agents. However, conventional solid-type zwitterions suffer from poor solubility in organic solvents due to strong intermolecular interactions, hindering uniform film formation and adversely affecting perovskite crystallization. In this study, a liquid-type zwitterion (LTZ) was designed to alleviate these limitations by tuning the intermolecular interactions of 3-(1-Pyridinio)-1-propanesulfonate. This modification significantly enhanced the solubility and processability of the zwitterion in common organic solvents. The uniform LTZ-passivated films facilitated superior charge transport and defect reduction compared to devices treated with solid-type zwitterions. Consequently, the LTZ-based PSC achieved an impressive power conversion efficiency (PCE) of 24.9% with outstanding thermal stability, retaining over 80% of its initial performance after 1968 hours at 60 °C in an inert N_2 atmosphere. Furthermore, a large-area module (active area of 32.7 cm^2) exhibited a notable PCE of 19.86%, accompanied by a high open-circuit voltage and fill factor. These findings highlight that LTZ-based interface engineering is a viable approach for realizing high-performance and durable PSCs.

References

[1] *Adv. Energy Mater.*, **2024**, *14*, 2401263

Morphology-Driven Degradation and Stress-Relief Design in Ni-Rich Cathodes: Single-Crystal vs. Refined Polycrystal

*Geurin Kim, Jeong Eun Kim,and Hoon-Hee Ryu**

Department of Chemical Engineering and Applied Chemistry, Chungnam National University, Daejeon, 34134, South Korea

Ni-rich layered $[Ni_{1-x-y}Co_x(Mn \text{ and/or } Al)_y]O_2$ (NCM, NCA, and NCMA) materials are mainstream for application as cathodes in next-generation EV batteries. However, the higher the Ni content in cathode materials, the poorer are their cycling stability and thermal stability, which adversely affect the reliability of LIBs. Especially, the microcracking of Ni-rich cathode materials in deeply charged states substantially increases the surface areas of the cathode materials exposed to parasitic side reactions, thus accelerating cathode deterioration and loss of electrochemical activity. Unlike conventional Ni-rich layered cathode particles that consist of numerous nano-sized grains, single-crystal cathode particles are promising because they are not vulnerable to microcracking due to the absence of intergranular boundaries. However, generally, a decrease in particle size increases the risk of surface degradation from the high surface-to-volume ratio. In addition, the kinetic properties of single-crystal cathodes are also largely influenced by the morphology and size distribution of the single crystals.

In this poster, we investigates a refined polycrystalline design (CSG-NCM90) with radially aligned primary grains, which is hypothesized to relieve internal stress and enhance both structural and electrochemical stability. Through a comparative analysis of SC, PC, and CSG morphologies under identical cycling conditions, we provide insights into morphology-driven degradation and propose CSG as a practical design solution for durable Ni-rich cathodes.

Doping Control of Mixed-Wall Carbon Nanotubes for Enhanced Thermoelectric Performance

Kanghyun Jo, Jihyun Kim, Byeonggwan Kim*

1. Department of Chemical Engineering and Applied Chemistry, Chungnam National University

*Corresponding author: Prof. Byeonggwan Kim, bg_kim@cnu.ac.kr

Thermoelectric generators (TEGs), which can effectively harvest waste heat from the human body to generate power, have emerged as a promising technology for self-driving wearable devices. In particular, robust mechanical flexibility and high thermoelectric performance are required for the implementation of flexible TEGs, and carbon-based materials have attracted much attention due to their high flexibility. Among them, carbon nanotubes (CNTs) have high electrical conductivity of over 1000 S cm^{-1}, and many studies have been conducted on their use. However, the practical application of TEGs has been hindered by the lack of stable p-type and n-type thermoelectric materials in air. In this study, we developed p-type and n-type thermoelectric materials with improved performance using mixed-wall carbon nanotubes (MWCNTs), which exhibit excellent electrical conductivity, high tensile strength, and excellent mechanical properties, and whose hydrophilic interactions are enhanced through oxidation. In particular, MWCNTs enable high-concentration uniform dispersion due to their enhanced hydrophilic interactions, enabling uniform coating when coated on PET films, and guaranteeing enhanced mechanical flexibility based on the high flexibility of PET, making them suitable as wearable TEG materials. In addition, molecular doping via drop-casting ensured stable thermoelectric performance and optimized charge transport. This study demonstrates that thermoelectric materials can be effectively produced through a method advantageous for large-area processing, and suggests new possibilities for the development of self-powered wearable TEGs.

