

# **14<sup>th</sup> Jilin-Korea-Waseda Alliance Annual Symposium**

**August 21 ~ 23, 2025**

**Yoo Imsoon Hall, Mediheal EES,  
Korea University**





## Organizers and Sponsors

- ✓ BK21 Four R&E Center for Chemistry, Korea University
- ✓ BK21 Four R&E Center for KU-KIST, Korea University
- ✓ The Institute of Basic Science, Korea University
- ✓ Office of Graduate School, Korea University
- ✓ Brain Korea 21 Four Program
- ✓ Department of Chemistry, Korea University
- ✓ Center for Advanced Molecular Science, Korea University



**4단계 BK21 화학교육연구단**  
BK21 FOUR R&E Center for Chemistry



**고려대학교 KU-KIST융합대학원**  
바이오혁신첨단소재교육연구단



**고려대학교 기초과학연구원**  
Korea University  
The Institute of Basic Science



**고려대학교 대학원혁신본부**  
Office of Graduate School, Korea University



**고려대학교 화학과**  
Department of Chemistry



# Program

## ► August 21, 2025, Thursday

18:00 – Registration and Welcome Reception

## ► August 22, 2025, Friday

08:50 – 09:00 Opening Address

Prof. Sungnam Park (Director, BK21 Chemistry, Korea University)

### Session Chair : Prof. Han Young Woo

09:00 – 09:30 Prof. Dong Hoon Choi (Korea University)

"From Blue to Green: Sterically Shielded MR-TADF Emitters for Solution Processed OLEDs"

09:30 – 10:00 Prof. Chuandong Dou (Jilin University)

"Boron-Containing Molecular Carbons"

10:00 – 10:30 Prof. Masahiro Kunimoto (Waseda University)

"Additive effects on mossy and dendritic growth of Zn as a negative electrode in aqueous electrolyte-based large-scale energy storage devices"

10:30 – 11:00 Coffee Break

### Session Chair : Prof. Chuandong Dou

11:00 – 11:30 Prof. Kenichi Oyaizu (Waseda University)

"Polymeric sulfur electrodes for high-density lithium sulfur batteries"

11:30 – 12:00 Prof. Guanglu Wu (Jilin University)

"Unveiling intermediate states and assembly mechanisms in multicomponent systems"

12:00 – 13:30 Lunch

**Session Chair : Prof. Kyoungsuk Jin**

13:30 – 14:00 Prof. Byoung-Hoon Lee (Korea University)  
"A Next-Generation Catalysis: Atomic Innovations for a Net-Zero World"

14:00 – 14:30 Prof. Wenke Zhang (Jilin University)  
"Application of Single-Molecule Force Spectroscopy in Studying the Mechanisms of Drug Action"

14:30 – 15:00 Prof. Seigo Watanabe (Waseda University)  
"Systematic Design of Low Dielectric Loss Poly(phenylene sulfide)s"

15:00 – 15:30 Prof. Yongju Kim (Korea University)  
"Architecting Bioactive Supramolecules: From Molecular Design to Functional Nanostructures"

15:30 – 15:50 Coffee Break

**Session Chair : Prof. Kenichi Oyaizu**

15:50 – 16:20 Prof. Kun Liu (Jilin University)  
"Biomolecular Induced Chiral Assembly of Plasmonic Nanoparticles"

16:20 – 16:50 Prof. Taeho Kang (Korea University)  
"Nickel-Catalyzed 1,2-Difunctionalization of Unactivated Alkenes Directed by Native Functional Groups"

16:50 – 17:20 Prof. Takamichi Matsuno (Waseda University)  
"Ordered Mesoporous Organosiloxane Elastomers using assemblies of Silica Nanospheres as Templates toward Nanoparticle Separation"

17:20 – 17:40 Prof. Dong-Kwon Lim (Korea University)  
"KU-KIST: Graduate School of Converging Science and Technology"

17:40 - 17:50 Closing Remark  
Prof. Dong-Kwon Lim (Director, BK21 KU-KIST, Korea University)

18:00 – Symposium Banquet

► **August 23, 2025, Saturday**

*Center Introduction and Future Cooperative Discussion*

10:00 – 10:30 Center for Advanced Molecular Science (CAMS, Korea University)

10:30 – 11:00 Top Global University Project & Leading Graduate Program  
(TGU/LGP, Waseda University)

11:00 – 11:30 State Key Laboratory of Supramolecular Structure & Materials  
(SKLSSM, Jilin University)

11:30 –        Closing

# Poster Session

*Friday, August 22, 2025*

*First Floor Lobby, Mediheal EES Hall,*

*Korea University*

*10:30 ~ 17:00*

P1. "Highly Coarse-Grained Patchy Ellipsoid Particle Model of Glucose"

Bin Li, You-Liang Zhu\*, Zhong-Yuan Lu\*, Jia-Li Gao\* (Jilin University)

P2. "Synthesis of an Ionic Aromatic Cyclodextrin for a Novel Host Molecule of Adapalene"

Dahee Jung, Yongju Kim (Korea University)

P3. "Soft Lewis Base-Containing Polymers for Solid Polymer Electrolytes with Unconventional Conduction Mechanism under Polymer-in-salt Conditions"

Akinari Chiba, Yuki Ogawa, Kenichi Oyaizu (Waseda University)

P4. "Development of a TPP-Conjugated Quercetin Probe for Enhanced Mitochondrial Targeting and Fluorescence Imaging"

Gayeon Nam, Yongju Kim (Korea University)

P5. "Highly conductive polymer electrolyte membranes with polyoxometalate hybrid nanodomains for high-temperature fuel cells"

Tingting Li, Haolong Li\* (Jilin University)

P6. "Polymer Exciplex Host-Driven TADF OLEDs via Non-Halogenated Solution Processing"

Subin Kwon, Ha Yeon Kim, Yeso Lee, Shinyoung Kim, Jong Bin Park, Han Young Woo, Chang Seop Hong, Sungnam Park, Min Ju Cho, Dong Hoon Choi (Korea University)

P7. "Analysis of lubrication mechanism at tribological interface using in-situ surface-enhanced Raman spectroscopy"

Subaru Sawaki (Waseda University)

P8. "Two-in-One Molecule as a Single-Molecule Exciplex Host for Enhancing Solution-Processed TADF-OLED Performance"

Yeseo Lee, Ha Yeon Kim, Haeun Kwak, Chae Yeong Park, Subin Kwon, Shinyoung Kim, Eunji Lim, Kyungsuk Jin, Chang Seop Hong, Weon-Sik Chae, Min Ju Cho, Sungnam Park, and Dong Hoon Choi (Korea University)

P9. "Conjugated Oligoelectrolyte-Driven Self-Assembled Monolayer for Bidirectional Interfacial Engineering in Sn–Pb Perovskite Solar Cells"

Jong Bin Park and Han Young Woo\* (Korea University)

P10. "Unveiling the Photoluminescence Mechanism of carbonized Polymer Dots: Evolution and Synergistic Photoluminescence of Multiple Molecular Fluorophores"

Xiao Han, Bai Yang\* (Jilin University)

P11. "Synthesis and Potential Application of the L/D-Cysteine-Induced Au 432 Helicoid I for Visible Light-Driven Asymmetric Reactions"

Joonwoo Seo, Dong-Kwon Lim\* (Korea University)

P12. "Deep learning model based on interpretable subgraph attention network"

Jinyong Park and Sungnam Park\* (Korea University)

P13. "Sn Incorporation into Layered Octosilicates using Tin(IV) Chloride"

Takeshi Iwakami, Takamichi Matsuno, and Atsushi Shimojima\* (Waseda University)

P14. "Size-dependent 2D materials: A comparative study on N2 fixation activity via Gas Chromatography"

Jijoe Samuel Prabagar and Dong-Kwon Lim (Korea University)

P15. "Bipolar Redox-active molecules for organic aqueous redox flow batteries"

Hyeong hui Kim and Han young Woo\* (Korea University)

P16. "Sulfur-Locked Multiple Resonance Emitters for High Performance Orange-Red/Deep-Red OLEDs"

Yexuan Pu, Yue Wang\* (Jilin University)

P17. "Enhanced dispersibility and prodrug conversion rate of Sulfasalazine by UV irradiation"

Sungchan Choi, Yongju Kim (Korea University)

P18. "Machine Learning Prediction of Optical Properties of Coumarin Derivatives"

Seokwoo Kim and Sungnam Park\* (Korea University)

P19. "Development of Poly(phenylene sulfide)-Based Charge-Transfer Complexes for Solid polymer electrolyte with high electrochemical stability"

Toshinori Kozakai, Kenichi Oyaizu (Waseda University)

P20. "Exploring Chiral Nanostructures via Self-Assembly of Pagoda[4]arene Derivatives"

Wonpyo Rhee, Yongju Kim (Korea University)

P21. "Tyrosine Nanoassembly as a Potent Ice Recrystallization Inhibition Activity"

Yong Duk Kim, Yedam Lee, Dong June Ahn\* and Dong-Kwon Lim\* (Korea University)

P22. "Poly(p-phenylene sulfide)-based Block Copolymers for PPS/Hydrophilic Interface Adhesion"

Yugo Tosaki, Yuki Yoshida, Seigo Watanabe, Kenichi Oyaizu (Waseda University)

P23. "Assembly-driven enhanced anticancer effect of berberine by guaiazulene sulfonate"

Yeojin Choi, Yongju Kim (Korea University)

P24. "Differential Regulation of Glucose Transporter 1 (GLUT1) Expression and Antioxidant Activity by Micelle and Chiral Sheet Structures"

Yerim Kim, Yongju Kim (Korea University)

# **Abstract**

## **(Oral Presentation)**

**Presentation Title:** From Blue to Green: Sterically Shielded MR-TADF Emitters for Solution Processed OLEDs

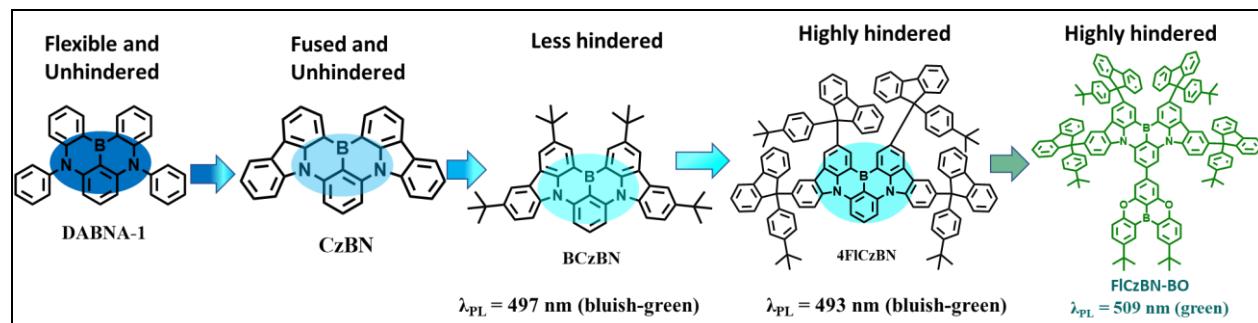
**Authors:** Dong Hoon Choi

**Affiliation:** Department of Chemistry, Korea University, Seoul 02841, Republic of Korea

**Email:** dhchoi8803@korea.ac.kr

**Abstract:**

In this research series, we developed a unified design strategy for multiple-resonance (MR) thermally activated delayed fluorescence (TADF) emitters incorporating steric shielding to achieve efficient and narrowband emission. Initially, we synthesized a blue-emitting MR emitter, **4FICzBN**, by decorating a BCzBN core with four bulky 9-phenylfluorene substituents. This steric encapsulation effectively reduced aggregation-caused quenching (ACQ), and improved solubility, enabling stable electroluminescence across a wide doping range. The resulting solution-processed OLEDs exhibited high color purity (FWHM = 28–30 nm) and notable device efficiency with an EQE of up to 12.2%, especially when used with a TADF sensitizer. Building upon this foundation, we further designed **FICzBN-BO**, a green-emitting dual MR-TADF emitter by integrating a BO-bridged acceptor (tDOBNA) with the FICzBN scaffold. This hybridization significantly lowered the HOMO-LUMO gap, resulting in a red-shifted yet still narrow emission (504 nm, FWHM = 31 nm). The steric hindrance from the phenyl-fluorene groups not only improved solubility but also induced core distortion, reducing the singlet-triplet energy gap ( $\Delta E_{ST} = 0.05$  eV) and enhancing the RISC rate ( $k_{RISC} = 1.6 \times 10^4$  s<sup>-1</sup>). Consequently, FICzBN-BO achieved high PLQY (92%) and an EQE of 16.26% in solution-processed OLEDs. Collectively, these studies demonstrate that steric shielding and MR framework hybridization represent a powerful strategy to realize high-performance, color-tunable MR-TADF materials for next-generation solution-processable OLED applications.



**Reference:**

1. N. Y. Kwon, C. W. Koh, S. H. Park, H. Kwak, H. Y. Kim, C. Y. Park, N. Peethani, J. Y. Park, S. Kim, K. Jin, C. S. Hong, M. J. Cho, S. Park, D. H. Choi, "Dual Multi-Resonance green emitter with steric shielding and core distortion for Solution-Processed TADF-OLEDs" *Chem. Eng. J.* **2025**, 506, 160139.
2. N. Peethani, N. Y. Kwon, C. W. Koh, S. H. Park, J. M. Ha, M. J. Cho, H. Y. Woo, S. Park, D. H. Choi, "Rational Design of a TADF Emitter with Steric Shielding and Multiple Resonance for Narrowband Solution-Processed OLEDs" *Adv. Opt. Mater.* **2024**, 12, 2301217.

## Dong Hoon Choi (崔東勳)



Department of Chemistry,  
College of Science, Korea University, Seoul 02841,  
Republic of Korea

Phone: (+82) 2-3290-3140  
E-mail: dhchoi8803@korea.ac.kr

### EDUCATION and PROFESSIONAL EXPERIENCES

2005. 3	<b>Professor</b>
–present	Department of Chemistry College of Science, Korea University, Seoul, Korea
2020	<b>Fellow</b>
–present	The Korean Academy of Science & Technology, Korea
2021	<b>Fellow</b>
–present	The Polymer Society of Korea, Korea
1995–2005	<b>Professor</b> Kyung Hee University, Yongin, Korea
1992–1995	<b>Senior Scientist</b> Korea Institute of Science and Technology, Seoul, Korea
1986–1991	<b>Ph.D</b> , Polymer Chemistry Macromolecular Sci. & Eng. The University of Michigan, Ann Arbor, MI, USA Supervisor: Prof. Robert Zand

### CURRENT RESEARCH ACTIVITIES

Organic Semiconducting Materials : Organic Light Emitting Materials, Organic Field Effect Transistor, Organic Phototransistor, Organic Photovoltaic Cell. Nanostructured Materials; nanomaterials; Nano-sized objects of organic semiconductor

### SELECTIVE PUBLICATIONS

1. N. Kim, M. J. Kang, H. J. Lee, J. Y. Park, H. Kwak, C. Y. Park, H. J. Ahn, J.-Y. Kim, J.-H. Baek, H. Y. Kim, S. Park, M. J. Cho, D. H. Choi,\* T. G. Kim\* “Enhancing Narrowband Blue TADF OLED Performance with Adamantane Group-Integrated Spatially Hindered 1,3-Bis(N-Carbazolyl)Benzene-Based Host”, *Adv. Funct. Mater.*, **2024**, *34*, 2408491.
2. N. Y. Kwon, C. W. Koh, S. H. Park, H. Kwak, H. Y. Kim, C. Y. Park, N. Peethani, J. Y. Park, S. Kim, K. Jin, C. S. Hong, M. J. Cho\*, S. Park\*, D. H. Choi\* Dual Multi-Resonance green emitter with steric shielding and core distortion for Solution-Processed TADF-OLEDs” *Chem. Eng. J.* **2025**, *506*, 160139.
3. S. H. Park, N. Y. Kwon, C. W. Koh, J. Y. Park, M. J. Kang, H. Kwak, C. Y. Park, S. Park\*, M. J. Cho\*, D. H. Choi\*, “Eco-friendly solution-processed narrowband OLEDs using non-halogenated aliphatic solvent systems”, *Chem. Eng. J.*, **2024**, *481*, 148484.
4. N. Peethani, N. Y. Kwon, C. W. Koh, S. H. Park, J. M. Ha, H. Y. Woo, M. J. Cho\*, S. Park\*, D. H. Choi\*, “Rational Design of a TADF Emitter with Steric Shielding and Multiple Resonance for Narrowband Solution-Processed OLEDs” *Adv. Opt. Mater.* **2024**, *12*, 2301217.
5. H. J. Kim, H. Kang, J.-E. Jeong, S. H. Park, C. W. Koh, C. W. Kim, H. Y. Woo, M. J. Cho,\* S. Park,\* D. H. Choi, Ultra-Deep-Blue Aggregation-Induced Delayed Fluorescence Emitters: Achieving Nearly 16% EQE in Solution-Processed Nondoped and Doped OLEDs with CIEy < 0.1” *Adv. Funct. Mater.* **2021**, *31*, 2102588.

**Presentation Title:** Boron-Containing Molecular Carbons

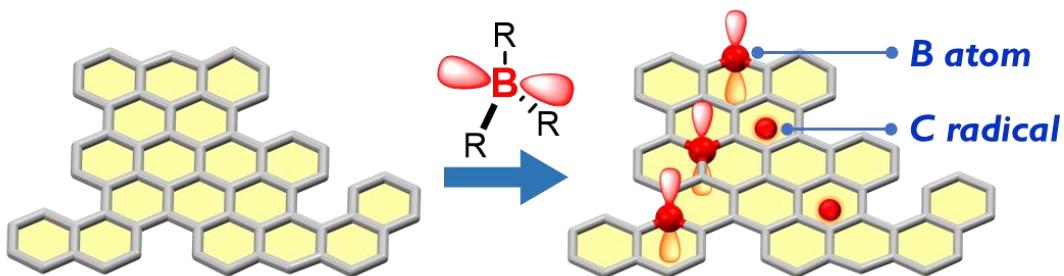
**Authors:** Chuandong Dou

**Affiliation:** State Key Laboratory of Supramolecular Structure and Materials, College of Chemistry, Jilin University, Changchun 130012, P. R. China

**Email:** chuandong@jlu.edu.cn

**Abstract:**

Molecular carbons, namely molecular cutout of carbon materials, are of importance for understanding accurate structures of carbon allotropes and developing functional  $\pi$ -electron materials. Doping the boron atoms into  $\pi$ -conjugated skeletons of molecular carbons enables the construction of boron-doped molecular carbons (BMCs), further leading to new chemistry and attractive material systems, which are distinct from carbon-based and other heteroatom-doped molecular carbons. Herein, our group focuses on the synthesis and functions of boron-containing molecular carbons, and promotes the development of heterocyclic material chemistry and organic functional materials. 1) By developing the synthetic method of selective borylation for organoborane building blocks, we have constructed boron-doped functional motif platform, and then realized precise boron-doping of molecular carbons. 2) By proposing controlled cyclization on organoboranes, we have developed boron-doped molecular nanocarbon systems, and obtained narrowband photoluminescence and electroluminescence as well as single-molecule conduction function. 3) By proposing quinoidal conjugation induced open-shell state of organoboranes, we have developed boron-containing open-shell molecular carbons and successfully explored photothermal conversion properties and applications.



**Reference:**

1. X. Tian, Z. Fan, Z. Li, S. Zhang, Z. Li, X. Zhuang, Y. Wang, C. Dou, "Polycyclic Aromatic Hydrocarbons with a Boron-Doped Zigzag/Armchair Topology: A Boron-Edging Strategy for Organic Narrowband Emitters", *Angew. Chem. Int. Ed.* 2025, 64, e202500110.
2. Y. Liu, X. Tian, Z. Li, T. Zhang, L. Yuan, Y. Wang, C. Dou, "Spiro-Fused vs 575-Ringed Boron-Doped Polycyclic  $\pi$ -Systems: Selective Synthesis, Reactivity and Properties", *Angew. Chem. Int. Ed.* 2025, 64, e202422031.
3. Z. Fan, Y. Liu, T. Zhang, Y. Wang, C. Dou, "Cove-Edged Boron-Doped peri-Acenes via Alkyne-Enabled Cyclization", *CCS Chem.* 2025, 7, 256.

# Chuandong Dou (窦传冬)



State Key Laboratory of Supramolecular Structure and Materials  
College of Chemistry, Jilin University  
2699 Qianjin Street, Changchun 130012, P. R. China  
Phone: (+86) 13604330884  
E-mail: chuandong@jlu.edu.cn

## EDUCATION and PROFESSIONAL EXPERIENCES

2020. 3      **Professor**  
–present      College of Chemistry,  
                  Jilin University, China

2013–2020      **Associate and Full Professor**  
                  Chemistry Changchun Institute of Applied Chemistry,  
                  Chinese Academy of Sciences, China

2011–2013      **Postdoc Researcher**  
                  Department of Chemistry, Nagoya University, Japan  
                  Supervisor: Prof. Shigehiro Yamaguchi

2006–2011      **Ph.D, Organic Chemistry**  
                  College of Chemistry, Jilin University, China  
                  Supervisor: Prof. Yue Wang

## CURRENT RESEARCH ACTIVITIES

Organic and polymeric optoelectronic materials; Organoboron chemistry; Molecular carbon chemistry and materials; Radical chemistry.

## SELECTIVE PUBLICATIONS

1. X. Tian, Z. Fan, Z. Li, S. Zhang, Z. Li, X. Zhuang\*, Y. Wang, C. Dou\*, “Polycyclic Aromatic Hydrocarbons with a Boron-Doped Zigzag/Armchair Topology: A Boron-Edging Strategy for Organic Narrowband Emitters”, *Angew. Chem. Int. Ed.*, **2025**, 64, e202500110.
2. Y. Liu, X. Tian, Z. Li, T. Zhang, L. Yuan, Y. Wang, C. Dou\*, “Spiro-Fused vs 575-Ringed Boron-Doped Polycyclic  $\pi$ -Systems: Selective Synthesis, Reactivity and Properties”, *Angew. Chem. Int. Ed.*, **2025**, 64, e202422031.
3. L. Yuan, J. Yang, S. Qi, Y. Liu, X. Tian, T. Jia, Y. Wang, C. Dou\*, “Diradicaloid Boron-Doped Molecular Carbons Achieved by Pentagon-Fusion”, *Angew. Chem. Int. Ed.*, **2023**, 62, e202314982.
4. Y. Liu, L. Yuan, J. Guo, W. Sun, Y. Wang, C. Dou\*, “Photonic Modulation Enabled by Controlling the Edge Structures of Boron-Doped Molecular Carbons”, *Angew. Chem. Int. Ed.*, **2023**, 62, e202306911.
5. W. Sun, J. Guo, Z. Fan, L. Yuan, K. Ye, C. Dou\*, Y. Wang, “Ribbon-Type Boron-Doped Polycyclic Aromatic Hydrocarbons: Conformations, Dynamic Complexation and Electronic Properties”, *Angew. Chem. Int. Ed.*, **2022**, 61, e202209271.
6. J. Guo, Y. Yang, C. Dou\*, Y. Wang, “Boron-Containing Organic Diradicaloids: Dynamically Modulating Singlet Diradical Character by Lewis Acid–Base Coordination”, *J. Am. Chem. Soc.*, **2021**, 143, 18272–18279.

**Presentation Title:** Additive effects on mossy and dendritic growth of Zn as a negative electrode in aqueous electrolyte-based large-scale energy storage devices

**Authors:** Masahiro Kunimoto, Ayumu Komiya, Takayuki Homma

**Affiliation:** Faculty of Science and Engineering, Waseda University, 3-4-1 Okubo, Shinjuku, Tokyo, Japan

**Email:** m.kunimoto@aoni.waseda.jp

### Abstract:

Zn is a promising material for the negative electrode in next-generation large-scale energy storage devices using aqueous electrolytes. A major challenge associated with Zn electrodes is the shape change during cycling, particularly the formation of mossy and dendritic structures, which significantly degrades charge/discharge efficiency. Researchers in the field of electrodeposition process have explored various kinds of additives to regulate the surface morphology of deposited materials. These additives are believed to be effective in battery electrodes, where they can suppress irregular Zn deposition. The objective of our research is to identify and design high-performance additive capable of controlling the morphology of deposited Zn, thereby mitigating mossy and dendrite during the charge process. To achieve this, we investigate the underlying mechanism of Zn morphological growth through a combination of density functional theory calculations and statistical Monte Carlo simulations. This theoretical framework provides insights to propose effective additives<sup>1</sup>. Our findings indicate that dendritic growth during charging is closely linked to the property of the ZnO layer formed during discharge. Based on these insights, we have focused on Li as a promising additive for the suppression of both mossy and dendritic growth<sup>2,3</sup>.

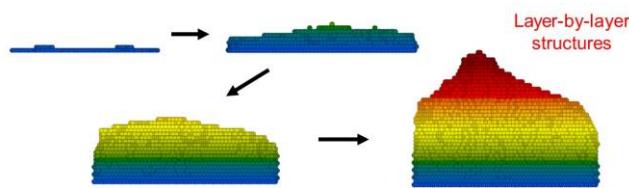


Figure 1. Results of DFT-base kinetic Monte-Carlo simulation to analyze Zn deposition that leads to protrusion structure.

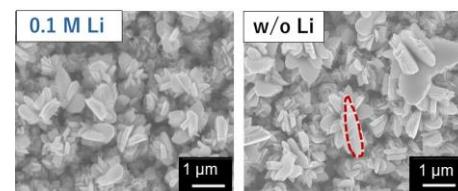


Figure 2. SEM images of Zn deposited surface of negative electrode with and without Li as additive.

### Reference:

1. Y. Onabuta, M. Kunimoto, S. Wang, Y. Fukunaka, H. Nakai, T. Homma, "Multiscale Simulation of Irregular Shape Evolution during the Initial Stage of Zn Electrodeposition on a Negative Electrode Surface", *J. Phys. Chem. C*, **2022**, 126, 5224.
2. Y. Onabuta, M. Kunimoto, S. Wang, Y. Fukunaka, H. Nakai, T. Homma, "Effect of Li<sup>+</sup> Addition during Initial Stage of Electrodeposition Process on Nucleation and Growth of Zn", *J. Electrochem. Soc.*, **2022**, 169, 92504.
3. A. Komiya, T. Wang, M. Kunimoto, T. Asano, Y. Nishikitani, T. Homma, "Additive Effect of Li on Electrical Property of ZnO Passivation Layer to Control Dendritic Growth of Zn during Recharge Processes", *J. Power Sources*, **2024**, 626, 235714.

# Masahiro Kunimoto (國本雅宏)

Global Center for Science and Engineering,  
Faculty of Science and Engineering, Waseda University,  
3-4-1 Okubo, Shinjuku, Tokyo, Japan  
Phone: (+81) 3-5286-3209  
E-mail: m.kunimoto@aoni.waseda.jp



## EDUCATION and PROFESSIONAL EXPERIENCES

2023. 10      **Associate Professor**  
–present      Global Center for Science and Engineering,  
                    Faculty of Science and Engineering, Waseda University, Tokyo, Japan

2023      **Associate Professor**  
                    Yamanashi University, Yamanashi, Japan

2018–2023      **Assistant Professor**  
                    Department of Applied Chemistry, Waseda University, Tokyo, Japan

2013–2018      **Postdoc Researcher**  
                    Research Organization for Nano & Life Innovation, Waseda University, Tokyo, Japan

2011–2013      **Research Associate**  
                    Department of Applied Chemistry, Waseda University, Tokyo, Japan

2009–2012      **Ph.D, Doctor of Engineering**  
                    Department of Nanoscience and Nanoengineering, Waseda University, Tokyo, Japan  
                    Supervisor: Prof. Takayuki Homma

## CURRENT RESEARCH ACTIVITIES

Interfacial analyses and electrochemical process developments; surface enhanced Raman spectroscopy, density functional theory, quantum chemical calculation, Monte Carlo simulation, electrolytic/electroless deposition process, large scale energy storages, additives, water splitting for renewable energy technology.

## SELECTIVE PUBLICATIONS

1. M. Kunimoto, H. Shoji, M. Yanagisawa, M. Morita, T. Abe, T. Homma, “Spectroelectrochemical Measurement Method of In Situ Surface-Enhanced Raman Spectroscopy for Various Electrode Materials Using a Transmission-Type Plasmonic Sensor”, *Energy Environ. Mater.* **2025**, in press.
2. K. Guo, M. Kunimoto, T. Homma, “Electroless-deposited NiFeP catalyst-coated-membrane cathodes for anion exchange membrane water electrolysis”, *J. Mater. Chem. A*, **2025**, 13, 7313.
3. Komiya, T. Wang, M. Kunimoto, T. Asano, Y. Nishikitani, T. Homma, “Additive Effect of Li on Electrical Property of ZnO Passivation Layer to Control Dendritic Growth of Zn during Recharge Processes”, *J. Power Sources*, **2024**, 626, 235714.
4. T. Wang, M. Kunimoto, M. Yanagisawa, M. Morita, T. Abe, T. Homma, “Zn dissolution-passivation behavior with ZnO formation via in-situ characterizations”, *Energy & Environ. Mater.* **2024**, 7, e12481.
5. Y. Onabuta, M. Kunimoto, S. Wang, Y. Fukunaka, H. Nakai, T. Homma, “Multiscale Simulation of Irregular Shape Evolution during the Initial Stage of Zn Electrodeposition on a Negative Electrode Surface”, *J. Phys. Chem. C*, **2022**, 126, 5224.