References

[1] Ji Y., Jang J. M., Kim J. Y., Choi E., Jeong H., Lee C. H., Lee S., Kwak Y., Cho Y., Lee H., Myung J.-h., Kim B., Kim S. J., Kim D. W. SWCNT/MWCNT binderless hybrid hydrogel: Towards large-scale high-performance EMI shielding coating at commercial level. *Carbon* **238**, 120250, (2025).

Electrodeposited $Co(OH)_2$ nanoflakes on O_2 plasma-modified activated carbon for high performance supercapacitors

Eunseon Chae[1], In Woo Lee[1], Seoyeong Cheon[1], Minah Kang[1], Yangseop Lee, Young-Seak Lee[1,2*]

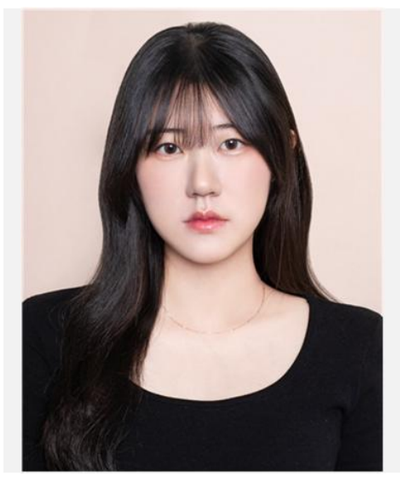
1. Department of Chemical Engineering and Applied Chemistry,
Chungnam National University, Daejeon, 34134, Republic of Korea
2. Institute of Carbon Fusion Technology (InCFT),
Chungnam National University, Daejeon, 34134, Republic of Korea
*Corresponding author: Prof. Lee, youngslee@cnu.ac.kr

$Co(OH)_2$ has attracted attention as a promising material for supercapacitors. However, its practical performance is limited compared to its theoretical capacity due to its inherent low electrical conductivity and particle aggregation. In this study, $Co(OH)_2$ nanoflakes were electrodeposited on an oxygen plasma treated activated carbon (OAC) electrode to solve this problem. The oxygen plasma treatment not only increased the specific surface area and mesopore volume of the activated carbon and introduced oxygen functional groups, but also improved the efficiency of the subsequent electrodeposition process. This enabled the rapid and uniform growth of $Co(OH)_2$ nanoflakes through strong interactions with the surface oxygen functional groups. The resulting OAC@$Co(OH)_2$ electrode exhibited a high specific capacitance of 163.4 F g^{-1} at 0.5 A g^{-1} and excellent cycling stability with a capacitance retention of 88.9% after 10,000 cycles. Furthermore, the asymmetric supercapacitor (OAC@Co600//AC) exhibited an energy density of 44.6 Wh kg^{-1} at a power density of 700 W kg^{-1}. These outstanding electrochemical properties are attributed to the synergistic effects of hydrophilic OAC and uniformly deposited $Co(OH)_2$. This study provides an efficient and scalable strategy to fabricate high-performance hydrophilic AC-based $Co(OH)_2$ electrodes via electrodeposition

References

[1] Gao, P., Zeng, Y., Tang, P., Wang, Z., Yang, J., Hu. A. & Liu, J. Understanding the Synergistic Effects and Structural Evolution of Co(OH)2 and Co3O4 toward Boosting Electrochemical Charge Storage. Adv. Funct. Mater. **32**, 2108644, (2022).

Preparatin of SiO_x-void@C with a controlled SiO_x composition via NF_3 fluorination as a lithium-ion batteries anode material



Seoyeong Cheon[1], Seongjae Myeong[1], In Woo Lee[1], Young-Seak Lee[1,2,*]

1. Department of Chemical Engineering and Applied Chemistry, Chungnam National University, Daejeon 34134, Republic of Korea

2. Institute of Carbon Fusion Technology (InCFT), Chungnam National University, Daejeon, 34134, Republic of Korea

*Corresponding author: Prof. Young-seak Lee, youngslee@cnu.ac.kr

This research focused on enhancing the electrochemical performance of SiO_x-based lithium-ion batteries anode material by improving both the stability and capacity. A SiO_x-void@C architecture was engineered, featuring internal voids between the SiO_x core and an outer carbon shell. This structure was achieved through coating with carbon and applying NF_3 gas fluorination to control the O/Si ratio of SiO_x. The NF_3 fluorination not only etched the SiO_x matrix to form voids but also introduced nitrogen and fluorine functional groups on the carbon surface. This design effectively accommodated the volume changes of silicon during lithiation/delithiation, while the reduced oxygen content enhanced capacity. In addition, fluorination generated SiO_xF_y species that provided additional capacity contributions during cycling. Among the samples, SiO_x@C_NF450 synthesized at an optimized temperature, exhibited a capacity increase of about 23% at a current density of 50 mA g^{-1} and a much bigger capacity increase of about 40% at a high current density of 5000 mA g^{-1} compared to SiO_x@C, demonstrating superior rate capability. It also maintained its initial capacity over 500 cycles at current density of 2000 mA g^{-1}. These results highlight the potential of N/F co-doped SiO_x-void@C materials, prepared via NF_3 fluorination, as high-performance anodes for next-generation lithium-ion batteries.

References

[1] Fan, S., Zhou, X., Tang, J., Ma, Y., & Yang, J. Insights to the variation of oxygen content and reasons for improved electrochemical performance of annealing SiOx anodes for Li-ion battery. *App. Surf. Sci.* **579**, 152179, (2022).

Encapsulation Characteristics of Diverse Biomolecules in Membrane-Less Vesicle-Like Condensates Formed by Coacervate Rearrangement

Hyunsuk Choi[1], Yoo Seong Choi[1,*]

1. Department of Chemical Engineering and Applied Chemistry, Chungnam National University

*Corresponding author: Prof. Yoo Seong Choi, biochoi@cnu.ac.kr

Membrane-less vesicle-like biomolecular condensates formed by liquid–liquid phase separation of two bioengineered proteins provide a simple, tunable platform for compartmentalization without lipid membranes. In this study, an anionic intrinsically disordered protein (GG1234) and a cationic, hydrophobic variant of bone morphogenetic protein 2 (bhBMP-2) were mixed sequentially to induce simple and complex coacervation, yielding hollow condensates with a liquid interior and a gel-like shell. To evaluate cargo uptake, we employed two loading strategies—pre-loading fluorescent probes with GG1234 before bhBMP-2 addition and post-loading by diffusion into preformed vesicles—and tested various cargo molecules with different sizes and hydrophobicities, including fluorescent proteins and fluorescently labeled compounds. The vesicle-like compartments can encapsulate a broad range of substances, based on the characteristics of the target molecules and their distribution between the core and shell depending on the method used. These tunable partitioning behaviors highlight the potential of coacervate-derived vesicles as customizable carriers for biomolecules and small-molecule drugs. Overall, our study demonstrates that sequence-engineered proteins can form dynamic, membrane-less compartments with programmable cargo loading, offering a new route to design functional biomolecular containers for applications in synthetic biology and targeted delivery.

Reference

[1] Choi, H., Hong, Y., Najafi, S., Kim, S. Y., Shea, J.-E., Hwang, D. S. & Choi, Y. S. Spontaneous Transition of Spherical Coacervate to Vesicle-Like Compartment. *Adv. Sci.* **11**, 2305978, (2024).

Biochemical Characterization of csTyr, an Organic Solvent–Tolerant Tyrosinase, for Enhanced Catechol Biosynthesis

Jaemin Han[1], Jiyeong Lee[1], Yoo Seong Choi[1,*]

1. Department of Chemical Engineering and Applied Chemistry, Chungnam National University

*Corresponding author: Prof. Yoo Seong Choi, biochoi@cnu.ac.kr

Tyrosinases are attractive biocatalysts for the ortho-hydroxylation of monophenols to valuable catechol derivatives, yet their poor stability in organic media has hampered practical applications. In this work, we report the discovery, recombinant expression, and detailed biochemical analysis of csTyr, a halophilic tyrosinase from *Citreicella* sp. SE45, produced in *Escherichia coli*. Remarkably, csTyr is inactive in purely aqueous buffers but becomes catalytically active upon addition of primary alcohol cosolvents—most notably 50 % (v/v) ethanol—where it achieves activity and long-term stability comparable to conventional tyrosinases in water. Under these optimized conditions, csTyr catalyzes the ortho-hydroxylation of acetaminophen and resveratrol to give 3-hydroxy-acetaminophen and piceatannol, respectively, with high conversion efficiency and minimal enzyme inactivation. These findings highlight csTyr as a robust “organophilic” biocatalyst capable of overcoming traditional solvent-stability limitations, opening new avenues for sustainable biosynthesis of catechol-based fine chemicals.

Reference

[1] Bae, G., Lee, J., Kim, H., Yeon, Y. J. & Choi, Y. S. Tyrosinase from *Citreicella* sp. as an organophilic enzyme for catechol biosynthesis. *Biochem. Eng. J.* **201**, 109123, (2024).