**Presentation Title:** Polymeric sulfur electrodes for high-density lithium sulfur batteries

**Authors:** Kenichi Oyaizu

**Affiliation:** Department of Applied Chemistry, Waseda University, Tokyo 169-8555, Japan

**Email:** oyaizu@waseda.jp

**Abstract:**

Lithium-sulfur batteries have attracted significant attention due to the high capacity of sulfur as the cathode-active material. When a solid electrolyte is employed, concerns regarding the elution of polysulfide ions into the electrolyte dissipate. However, the charge/discharge rate characteristics of the solid-state lithium-sulfur batteries are lower than those with an organic electrolyte. In this study, we synthesized a sulfur-containing elastomer polymer, which exhibits enhanced flexibility compared to elemental sulfur. Our findings demonstrate that this polymer significantly improves the rate characteristics by reducing the interfacial resistance.

The sulfur-containing polymer was synthesized by inverse vulcanization, a process in which cyclic sulfur opens up to form a radical, and the monomer polymerizes to yield a polymer with a polysulfide structure. A linear polymer was obtained by using a monomer with one C=C double bond and elemental sulfur, to which was added a cross-linking agent to produce the cross-linked polymer. The mixture of a monomer Span 80, elemental sulfur, and zinc diethyldithiocarbamate as a catalyst was stirred under heating conditions. Subsequently, a cross-linking agent, bisphenol A diglycidyl ether, was incorporated, and the mixture was subjected to further heating to yield the desired product. The cross-linking densities were tuned by incorporating different equivalents of the cross-linking agent.

Elemental sulfur demonstrated a discharge capacity of ca. 1500 mAh/g at 0.1 mA/cm<sup>2</sup>, but it decreased at higher current densities. The discharge capacity of the densely cross-linked polymer remained low; however, the less cross-linked polymers with relatively low Young's modulus and storage modulus exhibited larger capacities than that of pure sulfur at all current densities. The softness of the sulfur cathode seemed to facilitate contact at the solid-solid interface, thereby maintaining a conductive path.

**Reference:**

1. K. Zhang, X. Lin, Y. Shi, K. Oyaizu, Z. Jia, “Two-electron Redox Chemistry of Nitroxide Radicals: Fundamental Mechanisms and Applications in Energy Storage”, *ACS Electrochem.* **2025**, 1, 123.
2. K. Oyaizu, “Reversible and High-density Energy Storage with Polymers Populated with Bistable Redox Sites”, *Polym. J.* **2024**, 56, 127.
3. K. Hatakeyama-Sato, K. Oyaizu, “Redox: Organic Robust Radicals and Their Polymers for Energy Conversion/Storage Devices”, *Chem. Rev.* **2023**, 123, 11336.
4. K. Oyaizu, “Organic Radical Systems”, *Encyclopedia of Electrochemical Power Sources*, ed by J. Garche, Second Edition, Elsevier (2025), vol. 4, pp. 941-948.
5. K. Oyaizu, “Energy Conversion Materials”, *Functional Macromolecular Complexes*, ed by K. Yamamoto, H. Nishihara, Royal Society of Chemistry (2024), chapter 13, pp. 252-270.

## Kenichi Oyaizu (小柳津 研一)

Department of Applied Chemistry,  
Waseda University, Tokyo 169-8555, Japan  
Phone: (+81) 3-5286-3120  
E-mail: oyaizu@waseda.jp



### EDUCATION and PROFESSIONAL EXPERIENCES

2012. 4	<b>Professor</b>
–present	Waseda University, Tokyo, Japan
2007–2012	<b>Associate Professor</b> Department of Applied Chemistry, Waseda University, Tokyo, Japan
2003–2007	<b>Associate Professor</b> Institute of Colloid and Interface Science, Tokyo University of Science, Chiba, Japan
1995	<b>Ph.D.</b> Department of Applied Chemistry, Waseda University, Japan Supervisor: Prof. Eishun Tsuchida

### CURRENT RESEARCH ACTIVITIES

Development of functional polymers for use in energy-, optical-, and dielectric-related materials and devices.

### SELECTIVE PUBLICATIONS

1. K. Ishigami, S. Mori, K. Oyaizu, “Approach to Tuning the Dispersion Stability of TEMPO-substituted Polymer Nanoparticles for Aqueous Organic Redox Flow Batteries”, *ChemSusChem.* **2025**, in press. DOI: 10.1002/cssc.202500911
2. S. Watanabe, Z. An, H. Nishio, Y. Tsunekawa, K. Oyaizu, “Poly(dibenzothiophenylene sulfide)s: Sulfur-rich Annulated Frameworks with a Wide-range Ultrahigh Refractive Index”, *J. Mater. Chem. C* **2025**, 13, 7933.
3. S. Watanabe, Y. Tsunekawa, K. Oyaizu, “High Refractive Index Aromatic and Ether-containing Polythioureas: Improving Transparency and Mechanical Properties via Reciprocal Hydrogen Bonds”, *Macromol. Chem. Phys.* **2025**, 226, 2400456.
4. K. Kisu, A. Dorai, K. Hatakeyama-Sato, T. Takano, S. Takagi, K. Oyaizu, S. Orimo, “Enhanced Durability of Ca Metal Battery with Dual Salt: Synergistic Effect on Solid Electrolyte Interphase and Solvation Structure for Improved Electrodeposition”, *ACS Appl. Mater. Interfaces* **2025**, 17, 1322.
5. S. Watanabe, T. Yano, Z. An, K. Oyaizu, “Aromatic Poly(dithioacetal)s: Spanning Degradability, Thermostability, and High Refractive Index Towards Eco-friendly Optics”, *ChemSusChem.* **2025**, 18, e202401609.
6. S. Watanabe, L. M. Cavinato, V. Calvi, R. van Rijn, R. D. Costa, K. Oyaizu, “Polarizable H-bond Concept in Aromatic Poly(thiourea)s: Unprecedented High Refractive Index, Transmittance and Degradability at Force to Enhance Lighting Efficiency”, *Adv. Funct. Mater.* **2024**, 34, 2404433.
7. Y. Igarashi, K. Hatakeyama-Sato, K. Kitagawa, R. Shinozaki, K. Oyaizu, “Precise Potential Tuning for Polymer-mediated Aqueous Redox Flow Battery with Lithium Iron Phosphate as Target Cathode”, *ACS Appl. Polym. Mater.* **2024**, 6, 10113.

**Presentation Title:** Unveiling intermediate states and assembly mechanisms in multicomponent systems

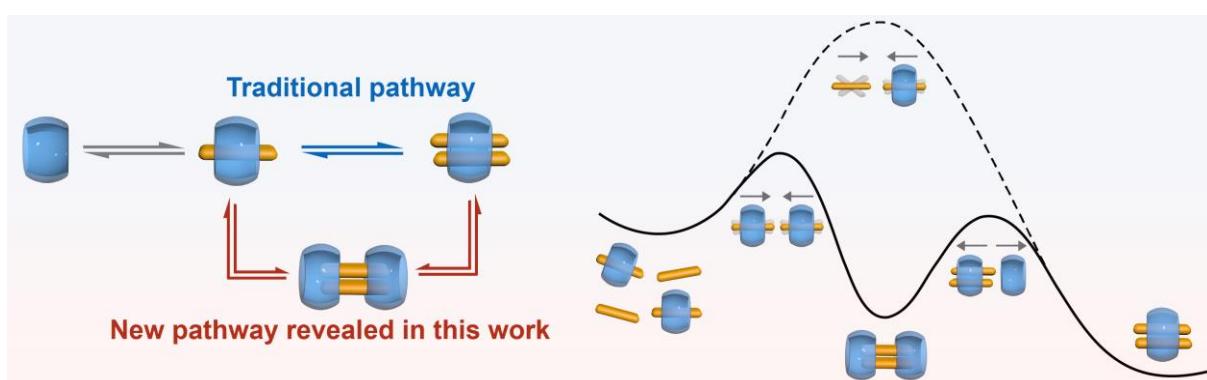
**Authors:** Guanglu Wu

**Affiliation:** State Key Laboratory of Supramolecular Structure and Materials, College of Chemistry, Jilin University, Changchun 130012, P R China

**Email:** guanglu@jlu.edu.cn

**Abstract:**

Cucurbit[8]uril (CB[8]) is widely recognized for its ability to form diverse assembly structures with various guest molecules and is often used as a model system for studying assembly mechanisms and structure-assembly relationships. CB[8]-mediated multicomponent complexes, in particular, have garnered significant attention due to their unique photophysical properties and the complexity of their assembly. Previous studies have primarily focused on revealing the thermodynamic equilibrium products of these complexes, with little exploration into their kinetic processes, primarily due to the rapid nature of the assembly. To study the kinetics and mechanisms of assembly, it is necessary to design molecular systems with slower assembly properties. In this work, we have developed a series of slow-assembling systems, synthesizing and assembling them for detailed kinetic studies. Employing time-resolved NMR and stopped-flow spectrophotometry, this study successfully observed intermediates in the assembly process and revealed unconventional pathways in the formation of these complexes. This work provides an expandable research system and methodology for understanding the assembly mechanisms in multicomponent systems.



**References:**

1. T. Y. Yang, Y. C. Shen, H. Y. Qu, B. Li, Y. B. Sun, **G. L. Wu\*** “Quaternary 2:2 Complexes as Kinetic Intermediates: Unveiling an Overlooked Pathway in Cucurbit[8]uril-Mediated Assembly” *CCS Chem.* **2025**, accepted.
2. J. Liu, X. J. Han, N. X. Han, B. Li, Y. B. Sun, M. Wang, **G. L. Wu\*** “One-Pot ‘Click’ Synthesis of Ring-in-Rings Complexes with Customizable  $\pi$ -Stacked Dyads”, *J. Am. Chem. Soc.* **2025**, 147, 15838–15846.
3. **G. L. Wu\***, F. Li, B. H. Tang, X. Zhang\* “Molecular Engineering of Noncovalent Dimerization”, *J. Am. Chem. Soc.* **2022**, 144, 14962–14975.

# Guanglu Wu (吴光鹭)

State Key Laboratory of Supramolecular Structure and Materials  
College of Chemistry, Jilin University  
2699 Qianjin Street, Changchun 130012, P. R. China  
Phone: (+86) 13810971479  
E-mail: [guanglu@jlu.edu.cn](mailto:guanglu@jlu.edu.cn)



## EDUCATION and PROFESSIONAL EXPERIENCES

2020. 9      **Associate and Full Professor**  
–present      College of Chemistry  
                  Jilin University, China

2014–2020    **Postdoc Researcher**  
                  Department of Chemistry, University of Cambridge, UK  
                  Supervisor: Prof. Oren A Scherman

2013–2014    **Postdoc Researcher**  
                  Department of Chemistry, Tsinghua University, China  
                  Supervisor: Prof. Xi Zhang

2007–2013    **Ph.D, Chemistry**  
                  Department of Chemistry, Tsinghua University, China  
                  Supervisor: Prof. Xi Zhang

## CURRENT RESEARCH ACTIVITIES

His research focuses on the complexity of supramolecular multicomponent systems, encompassing systematic studies from construction strategies and assembly mechanisms to functional regulation.

## SELECTIVE PUBLICATIONS

1. J. Liu, X. J. Han, N. X. Han, B. Li, Y. B. Sun, M. Wang, **G. L. Wu\***, “One-Pot ‘Click’ Synthesis of Ring-in-Rings Complexes with Customizable  $\pi$ -Stacked Dyads”, *J. Am. Chem. Soc.* **2025**, 147, 15838–15846.
2. J. Liu, X. J. Han, X. Wen, H. Yu, B. Li, M. Wang, M. H. Liu\*, **G. L. Wu\***, “Chiral Ring-in-Ring Complexes with Torsion-Induced Circularly Polarized Luminescence”, *Chem. Sci.* **2025**, 16, 7858–7863.
3. **G. L. Wu\***, F. Li, B. H. Tang, X. Zhang\*, “Molecular Engineering of Noncovalent Dimerization”, *J. Am. Chem. Soc.* **2022**, 144, 14962–14975.
4. **G. L. Wu**, Z. H. Huang, O. A. Scherman\*, “Quantitative Supramolecular Heterodimerization for Efficient Energy Transfer”, *Angew. Chem. Int. Ed.* **2020**, 59, 15963–15967.
5. **G. L. Wu**, Y. J. Bae, M. Olesińska, D. Antón-García, I. Szabó, E. Rosta, M. R. Wasielewski, O. A. Scherman\*, “Controlling the Structure and Photophysics of Fluorophore Dimers Using Multiple Cucurbit[8]uril Clampings”, *Chem. Sci.* **2020**, 11, 812–825.
6. **G. L. Wu**, M. Olesińska, Y. C. Wu, D. Matak-Vinkovic, O. A. Scherman\*, “Mining 2:2 Complexes from 1:1 Stoichiometry: Formation of Cucurbit[8]uril-Diarylviologen Quaternary Complexes Favored by Electron-Donating Substituents”, *J. Am. Chem. Soc.* **2017**, 139, 3202–3208.