Enhanced OER Performance of Zn-NiFe LDH Electrode Synthesized using One-pot precipitation in Alkaline water electrolysis

Jueun Hwang, Hyemi Song, Sungtak Kim*

Department of Chemical Engineering and Applied Chemistry, Chungnam National University, Daejeon, Korea

*Corresponding author: Prof. Sungtak Kim, sunnykim@cnu.ac.kr

Renewable energy is receiving increasing attention due to fossil fuel depletion and accelerating global warming. Among them, Hydrogen is increasing attention as a future-generation energy source. its abundance and energy density on Earth. Water electrolysis is a promising technology for producing green hydrogen. In particular, alkaline water electrolysis is a simple and economical technology because it uses a non-noble metal catalyst. However, The oxygen evolution reaction (OER) is a complex process involving the transfer of four electron. it causes an overpotential due to slow dynamics. For this reason, there is a limit to the efficiency and commercialization of the entire water electrolysis reaction. Therefore, it is essential to develop a high efficiency and high durability OER electrode catalyst. Layered double hydroxide (LDH), particularly NiFe-based catalyst, have demonstrated excellent OER activity due to their abundant active sites, tunable metal composition, and conductive layered structures.

In this study, Zn-NiFe LDH was synthesized using a simple one-pot precipitation method. The incorporation of Zn into the NiFe-LDH structure enhanced OER performance by increasing surface area and modulating the electronic structure. The Z1N25 with a Ni^{2+} to Zn^{2+} ratio of 25:1 exhibited a low overpotential of 225 mV at 10 mA cm^{-2}, significantly improved compared to pristine NiFe LDH, which required 277 mV. During cyclic voltammetry (CV) activation, the overpotential further decreased to 201.6 mV and 186.4 mV after 1,000 and 2,000 cycles, respectively, which is attributed to Zn leaching that increased the surface area while maintaining the LDH structure. The Tafel slope also decreased from 57.8 mV dec^{-1} to 45.2 mV dec^{-1}, indicating enhanced catalytic kinetics due to Zn doping. Long-term chronoamperometric tests demonstrated excellent stability over 140 hours of continuous operation. X-ray photoelectron spectroscopy (XPS) analysis revealed an increase in the oxidation state of Ni, growth in M–OH peaks, and a red shift

in Fe 2p binding energy, confirming improved OER activity driven by favorable electronic restructuring. The one-pot precipitation strategy simplifies the synthesis process by utilizing oxygen corrosion of the Fe substrate, significantly reducing time and cost for electrode preparation. These findings highlight Zn-NiFe LDH as a cost-effective and high-performance catalyst, offering both high catalytic activity and long-term durability essential for sustainable hydrogen production via alkaline water electrolysis.

The 4th CNU-SU Joint Symposium

DATE August,1st 2025

VENUE Central Library

Guidelines of Symposium

1 **Presentation Time** (15 min talk , Q&A 5 min)

2 **A/V Equipment**

- Laptop with Powerpoint will be provided, with your preseintation files preladed.
- HDMI cables and power outlets will be available at the venue.

3 **Wi-Fi Information**

Please use the provided one-day Wi-Fi information (ID and password) available inside the venue.

4. **Access the Venue**

Please use the QR code posted at the entrance of the Central Library to access the event venue.

Transportation to the Venue

5. To ensure smooth progress of the event, shuttle bus will be arranged for all schedules on August 1 (Fri).
Hotel Shuttle Departure Time: August 1 at 8:20 AM.

Reception & Banquet

6.

July 31, 2025 (Thu) 6:00 PM
알텐데 ALTENDE (1st Floor, Yuseong Bldg, 34 Oncheon-ro, Yuseong-gu, Daejeon)
For Professors Only

August 1, 2025 (Fri) 11:40 AM
베니스 레스토랑 Venice Restaurant (23rd Floor, 31 Daehak-ro, Yuseong-gu, Daejeon)
For Professors and Student Presenters

August 1, 2025 (Fri) 6:30 PM
옛터 민속박물관 Yetter Folk Museum (321-35, Sannae-ro, Dong-gu, Daejeon)
For Professors Only

August 1, 2025 (Fri) 6:00 PM
황토가마 Hwangto Gama (1st Floor, 35 Daehak-ro 145beon-gil, Yuseong-gu, Daejeon)
For Student Presenters

Accommodations

7. July 31, 2025(Thu) ~ August 2, 2025(Sat) LAMADA Daejoen Hotel