## Presentation Title: A Next-Generation Catalysis: Atomic Innovations for a Net-Zero World

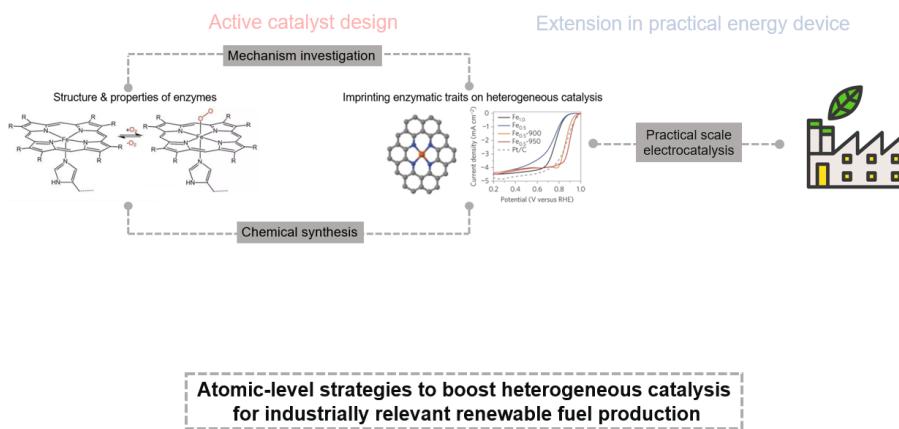
Authors: Byoung-Hoon Lee

Affiliation: KU-KIST Graduate School of Converging Science and Technology  
Department of Integrative Energy Engineering, College of Engineering  
Korea University, Seoul, Korea

Email: bhlee90@korea.ac.kr

### Abstract:

This seminar presents a material-focused approach to achieving net-zero carbon emissions, with a strong emphasis on atomic-scale catalyst design. We begin by reviewing current strategies for carbon reduction and identifying key technological bottlenecks. Next, we explore how catalysts engineered at the atomic level—supported by deep mechanistic understanding—can overcome these challenges, offering improved efficiency and selectivity. In the following section, we highlight recent system-level advances in electrochemical, photochemical, and thermochemical processes, illustrating how atomic-level innovations in materials can enable industrial-scale operations with minimal carbon output. The seminar concludes with case studies on practical fuel synthesis, along with assessments of carbon footprint, energy usage, and techno-economic performance, demonstrating how atomic-scale materials engineering can drive the transition to a carbon-neutral future.



### Reference:

1. J. Shim†, K. Lee†, Y. Yu, H. S. Lee, H. Shin, K. S. Lee, M. S. Bootharaju, S. Han, G. S. Yi, H. Ko, S. Lee, J. Ryu, M. Kim\*, **B. H. Lee\***, T. Hyeon\*, Y. E. Sung\* "Atomically Dispersed High-Valent d<sup>0</sup>-Metal Breaks the Activity–Stability Trade-Off in Proton Exchange Membrane Water Electrolysis" *J. Am. Chem. Soc.* 2025, 147, 16179.
2. C. W. Lee†, **B. H. Lee†\***, S. Park†, Y. Jung, J. Han, J. Heo, K. Lee, W. Ko, S. Yoo, M. Bootharaju, J. Ryu, K. T. Nam, M. Kim\*, T. Hyeon\* "Photochemical tuning of dynamic defects for high-performance atomically dispersed catalysts." *Nature Materials* 2024, 23, 552-559.
3. **B. H. Lee†**, H. Shin†, A. S. Rasouli†, H. Choubisa†, P. Ou, R. Dorakhan, I. Grigioni, G. Lee, E. Shirzadi, R. K. Miao, J. Wicks, S. Park, J. Zhang, Y. Chen, Z. Chen, D. Sinton, T. Hyeon\*, Y. E. Sung\*, E. H. Sargent\* "Supramolecular tuning of supported metal phthalocyanine catalysts for hydrogen peroxide electrosynthesis." *Nature Catalysis* 2023, 6, 234-243.
4. E. Jung†, H. Shin†, **B. H. Lee†**, V. Efremov, S. Lee, H. S. Lee, J. Kim, W. H. Antink, S. Park, K. S. Lee, S. P. Cho, J. S. Yoo\*, Y. E. Sung\*, T. Hyeon\* "Atomic-level Tuning of Co-N-C Catalyst for High-Performance Electrochemical H<sub>2</sub>O<sub>2</sub> Production." *Nature Materials* 2020, 19, 436-442.

## Byoung-Hoon Lee

KU-KIST Graduate School of Converging Science and Technology  
Department of Integrative Energy Engineering, College of Engineering  
Republic of Korea

Phone: (+82) 2-3290-5966  
E-mail: bhlee90@korea.ac.kr



### EDUCATION and PROFESSIONAL EXPERIENCES

2023. 9	<b>Assistant Professor</b>
–present	KU-KIST Graduate School of Converging Science and Technology Korea University, Seoul, Korea
2021–2023	<b>Postdoctoral Researcher</b> Department of Electrical and Computer Engineering, University of Toronto, Canada Supervisor: Prof. Edward H. Sargent
2019–2021	<b>Postdoctoral Researcher</b> Department of Chemical and Biological Engineering, Seoul National University, Korea Supervisor: Prof. Taeghwan Hyeon
2015–2019	<b>Ph.D. in Chemical and Biological Engineering</b> Department of Chemical and Biological Engineering, Seoul National University, Korea Supervisor: Prof. Taeghwan Hyeon

### CURRENT RESEARCH ACTIVITIES

Energy Materials; Nano Materials; Electrochemical CO<sub>2</sub> capture; Heterogeneous Catalysis; Electro Catalysis; Single Atom Catalysts; Water Electrolyzer; Electrochemical Energy Device

### SELECTIVE PUBLICATIONS

1. J. Shim†, K. Lee†, Y. Yu, H. S. Lee, H. Shin, K. S. Lee, M. S. Bootharaju, S. Han, G. S. Yi, H. Ko, S. Lee, J. Ryu, M. Kim\*, **B. H. Lee\***, T. Hyeon\*, Y. E. Sung\* "Atomically Dispersed High-Valent d<sup>0</sup>-Metal Breaks the Activity–Stability Trade-Off in Proton Exchange Membrane Water Electrolysis" *J. Am. Chem. Soc.* 2025, 147, 16179.
2. C. W. Lee†, **B. H. Lee†\***, S. Park†, Y. Jung, J. Han, J. Heo, K. Lee, W. Ko, S. Yoo, M. Bootharaju, J. Ryu, K. T. Nam, M. Kim\*, T. Hyeon\* "Photochemical tuning of dynamic defects for high-performance atomically dispersed catalysts." *Nature Materials* 2024, 23, 552-559.
3. **B. H. Lee†**, H. Shin†, A. S. Rasouli†, H. Choubisa†, P. Ou, R. Dorakhan, I. Grigioni, G. Lee, E. Shirzadi, R. K. Miao, J. Wicks, S. Park, J. Zhang, Y. Chen, Z. Chen, D. Sinton, T. Hyeon\*, Y. E. Sung\*, E. H. Sargent\* "Supramolecular tuning of supported metal phthalocyanine catalysts for hydrogen peroxide electrosynthesis." *Nature Catalysis* 2023, 6, 234-243.
4. E. Jung†, H. Shin†, **B. H. Lee†**, V. Efremov, S. Lee, H. S. Lee, J. Kim, W. H. Antink, S. Park, K. S. Lee, S. P. Cho, J. S. Yoo\*, Y. E. Sung\*, T. Hyeon\* "Atomic-level Tuning of Co-N-C Catalyst for High-Performance Electrochemical H<sub>2</sub>O<sub>2</sub> Production." *Nature Materials* 2020, 19, 436-442.

**Presentation Title:** Application of Single-Molecule Force Spectroscopy in Studying the Mechanisms of Drug Action

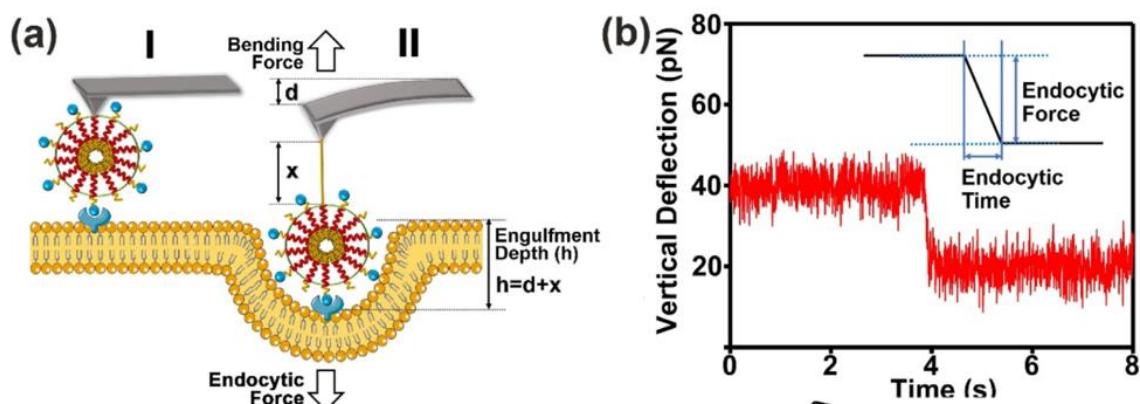
**Authors:** Wenke Zhang

**Affiliation:** State Key Laboratory of Supramolecular Structure and Materials, College of Chemistry, Jilin University, Changchun 130012, P R China

**Email:** zhangwk@jlu.edu.cn

**Abstract:**

Investigating the interaction mechanisms between drug molecules and their carriers with biomacromolecules (such as nucleic acids and proteins) and even living cells, at the molecular level, holds significant guiding implications for revealing drug action mechanisms, optimizing drug design, and developing new therapeutics. This presentation will introduce our research group's progress in the following areas: utilizing atomic force microscopy-based single-molecule force spectroscopy and related techniques to investigate the higher-order structures of nucleic acids and their dynamic transformations[1-3]; and the interaction mechanisms between nanomedicines and cells[4], bacteria[5], and viruses[6], as well as the structure-property relationships involved.



**Fig. 1** Single-molecule force spectroscopy study on the effect of PEGylation on the cell-nanomicelle interactions

**Reference:**

1. Y. Song, Z. W. Ma, W. K. Zhang, *Macromolecules*, 2022, 55, 4177–4199.
2. X. N. Zhang, W. K. Zhang, et al., *CCS Chem.*, 2022, 4, 3023–3035.
3. X. N. Zhang, W. K. Zhang, et al., *Nucleic Acids Res.*, 2020, 48, 6458–6470.
4. W. Zhang, W. K. Zhang, et al., *Acta Biomater.*, 2023, 157, 310–320.
5. Y. Q. Zhang, W. K. Zhang, et al., *ACS Materials Lett.*, 2024, 6, 2409–2415.
6. H. J. Wang, Y. Chen, W. K. Zhang, et al., *Nanoscale*, 2019, 11, 16368–16376.

## Wenke Zhang (张文科)

State Key Laboratory of Supramolecular Structure and Materials  
College of Chemistry, Jilin University  
2699 Qianjin Street, Changchun 130012, P. R. China  
Phone: (+86) 431-8515-9203  
E-mail: zhangwk@jlu.edu.cn



### EDUCATION and PROFESSIONAL EXPERIENCES

2007. 6      **Professor**  
–present      College of Chemistry  
                  Jilin University, Changchun, China

2003–2007      **Postdoc Researcher**  
                  School of Pharmacy, School of Chemistry, The University of Nottingham, UK

2001–2002      **Joint-training Ph. D.**  
                  Department of Physics, LMU, Germany   Supervisor: Prof. Hermann E. Gaub

1997–2002      **Ph.D, Chemistry**  
                  College of Chemistry, Jilin University, China   Supervisor: Prof. Xi Zhang

### CURRENT RESEARCH ACTIVITIES

Single-molecule force spectroscopy for supramolecular and polymer sciences; Polymer crystallization; Nanomedicine for the treatment of cancer or bacterial infection; Polymer mechanochemistry.

### SELECTIVE PUBLICATIONS

1. Y. Song, Z. Ma, W. K. Zhang\*, “Manipulation of a Single Polymer Chain: From the Nanomechanical Properties to Dynamic Structure Evolution”, *Macromolecules* **2022**, 55, 4177–4199.
2. X. Zhang, H. Zhang, S. Lu, Y. Song\*, W. K. Zhang\*, “Direct Detection of the Chain Trajectory and Long-Range Correlation in Crystalline–Amorphous Polymer Networks by Single-Molecule Force Spectroscopy”, *Macromolecules* **2025**, ASAP.
3. J. Hou, N. Li, W. Zhang\*, W. K. Zhang\*, “Exploring the Impact of PEGylation on the Cell-nanomicelle Interactions by AFM-based Single-Molecule Force Spectroscopy and Force Tracing”, *Acta Biomater.* **2023**, 157, 310–320.
4. Y. Zhang, W. Feng, W. K. Zhang\*, “Tetrahedral DNA Enhanced Antibacterial Effect of Lysozyme”, *ACS Materials Lett.* **2024**, 6, 2409–2415.
5. Z. Ma, H. Zhang, Y. Song, Q. Mei, P. Shi, J. W. Park, W. K. Zhang\*, “Increasing the Mechanical Stability of Polymer–Gold Interfacial Connection: A Parallel Covalent Strategy”, *ACS Macro Lett.* **2023**, 12, 421–427.
6. X. Liu, R. Yao, Z. Sun, H. Zhang, F. Yan\*, H. Li, W. K. Zhang\*, “Single-Molecule Study Reveals Ion-Dependent Conformational Change and Nanomechanical Property of Crown Ether-Based Polymer”, *Macromolecules* **2024**, 57, 3798–3806.

**Presentation Title:** Systematic Design of Low Dielectric Loss Poly(phenylene sulfide)s

**Authors:** Seigo Watanabe

**Affiliation:** Research Institute for Science and Engineering, Waseda University, 3-4-1 Okubo, Shinjuku-ku, Tokyo 169-8555, Japan.

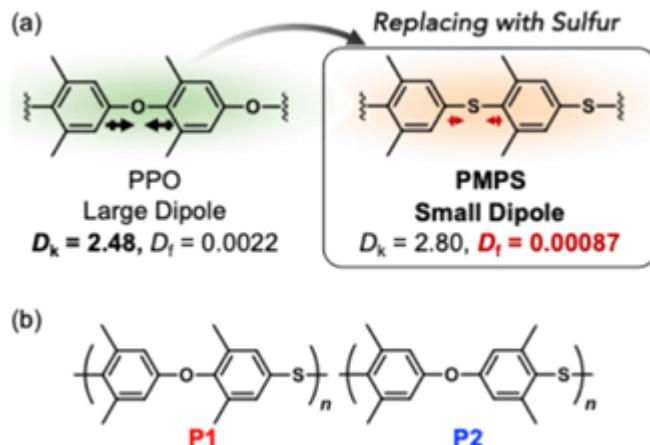
**Email:** swatanabe@aoni.waseda.jp

**Abstract:**

With the recent development in the Internet of Things (IoT) and artificial intelligence (AI), there has been a great demand for low-loss, high-frequency telecommunications, and in particular, insulating polymers with low dielectric constant ( $D_k$ ) and low loss tangent ( $D_f$ ) are essential.<sup>1</sup> Their molecular design typically involves introducing substructures with low polarizability, small dipoles, and high rigidity to reduce electric-field responsiveness, such as fluorine/siloxane-containing polyimides<sup>2,3</sup> and poly(phenylene oxide)s.<sup>4</sup> However, most low dielectric loss polymers consist of partially polar structures (e.g., imides, ethers) which induce microscopic polarity, suggesting an empirical limit in  $D_f$ .

In this context, we focused on poly(2,6-dimethyl-1,4-phenylenesulfide) (**PMPS**) as a promising low-dielectric-loss polymer candidate by lacking any polar structures in the repeating unit (**Figure 1**).<sup>5</sup> Regarding the dielectric loss of **PMPS** and its copolymers with PPO (**P1** and **P2**),  $D_f$  decreased and  $D_k$  increased systematically alongside increasing sulfur content. Importantly, **PMPS** displayed an exceptionally low  $D_f$  (0.00087 at 10 GHz), outperforming prior aromatic polymers owing to the low polarity of sulfide bonds.

Furthermore, we investigated the **PMPS/P1** polymer blends to adjust dielectric loss and thermal properties, succeeding in a simultaneous decrease in  $D_k$  and  $D_f$  due to the balanced ether and sulfide content. Also, we expanded the molecular design to thermosetting polymers, composed of **PMPS** and low-polar benzocyclobutene units<sup>6</sup> as cross-linkable moieties, achieving improved thermostability (glass transition temperature:  $T_g > 200$  °C) while maintaining low dielectric loss. Their detailed mechanisms and structure- $D_k/D_f$  relationships will also be discussed.



**Figure 1.** Research outline. (a) Comparison of dielectric properties for PPO and **PMPS**. (b) Structures of copolymers.

**References:**

1. H. Qiu *et al.*, *Macromol. Rapid Commun.* **2024**, *45*, e2300601.
2. C.-S. Hsu *et al.*, *ACS Appl. Mater. Interfaces* **2025**, *17*, 18931–18939.
3. T. Hayakawa *et al.*, *Macromol. Rapid. Commun.* **2025**, *46*, 2500115.
4. H. Yang *et al.*, *ACS Appl. Polym. Mater.* **2024**, *6*, 4708–4717.
5. S. Watanabe, S. Miura, T. Miura, Y. Tsunekawa, D. Ito, K. Oyaizu, *in revision*.
6. W. Fu *et al.*, *Macromol. Chem. Phys.* **2025**, *226*, 2400338.

## Seigo Watanabe (渡辺清瑚)



Research Institute for Science and Engineering  
Waseda University, 3-4-1 Okubo, Shinjuku-ku, Tokyo 169-8555, Japan.  
Phone: (+81) 3-5286-3120  
E-mail: swatanabe@aoni.waseda.jp

### EDUCATION and PROFESSIONAL EXPERIENCES

2024.04	<b>Junior Researcher (Assistant Professor)</b>
–present	Research Institute for Science and Engineering Polymer Chemistry Laboratory, Waseda University, Japan
2024	<b>Visiting Researcher</b> Supervisor: Prof. Rubén D. Costa, Technical University of Munich, Germany
2022–2024	JSPS Research Fellow (DC2)
2021–2024	<b>Ph. D. in Polymer Chemistry</b> Supervisor: Prof. Kenichi Oyaizu, Waseda University, Japan
2019–2021	<b>M. Eng. in Polymer Chemistry</b>
2015–2019	<b>B. Eng. in Polymer Chemistry</b> Department of Applied Chemistry, Waseda University, Japan Supervisor: Prof. Kenichi Oyaizu

### CURRENT RESEARCH ACTIVITIES

Synthesis of Sulfur-containing Polymers; High Refractive Index Polymers; Low Dielectric Loss Polymers; Adhesive Polymers; Polymer-inorganic Hybrid Materials; Degradable Polymers; Sustainable Polyelectrolytes for Light-emitting Devices

### SELECTIVE PUBLICATIONS

1. S. Watanabe, Z. An, H. Nishio, Y. Tsunekawa, K. Oyaizu, “Poly(dibenzothiophenylene sulfide)s: Sulfur-rich Annulated Frameworks with Wide-Range Ultrahigh Refractive Index”, *J. Mater. Chem. C* **2025**, *13*, 7933.
2. S. Watanabe, T. Yano, Z. An, K. Oyaizu, “Aromatic Poly(dithioacetal)s: Spanning Degradability, Thermostability, and High Refractive Index Towards Eco-friendly Optics”, *ChemSusChem* **2025**, *18*, e202401609.
3. S. Watanabe, L. M. Cavinato, V. Calvi, R. van Rijn, R. D. Costa, K. Oyaizu, “Polarizable H-bond Concept in Aromatic Poly(thiourea)s: Unprecedented High Refractive Index, Transmittance and Degradability at Force to Enhance Lighting Efficiency”, *Adv. Funct. Mater.* **2024**, *34*, 2404433.
4. S. Watanabe, Y. Tsunekawa, T. Takayama, K. Oyaizu, “Diverse Side-chain Transformation of High Refractive Index Methylthio-substituted Poly(phenylene sulfide)s”, *Macromolecules* **2024**, *57*, 2897–2904.
5. S. Watanabe, T. Takayama, K. Oyaizu, “Transcending the Trade-off in Refractive Index and Abbe Number for Highly Refractive Polymers: Synergistic Effect of Polarizable Skeletons and Robust Hydrogen Bonds”, *ACS Polym. Au* **2022**, *2*, 458–466.
6. S. Watanabe, K. Oyaizu, “Designing Ultrahigh-Refractive-Index Amorphous Poly(phenylene sulfide)s Based on Dense Intermolecular Hydrogen-Bond Networks”, *Macromolecules* **2022**, *55*, 2252–2259.

**Presentation Title:** Architecting Bioactive Supramolecules: From Molecular Design to Functional Nanostructures

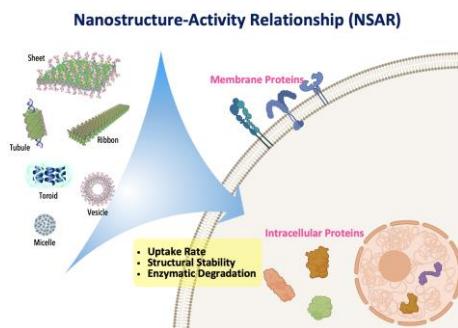
**Authors:** Yongju Kim

**Affiliation:** KU-KIST Graduate School of Converging Science and Technology  
Department of Integrative Energy Engineering, College of Engineering  
Korea University, Seoul, Korea

**Email:** yongjukim@korea.ac.kr

**Abstract:**

Supramolecular assemblies, defined by non-covalent interactions, are central to numerous biological processes due to their dynamic and adaptable structures. This study explores the intricate relationships between the molecular design of supramolecular assemblies and their biological functions. The arrangement and organization of these assemblies significantly influence their efficiency and specificity in various applications, including drug delivery, molecular recognition, and fluorescence imaging. Here, I present recent advancements in supramolecular materials and their ability to form diverse, functional nanostructures with targeted biological applications. Key highlights include tamoxifen-selective fluorescent assembly, 2D peptide assemblies, enhanced cGAMP stability, membrane-to-vesicle transformations, and a non-cytotoxic quercetin fluorophore. Our results demonstrate that even slight modifications in supramolecular components can lead to significant changes in their activity, underscoring the importance of precise molecular design in optimizing supramolecular systems for biological applications.



**Reference:**

1. T. Kim, J. Y. Park, J. Hwang, G. Seo, **Y. Kim\*** "Supramolecular Two-dimensional Systems and their Biological Applications" *Adv. Mater.* **2020**, 32, 2002405.
2. G. Seo, T. Kim, B. Shen, J. Kim, **Y. Kim\*** "Transformation of Supramolecular Membranes to Vesicles driven by Spontaneous Gradual Deprotonation on Membrane Surfaces" *J. Am. Chem. Soc.* **2022**, 144, 17341.
3. T. Kim, J. Hong, J. Kim, J. Cho, **Y. Kim\*** "Two-dimensional peptide assembly via arene–perfluoroarene interactions for proliferation and differentiation of myoblasts" *J. Am. Chem. Soc.* **2023**, 145, 1793.
4. J. Y. Park, M. Kang, S. Lim, H. Cho, S. Yang, S. Y. Baek, L. Tan, C. Song, M. Lee, B. Yeom, J. S. Ha, S. Lee\*, **Y. Kim\*** "Assembly of 2',3'-Cyclic Guanosine Monophosphate-Adenosine Monophosphate and Their Spontaneous Intracellular Disassembly for Enhanced Antitumor Immunity via Natural STING Pathway Activation" *Chem. Eng. J.* **2024**, 500, 157037.
5. J. Y. Park, J. Kim, J. S. Ha, **Y. Kim\*** "Self-Assembled Tamoxifen-Selective Fluorescent Nanomaterials Driven by Molecular Structural Similarity." *Eur. J. Org. Chem.* **2023**, 27, e202300807. *Nature Materials* 2020, 19, 436-442.

# **Yongju Kim (金容柱)**

KU-KIST Graduate School of Converging Science and Technology  
Department of Integrative Energy Engineering, College of Engineering  
Republic of Korea  
Phone: (+82) 2-3290-4618  
E-mail: yongjukim@korea.ac.kr



## **EDUCATION and PROFESSIONAL EXPERIENCES**

2019. 3      **Associate and Full Professor**  
–present      KU-KIST Graduate School of Converging Science and Technology  
                  Korea University, Seoul, Korea

2014–2019    **Associate and Full Professor**  
                  State Key Laboratory of Supramolecular Structure and Materials, Jilin University,  
                  China

2013–2014    **Postdoc Researcher**  
                  State Key Laboratory of Supramolecular Structure and Materials, Jilin University, China  
                  Supervisor: Prof. Myongsoo Lee

2005–2012    **Ph.D. in Organic Chemistry**  
                  Department of Chemistry, Seoul National University, Korea  
                  Supervisor: Prof. Seung Bum Park

## **CURRENT RESEARCH ACTIVITIES**

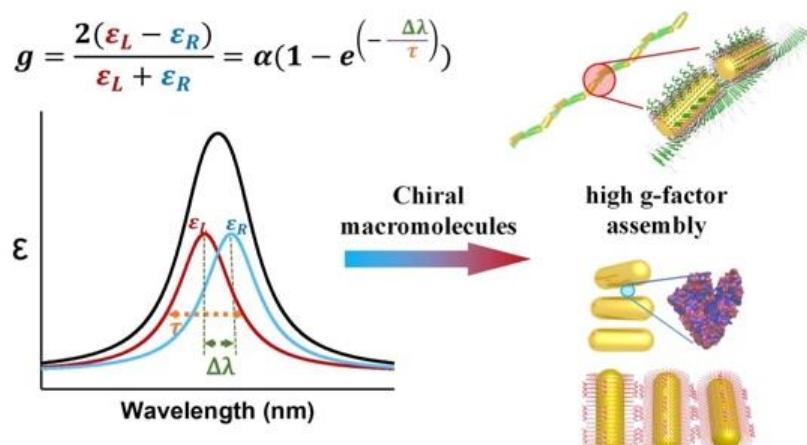
Supramolecular Medicinal Chemistry; Biomolecule-based Materials (peptides, proteins, nucleic acids, carbohydrates); Drug-Delivery Systems; Organic Synthesis and Chemical Biology; Nanostructure-Activity Relationship (NSAR) Study

## **SELECTIVE PUBLICATIONS**

1. J. Y. Park, M. Kang, S. Lim, H. Cho, S. Yang, S. Y. Baek, L. Tan, C. Song, M. Lee, B. Yeom, J. S. Ha, S. Lee\*, **Y. Kim\*** “Assembly of 2',3'-Cyclic Guanosine Monophosphate-Adenosine Monophosphate and Their Spontaneous Intracellular Disassembly for Enhanced Antitumor Immunity via Natural STING Pathway Activation.” *Chem. Eng. J.* **2024**, 500, 157037.
2. T. Kim, J. Hong, J. Kim, J. Cho, **Y. Kim\*** “Two-dimensional peptide assembly via arene–perfluoroarene interactions for proliferation and differentiation of myoblasts.” *J. Am. Chem. Soc.* **2023**, 145, 1793.
3. G. Seo, T. Kim, B. Shen, J. Kim, **Y. Kim\*** “Transformation of supramolecular membranes to vesicles driven by spontaneous gradual deprotonation on membrane surfaces.” *J. Am. Chem. Soc.* **2022**, 144, 17341.
4. T. Kim, J. Y. Park, J. Hwang, G. Seo, **Y. Kim\*** “Supramolecular two-dimensional systems and their biological applications.” *Adv. Mater.* **2020**, 32, 2002405.
5. B. Sun, **Y. Kim\***, Y. Wang, H. Wang, J. Kim, X. Liu, M. Lee\* “Homochiral porous nanosheets for enantiomer sieving.” *Nat. Mater.* **2018**, 17, 599–604.
6. **Y. Kim**, H. Li, Y. He, X. Chen, X. Ma, M. Lee “Collective helicity switching of a DNA-coat assembly.” *Nat. Nanotech.* **2017**, 12, 551–556.

**Presentation Title:** Biomolecular Induced Chiral Assembly of Plasmonic Nanoparticles**Authors:** Kun Liu**Affiliation:** Key Laboratory of Supramolecular Structure and Materials, College of Chemistry, Jilin University, P. R. China**Email:** kliu@jlu.edu.cn**Abstract:**

Irregular changes in chiral structures of biomolecules are closely related to many major diseases. However, the detection of irregular changes of biomolecules is highly challenging due to their weak chiroptical signals. The transfer and amplification of the chiroptical signals of biomolecules by using surface plasmonic nanoparticles hold great promise for the early diagnosis of major diseases. Our research has focused on bio-macromolecular mediated chiral assembly of plasmonic nanoparticles. In the present talk, I would like to share with you how we have derived a more universal equation to correlate the order of nanostructures with the asymmetric factor (g-factor), which was used to guide the chiral assembly nanostructures with long-range order and with giant g-factors (up to 0.12) We have also developed a series of new synthetic methods for chiral shaped nanoparticle enantiomers, of which the chiral assembly lead to a further increase of g-factors to 0.24. In addition, we have discovered the chiral morphology dependent of chiral cellular uptake for the chiral enantiomers. These works paved new paths for the transfer and amplification of the chiral signal of bio-molecules.

**Reference:**

1. Lu, J.; Yao Xue, Y.; Bernardino, K.; Zhang, N.-N.; Gomes, W. R.; Ramesar, N. S.; Liu, S.; Zheng Hu, Z.; Sun, T.; Farias de Moura, A.; Kotov, N. A.; Liu, K. *Science* **2021**, *371*, 1368.
2. Zhang, N.-N.; Sun, H.-R.; Liu, S.; Xing, Y.-C.; Lu, J.; Peng, F.; Han, C.-L.; Wei, Z.; Sun, T.; Yang, B.; Liu, K. *CCS Chemistry* **2022**, *4*, 660.
3. Kang, J.; Wang, Y.; Peng, F.; Zhang, N.-N.; Xue, Y.; Yang, Y.; Kumacheva, E.; Liu, K. *Angew. Chem. Int. Ed.* **2022**, *61*, e202202405.
4. Zhang, N.-N.; Shen, Z.-L.; Gao, S.-Y.; Peng, P.; Cao, Z.-J.; Wang, Y.; Wang, Z.-Z.; Zhang, W.; Yang, Y.; Liu, K.; Sun, T. *Adv. Optical Mater.* **2023**, *11*, 2203119.
5. Zhang, N.-N.; Mychinko, M.; Gao, S.-Y.; Yu, L.; Shen, Z.-L.; Wang, L.; Peng, F.; Wei, Z.; Wang, Z.; Zhang, W.; Zhu, S.; Yang, Y.; Sun, T.; Liz-Marzán, L. M.; Bals, S.; Liu, K. *Nano Letters* **2024**, *24*, 13027

## Kun Liu (刘堃)



State Key Laboratory of Supramolecular Structure and Materials  
College of Chemistry, Jilin University  
2699 Qianjin Street, Changchun 130012, P. R. China  
Phone: (+86) 431-89228926  
E-mail: kliu@jlu.edu.cn

### EDUCATION and PROFESSIONAL EXPERIENCES

2012. 10      **Professor**  
–present      State Key Laboratory of Supramolecular Structure and Materials  
                  College of Chemistry, Jilin University

2008–2012      **Postdoc Researcher**  
                  Department of Chemistry, University of Toronto, ON, CANADA  
                  Supervisor: Prof. Eugenia Kumacheva

1996–1999      **Ph.D, Chemistry**  
                  Department of Chemistry, University of Toronto, ON, CANADA  
                  Supervisor: Prof. Ian Manners

### CURRENT RESEARCH ACTIVITIES

Polymer Grafted Nanoparticles, Polynanomers (Polynanoparticles), Plasmonic Nanomaterials, Aluminum Nanoparticles, Chiral Nanomaterials.

### SELECTIVE PUBLICATIONS

1. Wang, J.; Chen, H.; Chen, D.; Luo, Y.; Shen, Z.-L.; Zhang, N.-N.; Dong, B.; Tian, W.; **Liu, K.**\* and Xu, B. Stabilizing Gold Nanotetrapods via In Situ Polymerization for Superior Photoacoustic and Photothermal Applications *Nano Lett.* **2025**, *21*, 8758–8767.
2. Zhang, N.-N.; Mychinko, M.; Gao, S.-Y.; Yu, L.; Shen, Z.-L.; Wang, L.; Peng, F.; Wei, Z.; Wang, Z.; Zhang, W.; Zhu, S.; Yang, Y.; Sun, T.-M.; Liz-Marzán, L. M.\*; Bals, S.\* and **Liu, K.**\* Self-Matching Assembly of Chiral Gold Nanoparticles Leads to High Optical Asymmetry and Sensitive Detection of Adenosine Triphosphate *Nano Lett.* **2024**, *24*, 13027–13036.
3. Zhang, N.-N.; Sun, H.-R.; Liu, S.; Xing, Y.-C.; Lu, J.; Peng, F.; Han, C.-L.; Wei, Z.; Sun, T.-M.; Yang, B.; **Liu, K.**\* Gold Nanoparticle Enantiomers and Their Chiral-Morphology Dependence of Cellular Uptake *CCS Chem.* **2022**, *4*, 660–670.
4. Kang, J.; Wang, Y.; Peng, F.; Zhang, N.-N.; Xue, Y.; Yang, Y.; Kumacheva, E.\* and **Liu, K.**\* Oxidative Elimination and Reductive Addition of Thiol-Terminated Polymer Ligands to Metal Nanoparticles *Angew. Chem. Int. Ed.* **2022**, *61*, e202202405.
5. Tao, X.; Li, Y.; Yu, L.; Zhang, Y.; Han, C.; Yang, Y.; Qian, H.; Lu, Z.\* and Liu, K.\* Two-Dimensional Polymer Networks Locking on Inorganic Nanoparticles *Angew. Chem. Int. Ed.* **2023**, *62*, e202216620.
6. Lu, J.; Xue, Y.; Bernardino, K.; Zhang, N.-N.; Gomes, R. W.; Ramesar, S. N.; Liu, S.; Hu, Z.; Sun, T.-M.; de Moura, A. F.\*; Kotov, A. N.\* and **Liu, K.**\* Enhanced Optical Asymmetry in Supramolecular Chiroplasmonic Assemblies with Long-Range Order *Science* **2021**, *371*, 1368–1374.

**Presentation Title:** Nickel-Catalyzed 1,2-Difunctionalization of Unactivated Alkenes Directed by Native Functional Groups.

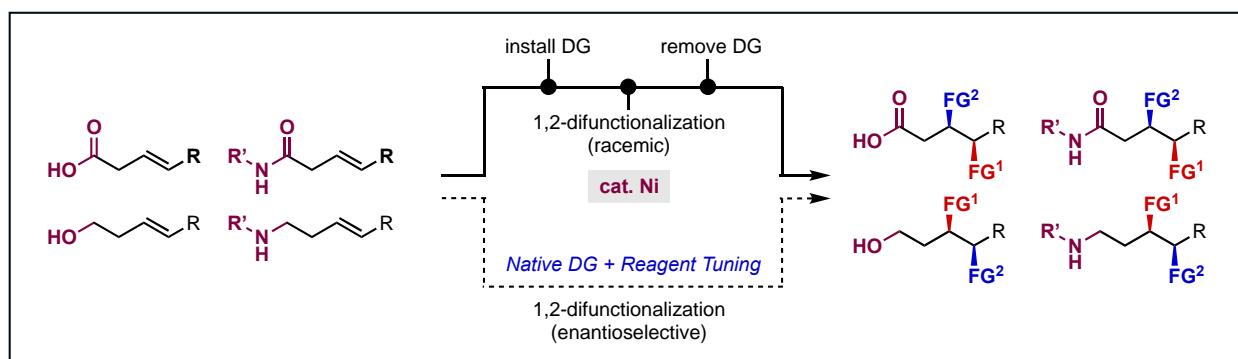
**Authors:** Taeho Kang

**Affiliation:** Department of Chemistry, Korea University, Seoul, Korea

**Email:** taehokang@korea.ac.kr

**Abstract:**

Transition-metal-catalyzed alkene difunctionalization is a powerful approach toward rapid assembly of molecular complexity. Traditionally, strategies using bidentate directing auxiliaries (e.g., 8-aminoquinoline) have been employed to control regioselectivity and stabilize metalacycle intermediates formed during the reaction. While use of this type of removable directing group has assisted development of a variety of unique alkene functionalization reactions, the necessity of at least two steps for installation and removal of the directing auxiliary significantly decreases the synthetic utility of these methods. To overcome this limitation, we became interested in translating auxiliary-based reactivity to substrates containing only native functional groups. To this end, we developed carboxylate/sulfonamide-directed dicarbofunctionalization, alcohol/amine/amide-directed carboamination of unactivated alkenes using a Ni catalyst. Under the optimized conditions, the desired products were obtained with excellent regio- and *syn*-stereoselectivity from simple alkenyl compounds in one step.



**Reference:**

1. Apolinar, O.<sup>†</sup>; **Kang, T.**<sup>†</sup>; Alturaifi, T. M.; Bedekar, P. G.; Rubel, C. Z.; Derosa, J.; Sanchez, B. B.; Wong, Q. N.; Sturgell, E. J.; Chen, J. S.; Wisniewski, S. R.; Liu, P.; Engle, K. M. Three-Component Asymmetric Ni-Catalyzed 1,2-Dicarbofunctionalization of Unactivated Alkenes via Stereoselective Migratory Insertion. *J. Am. Chem. Soc.* **2022**, *144*, 19337. (<sup>†</sup>Authors contributed equally.)
2. **Kang, T.**; González, J. M.; Li, Z.-Q.; Foo, K.; Cheng, P. T.; Engle, K. M. Alkene Difunctionalization Directed by Free Amines: Diamine Synthesis via Nickel-Catalyzed 1,2-Carboamination. *ACS Catal.* **2022**, *12*, 3890.
3. **Kang, T.**; Kim, N.; Cheng, P. T.; Zhang, H.; Foo, K.; Engle, K. M. Nickel-Catalyzed 1,2-Carboamination of Alkenyl Alcohols. *J. Am. Chem. Soc.* **2021**, *143*, 13962.
4. Derosa, J.<sup>†</sup>; **Kang, T.**<sup>†</sup>; Tran, V. T.; Wisniewski, S. R.; Karunananda, M. K.; Jankins, T. C.; Xu, K. L.; Engle, K. M. Nickel-Catalyzed 1,2-Diarylation of Alkenyl Carboxylates A Gateway to 1,2,3-Trifunctionalized Building Blocks. *Angew. Chem. Int. Ed.* **2020**, *59*, 1201. (<sup>†</sup>Authors contributed equally.)

# Taeho Kang (姜兌昊)

Department of Chemistry, Korea University  
Republic of Korea  
Phone: (+82) 2-3290-3130  
E-mail: taehokang@korea.ac.kr



## EDUCATION and PROFESSIONAL EXPERIENCES

2025. 3      **Assistant Professor**  
–present      Department of Chemistry, Korea University, Seoul, Korea

2023–2025      **Postdoctoral Associate**  
                    Department of Chemistry, Cornell University, USA  
                    Supervisors: Profs. Geoffrey W. Coates and Yadong Wang

2018–2023      **Ph.D. in Chemistry**  
                    Department of Chemistry, The Scripps Research Institute, USA  
                    Supervisor: Prof. Keary M. Engle

## CURRENT RESEARCH ACTIVITIES

Organic Synthesis; Organometallic Chemistry; Transition Metal Catalysis; Polymer Chemistry

## SELECTIVE PUBLICATIONS

1. Apolinar, O.<sup>†</sup>; **Kang, T.**<sup>†</sup>; Alturaifi, T. M.; Bedekar, P. G.; Rubel, C. Z.; Derosa, J.; Sanchez, B. B.; Wong, Q. N.; Sturgell, E. J.; Chen, J. S.; Wisniewski, S. R.; Liu, P.; Engle, K. M. Three-Component Asymmetric Ni-Catalyzed 1,2-Dicarbofunctionalization of Unactivated Alkenes via Stereoselective Migratory Insertion. *J. Am. Chem. Soc.* **2022**, *144*, 19337. (†Authors contributed equally.)
2. **Kang, T.**; González, J. M.; Li, Z.-Q.; Foo, K.; Cheng, P. T.; Engle, K. M. Alkene Difunctionalization Directed by Free Amines: Diamine Synthesis via Nickel-Catalyzed 1,2-Carboamination. *ACS Catal.* **2022**, *12*, 3890.
3. **Kang, T.**; Kim, N.; Cheng, P. T.; Zhang, H.; Foo, K.; Engle, K. M. Nickel-Catalyzed 1,2-Carboamination of Alkenyl Alcohols. *J. Am. Chem. Soc.* **2021**, *143*, 13962.
4. **Kang, T.**; Erbay, T. G.; Xu, K. L.; Gallego, G. M.; Burtea, A.; Nair, S. K.; Patman, R. L.; Zhou R.; Sutton, S. C.; McAlpine, I. J.; Liu, P.; Engle, K. M. Multifaceted Substrate–Ligand Interactions Promote the Copper-Catalyzed Hydroboration of Benzylidene cyclobutanes and Related Compounds. *ACS Catal.* **2020**, *10*, 13075.
5. Derosa, J.<sup>†</sup>; **Kang, T.**<sup>†</sup>; Tran, V. T.; Wisniewski, S. R.; Karunananda, M. K.; Jankins, T. C.; Xu, K. L.; Engle, K. M. Nickel-Catalyzed 1,2-Diarylation of Alkenyl Carboxylates A Gateway to 1,2,3-Trifunctionalized Building Blocks. *Angew. Chem. Int. Ed.* **2020**, *59*, 1201. (†Authors contributed equally.)

**Presentation Title:** Ordered Mesoporous Organosiloxane Elastomers using assemblies of Silica Nanospheres as Templates toward Nanoparticle Separation

**Authors:** Takamichi Matsuno

**Affiliation:** Department of Applied Chemistry, Faculty of Science and Engineering, Waseda University, 3-4-1 Okubo, Shinjuku-ku, Tokyo 169-8555, Japan

Kagami Memorial Research Institute for Materials Science and Technology, Waseda University, 2-8-26 Nishiwaseda, Shinjuku-ku, Tokyo 169-0051, Japan

**Email:** matsuno@aoni.waseda.jp

**Abstract:**

Elastic nanoporous materials are potentially useful for controlling the separation of various substances due to their reversible pore deformation.<sup>1</sup> Our group previously synthesized ordered nanoporous organosiloxane materials, including elastomers (~74 nm in pore diameter), using ordered assemblies of silica nanospheres (silica colloidal crystals, SCCs) as a template.<sup>2,3</sup> If the pore size can be further reduced to the mesoporous regime, it is expected to enable the separation of various sizes of substances, such as large molecules and nanoparticles. However, the pore structure collapsed when the size of the template nanospheres was reduced to ~50 nm. Herein, ordered mesoporous organosiloxane elastomers were successfully prepared by optimizing the template removal conditions, and nanoparticle separation was demonstrated.

A dispersion of 48 nm silica nanospheres was prepared and dried to obtain the SCCs based on our previous report.<sup>2,4</sup> Poly[(mercaptopropyl)methylsiloxane] (PMMS) and 2,4,6,8-tetramethyl-2,4,6,8-tetravinylcyclotetrasiloxane (D4V) were cross-linked by the thiol-ene reaction inside the nanopores of the SCCs. A highly ordered mesoporous structure was obtained by the preferential dissolution of silica using a base solution. The resulting powder samples were packed in the column and used for the nanoparticle separation.

The electron microscopy, small-angle X-ray scattering (SAXS), and N<sub>2</sub> adsorption–desorption analyses confirmed the three-dimensionally ordered spherical nanopores (~40 nm in diameter). The SAXS results showed an anisotropic pattern under compression, suggesting pore deformation. In the nanoparticle separation test, a mixed dispersion of silica nanospheres with diameters of 12 nm and 48 nm passed through the prepared column. The size exclusion chromatographic separation varied depending on whether the column packing was compressed or not.

**References:**

1. H. Nishihara, T. Simura, S. Kobayashi, K. Nomura, R. Berenguer, M. Ito, M. Uchimura, H. Iden, K. Arihara, A. Ohma, Y. Hayasaka, and T. Kyotani, *Adv. Funct. Mater.* **2016**, *26*, 6418.
2. N. Muramoto, T. Matsuno, H. Wada, K. Kuroda, and A. Shimojima, *Chem. Lett.* **2021**, *50*, 1038.
3. N. Muramoto, T. Sugiyama, T. Matsuno, H. Wada, K. Kuroda, and A. Shimojima, *Nanoscale* **2020**, *12*, 21155.
4. K.-M. Choi and K. Kuroda, *Chem. Commun.* **2011**, *47*, 10933.

## Takamichi Matsuno (松野敬成)

Department of Applied Chemistry,  
Faculty of Science and Engineering, Waseda University, 3-4-1 Okubo,  
Shinjuku-ku, Tokyo  
Phone: (+81) 3-5286-3281  
E-mail: matsuno@aoni.waseda.jp



### EDUCATION and PROFESSIONAL EXPERIENCES

2021–present **Assistant Professor**  
Department of Applied Chemistry, Faculty of Science and Engineering, Waseda University

2018–2021 **Ph.D, Applied Chemistry**  
Department of Applied Chemistry, Faculty of Science and Engineering, Waseda University  
Supervisor: Prof. Kazuyuki Kuroda

2015–2018 **Researcher**  
Teijin Limited (development of polymer materials)

### CURRENT RESEARCH ACTIVITIES

Inorganic synthetic chemistry, especially the precise synthesis of crystalline nanoporous materials with ordered nanopores and controlled crystallite size for understanding the correlation between nanostructures and physicochemical properties; Design of functional nanoporous oxide materials, including catalysts, thermoelectric materials, and adsorbents/separators.

### SELECTIVE PUBLICATIONS

1. D. Oka, K. Takaoka, A. Shimojima, T. Matsuno\*, “Quasi-Single-Crystalline Inverse Opal  $\alpha$ -Fe<sub>2</sub>O<sub>3</sub> Prepared via Diffusion and Oxidation of FeCl<sub>3</sub> Precursor in Nanospaces”, *Chem. Mater.* **2025**, in press.
2. K. Takaoka, T. Matsuno\*, M. Koike, N. Muramoto, H. Wada, K. Kuroda, and A. Shimojima\*, “Zeolite Crystallization inside Chemically Recyclable Ordered Nanoporous Co<sub>3</sub>O<sub>4</sub> Scaffold: Precise Replication and Accelerated Crystallization”, *Small* **2025**, *21*, 202405280.
3. Y. Saito‡, T. Matsuno‡, Q. Guo, T. Mori, M. Kashiwagi, A. Shimojima, H. Wada, and K. Kuroda\*, “Preparation of Ordered Nanoporous Indium Tin Oxides with Large Crystallites and Individual Control over Their Thermal and Electrical Conductivities”, *ACS Appl. Mater. Interfaces* **2021**, *13*, 15373–15382. (‡: These authors contributed equally to this work)
4. N. Muramoto, T. Matsuno, H. Wada, K. Kuroda, and A. Shimojima\*, “Preparation of an Ordered Nanoporous Silicone-based Material Using Silica Colloidal Crystals as a Hard Template”, *Chem. Lett.* **2021**, *50*, 1038–1040.
5. T. Matsuno, Y. Kuroda, M. Kitahara, A. Shimojima, H. Wada, and K. Kuroda\*, “A Single-Crystalline Mesoporous Quartz Superlattice”, *Angew. Chem. Int. Ed.* **2016**, *55*, 6008–6012.

# **Abstract**

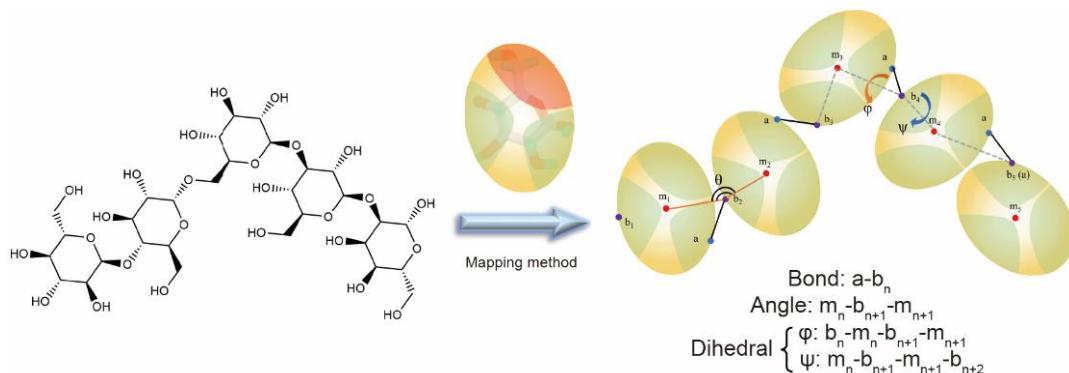
## **(Poster Presentation)**

**Presentation Title:** Highly Coarse-Grained Patchy Ellipsoid Particle Model of Glucose**Authors:** Bin Li, You-Liang Zhu\*, Zhong-Yuan Lu\*, Jia-Li Gao\***Affiliation:** Institute of Theoretical Chemistry, State Key Laboratory of Supramolecular Structure and Materials, Jilin University, Changchun, 130021, China

Institute of Systems and Physical Biology, Shenzhen Bay Laboratory, Shenzhen, 518000, China

**Email:** youliangzhu@jlu.edu.cn, luzhy@jlu.edu.cn, jiali@jialigao.org**Abstract:**

Glycan chains are widely present in living organisms, with specific glycan structures encoding vital biological functions. However, the structural diversity and conformational variability of glycans present significant challenges in linking molecular properties to functional outcomes. To address these challenges and enable larger-scale simulations, coarse-graining of molecules is a widely adopted strategy. The Martini force field, through extensive parameter optimization for carbohydrates, accurately captures their conformational properties and some functional characteristics. However, simulations for high-concentration monosaccharide solutions at large spatial scales still require higher coarse-graining level model. This study proposes a novel coarse-graining scheme for glucose molecules, simplifying them into patchy ellipsoid particles and fitting non-bonded interactions using the Gay-Berne (GB) potential. By constructing glucose dimer models with various glycosidic linkages and performing flexible scans of bond lengths, bond angles, and dihedral angles using the MP2/6-311G(d,p) method, harmonic functions were fitted to determine the corresponding spring constants, equilibrium bond lengths, and bond angles. Additionally, dihedral potential terms were obtained through decoupling and averaging systematic calculations. This scheme holds promise for high-quality simulations of larger-scale glycolipid or glycoprotein systems.

**References:**

1. V. Lutsyk, P. Wolski, W. Plazinski, "Extending the Martini 3 coarse-grained force field to carbohydrates", *Chem. Theory Comput.* **2022**, 18, 5089-5107.
2. F. Grünwald, M. H. Punt, S. J. Marrink, et al., "Martini 3 coarse-grained force field for carbohydrates", *Chem. Theory Comput.* **2022**, 18, 7555-7569.
3. Z.-W. Li, Y.-L. Zhu, Z.-Y. Lu, Z.-Y. Sun, "General patchy ellipsoidal particle model for the aggregation behaviors of shape- and/or surface-anisotropic building blocks", *Soft Matter* **2018**, 14, 7625-7633.

**Presentation Title:** Synthesis of an Ionic Aromatic Cyclodextrin for a Novel Host Molecule of Adapalene

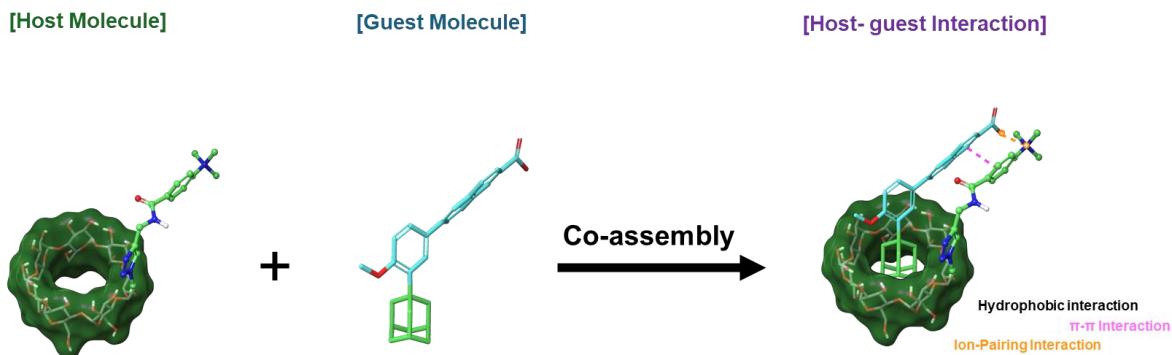
**Authors:** Dahee Jung, Yongju Kim

**Affiliation:** KU-KIST Graduate School of Converging Science and Technology  
Korea University, Seoul, Korea

**Email:** jdh0009@korea.ac.kr

**Abstract:**

Adapalene is a third-generation topical retinoid that effectively treats acne through cell differentiation, keratinization modulation, and anti-inflammatory effects. However, its clinical use is limited due to safety concerns related to light sensitivity and potential skin irritation. Cyclodextrins (CD) are cyclic oligosaccharides that can form inclusion complexes with hydrophobic drugs such as adapalene. In this study, we report a novel synthetic CD that improves the host-guest interaction with adapalene through additional aromatic and electrostatic interactions. The addition of synthetic CD enhances the light stability of adapalene, potentially reducing side effects and overcoming its limitations.



### P3

**Presentation Title:** Soft Lewis Base-Containing Polymers for Solid Polymer Electrolytes with Unconventional Conduction Mechanism under Polymer-in-salt Conditions

**Authors:** Akinari Chiba, Yuki Ogawa, Kenichi Oyaizu

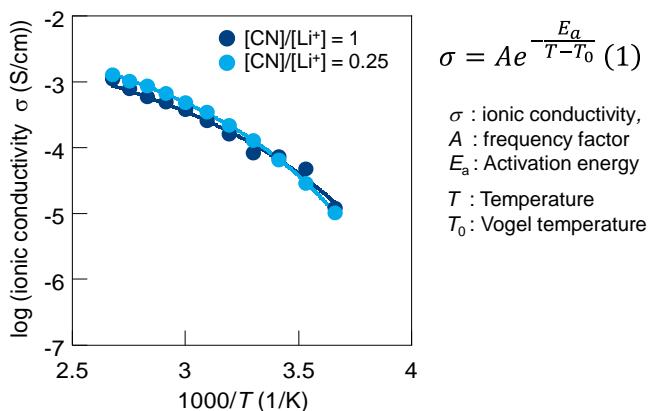
**Affiliation:** Department of Applied chemistry, Waseda University, 3-4-1 Okubo, Shinjuku-ku, Tokyo, Japan

**Email:** Akinarichiba@suou.waseda.jp

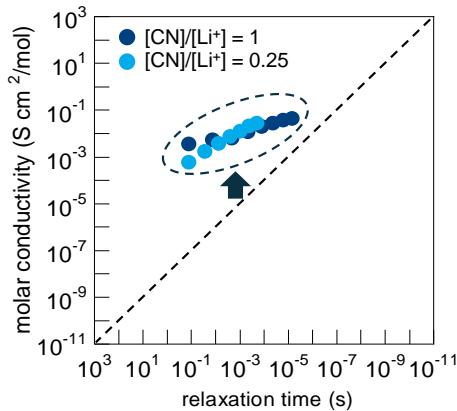
#### Abstract:

Solid polymer electrolytes (SPEs) have attracted much attention as electrolytes for all-solid-state batteries due to their lower interfacial resistance between the electrolyte and the electrode than that of other solid electrolytes (i.e. oxides and sulfides) and high formability. However, ion transportation in the conventional PEO-based SPEs is restricted by the segmental motion of polyethers and dramatic conductivity improvement is challenging. To solve this problem, we examined polymer-in-salt conditions where polymers were mixed with excess amount of lithium salt, based on previous reports of high conductivity due to weakly solvated structure of lithium ions<sup>1)</sup>. In this report, we present the ionic conductivity and ion conduction mechanisms of SPEs with soft Lewis base-containing polymers which interact with lithium-ions moderately.

SPEs with poly(acrylonitrile) (PAN) and Lithium (fluorosulfonyl)(trifluoromethanesulfonyl)imide (LiFTFSI) ( $[CN]/[Li^+] = 1, 0.25$ ) were prepared and their temperature dependence of ionic conductivity and viscoelastic behavior were evaluated. The temperature dependence of ionic conductivity followed the VTF equation (eq. 1) which assumed ion conduction in the amorphous phase, and high ionic conductivity above  $10^{-4}$  S/cm was observed at 40 °C (Fig. 1). Walden plots obtained with the results of conductivity and viscoelasticity measurements are shown in Fig. 2. Decoupling of ion conduction and viscoelastic behavior was clearly observed, which suggested the ion conduction mechanism independent of the segmental motion of the polymer chain. Detailed conduction mechanisms will also be discussed in the presentation.



**Fig. 1** Temperature dependence of ionic conductivity of PAN/LiFTFSI.



#### References:

1. W. Tan Y. Tominaga, *Electrochim. Acta*, **2023**, 464, 142875.

**Presentation Title:** Development of a TPP-Conjugated Quercetin Probe for Enhanced Mitochondrial Targeting and Fluorescence Imaging

**Authors:** Gayeon Nam, Yongju Kim

**Affiliation:** KU-KIST Graduate School of Converging Science and Technology  
Korea University, Seoul, Korea

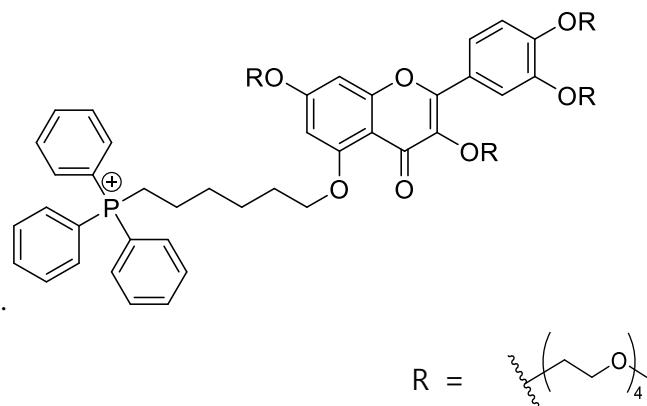
**Email:** skark26@korea.ac.kr

**Abstract:**

Bright fluorescent materials are essential for high-resolution bioimaging. To enhance mitochondrial fluorescence, we developed a quercetin-based probe that amplifies fluorescence intensity when co-stained with MitoTracker, a commonly used mitochondria-selective dye.

Quercetin, a flavonoid with five hydroxyl groups, allows selective modifications that influence its optical properties. Our group previously reported that the pentasubstituted form exhibits strong fluorescence.

To ensure mitochondrial localization, we conjugated quercetin with triphenylphosphonium (TPP), enabling targeted imaging while maintaining fluorescence intensity. Notably, co-treatment with MitoTracker significantly enhanced mitochondrial fluorescence, demonstrating the potential of this probe for improved mitochondrial visualization in live-cell imaging. This approach offers new possibilities for designing fluorescence-enhancing probes for advanced bioimaging applications.



**References:**

1. Y.Kim, Y.Kim. Synthesis of Penta and Tetra Substituted Quercetin and Their Fluorescent Properties, Eur.J.Org.Chem.2023, e202300807

**Presentation Title:** Highly conductive polymer electrolyte membranes with polyoxometalate hybrid nanodomains for high-temperature fuel cells

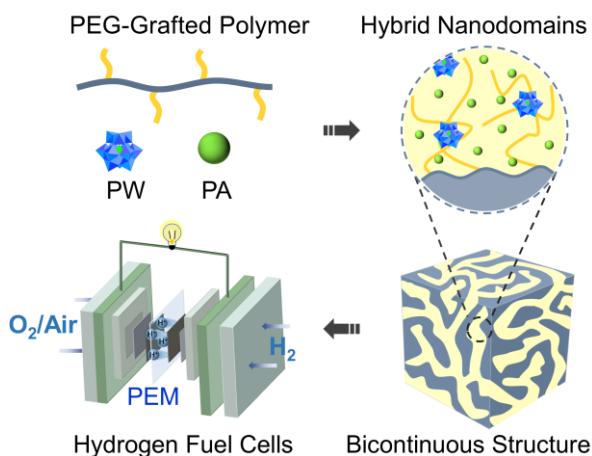
**Authors:** Tingting Li, Haolong Li\*

**Affiliation:** State Key Laboratory of Supramolecular Structure and Materials, College of Chemistry, Jilin University, Changchun 130012, China

**Email:** hl\_li@jlu.edu.cn

**Abstract:**

Phosphoric acid (PA)-doped polymer electrolyte membranes represent the most widely used high-temperature proton exchange membranes (HT-PEMs) in fuel cells. However, these materials face a significant challenge in achieving high proton conductivity under low PA content. Here, we report the fabrication of highly conductive nanodomains in HT-PEMs to solve this issue. A comb polymer with poly(ethylene glycol) (PEG) side chains was assembled with polyoxometalate nanoclusters (POMs) and PA, forming hybrid membranes with continuous nanodomains and dense hydrogen-bonding networks, which enabled efficient proton conduction and suppressed PA leaching. These membranes exhibited superior proton conductivity ( $109 \text{ mS cm}^{-1}$  at  $180^\circ\text{C}$ ) and high cell performance ( $1287 \text{ mW cm}^{-2}$  at  $160^\circ\text{C}$ , 2.2 times of commercial PBI/PA membrane) at low PA uptake (160%). Additionally, POMs acted as electrostatic crosslinkers, enhancing both mechanical strength and PA retention. This work demonstrates the potential of POM-polymer hybridization strategy in developing advanced HT-PEMs for energy applications.



**References:**

1. H. He, S. Song, L. Zhai, Z. Li, S. Wang, P. Zuo, Y. Zhu, H. Li, "Supramolecular Modifying Nafion with Fluoroalkyl-Functionalized Polyoxometalate Nanoclusters for High-Selective Proton Conduction", *Angew. Chem., Int. Ed.* **2024**, 63, e202409006.
2. S. Lee, J. G. Seong, Y. Jo; S.-J. Hwang, G. Gwak, Y. Park, Y. C. Kim, K. H. Lim, H.-Y. Park, J. H. Jang, H.-J. Kim, S.-W. Nam, S. Y. Lee, "Self-assembled network polymer electrolyte membranes for application in fuel cells at 250 °C", *Nat. Energy* **2024**, 9, 849-861.
3. X. Yang, Z. Feng, M. Alshurafa, M. Yu, A. B. Foster, H. Zhai, T. Yuan, Y. Xiao, C. D'Agostino, L. Ai, M. Perez-Page, K. Smith, F. Foglia, A. Lovett, T. S. Miller, J. Chen, P. M. Budd, S. M. Holmes, "Durable Proton Exchange Membrane Based on Polymers of Intrinsic Microporosity for Fuel Cells", *Adv. Mater.* **2025**, 37(19), 2419534.

**Presentation Title:** Polymer Exciplex Host-Driven TADF OLEDs via Non-Halogenated

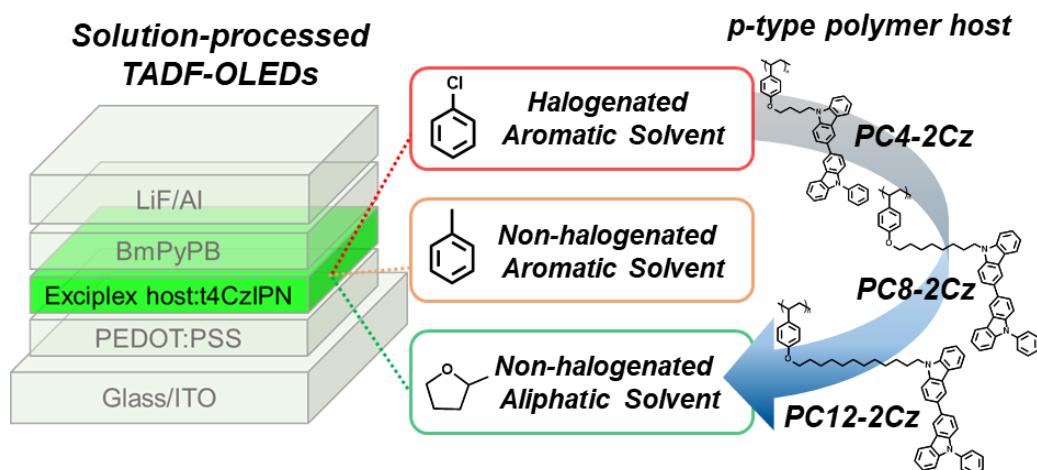
**Authors:** Subin Kwon, Ha Yeon Kim, Yeso Lee, Shinyoung Kim, Jong Bin Park, Han Young Woo, Chang Seop Hong, Sungnam Park, Min Ju Cho, Dong Hoon Choi

**Affiliation:** Department of Chemistry, Korea University, 145 Anam-ro, Seongbuk-gu, Seoul, 02841, Republic of Korea

**Email:** subink16@korea.ac.kr

**Abstract:**

We report high-performance green TADF OLEDs based on polymeric exciplex hosts that enable solution processing using non-halogenated solvents. Three biscarbazole-based p-type polymers (PC4-2Cz, PC8-2Cz, and PC12-2Cz) were synthesized with systematically varied alkylene spacers, achieving tunable solubility from halogenated aromatic to non-halogenated aliphatic solvents. When blended with tPDPA as the n-type component, the polymers formed stable exciplex hosts, enabling efficient green electroluminescence with maximum external quantum efficiencies (EQEs) up to 16.8%. Notably, devices fabricated using non-halogenated solvents such as toluene and 2-methyltetrahydrofuran exhibited performance comparable to those processed with chlorobenzene. These results highlight a sustainable molecular design strategy for scalable, environmentally friendly OLED fabrication without sacrificing device efficiency.



**References:**

1. S. Kwon, H. Y. Kim, S. Cho, H. Kwak, C. Y. Park, Y. Lee, S. Kim, J. B. Park, H. Y. Woo, C. S. Hong, S. Park, M. J. Cho, D. H. Choi, *J. Mater. Chem. C*, 2025, 13, 11950–11961.
2. S. Cho, N. Y. Kwon, C. W. Kim, H. Lee, J. M. Ha, H. J. Kim, H. Y. Woo, S. Park, M. J. Cho, D. H. Choi, *Polym. Chem.*, 2022, 13, 1824–1830.
3. H. Nakanotani, K. Masui, J. Nishide, T. Shibata, C. Adachi, *Sci. Rep.*, 2013, 3, 2127.
4. C.-Y. Chan, M. Tanaka, H. Nakanotani, C. Adachi, *Nat. Commun.*, 2018, 9, 5036.

**Presentation Title:** Analysis of lubrication mechanism at tribological interface using in-situ surface-enhanced Raman spectroscopy

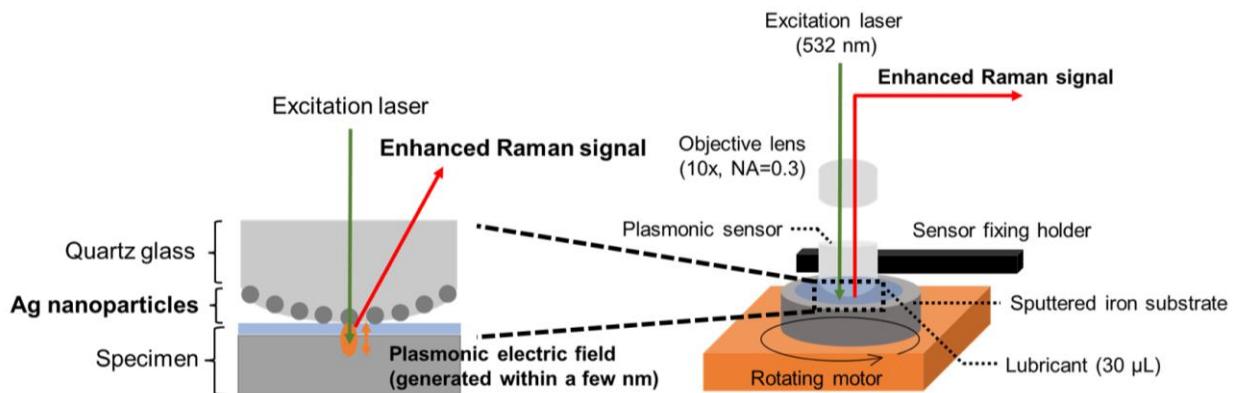
**Authors:** Subaru Sawaki

**Affiliation:** Department of Advanced Science and Engineering, Waseda University, Tokyo 169-8555, Japan

**Email:** tbxblj0323@akane.waseda.jp

**Abstract:**

Lubricants play a vital role in reducing energy consumption in the machinery industry. To meet rising global energy demands, high-performance lubricants should be developed. This requires molecular-level analysis of lubrication and degradation mechanisms, particularly through direct observation during sliding. In previous studies, such observations have been conducted using spectroscopic techniques such as infrared spectroscopy (IR) and sum frequency generation vibrational spectroscopy (SFG) <sup>[1][2]</sup>. However, IR is insensitive to chemical bonds at nanometer-scale interfaces. Moreover, SFG has limited sensitivity to functional groups critical to lubrication. In addition, these methods suffer from low temporal resolution, leaving lubrication mechanisms still poorly understood. Surface-enhanced Raman spectroscopy (SERS) provides high sensitivity to molecular vibrations at nanometer-scale interfaces and enables high temporal resolution. Our laboratory has developed a plasmonic sensor, composed of silver nanoparticles on a convex transparent glass substrate. This allows in-situ SERS measurements during sliding without damaging the specimen, as shown in the figure below <sup>[3]</sup>. In this presentation, we will introduce the in-situ measurement methodology, chemical structures observed at the interface during sliding, and the proposed lubrication mechanism based on these observations.



**References:**

1. R. R. Sahoo, S. K. Biswas “Frictional response of fatty acids on steel”, *J. Colloid Interface Sci.*, 2009, 333, 707.
2. S. Watanabe, M. Nakano, K. Miyake, S. Sasaki “Analysis of the interfacial molecular behavior of a lubrication film of n-dodecane containing stearic acid under lubricating conditions by sum frequency generation spectroscopy”, *Langmuir*, 2016, 32, 13649.
3. S. Sawaki, M. Yanagisawa, M. Kunimoto, T. Homma, “In-situ molecular-level observation of lubricant species at tribological interface using surface-enhanced Raman spectroscopy”, *Tribol. Int.*, 2025, 209, 110695.

**Presentation Title:** Two-in-One Molecule as a Single-Molecule Exciplex Host for Enhancing Solution-Processed TADF-OLED Performance

**Authors:** Yeseo Lee, Ha Yeon Kim, Haeun Kwak, Chae Yeong Park, Subin Kwon, Shinyoung Kim, Eunji Lim, Kyungsuk Jin, Chang Seop Hong, Weon-Sik Chae, Min Ju Cho, Sungnam Park, and Dong Hoon Choi

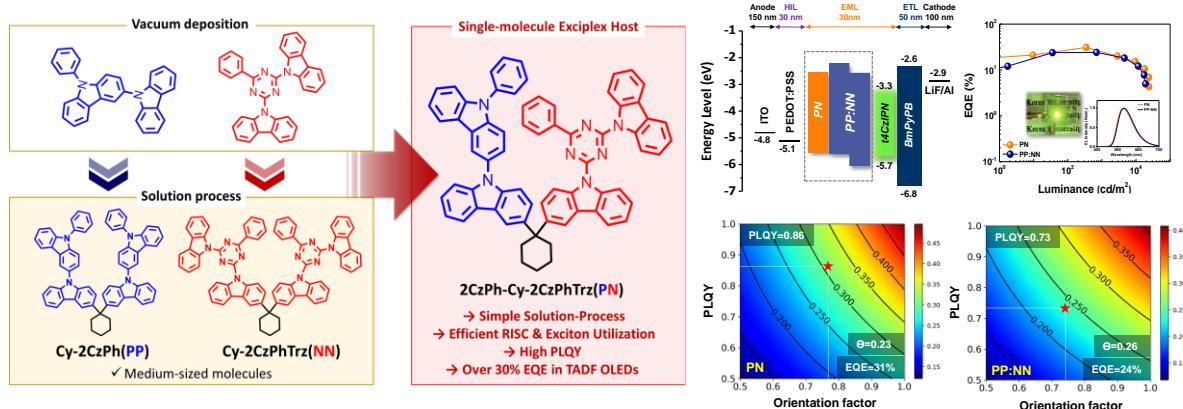
**Affiliation:** Department of Chemistry, Korea University, Seoul 02841, Republic of Korea

**Email:** okysl2000@korea.ac.kr

**Abstract:**

Exciplex hosts enhance charge balance in OLEDs, improving efficiency and stability. Traditional ternary EMLs with a donor, acceptor, and emitter require precise control in vacuum deposition, complicating fabrication. Solution processing offers scalability and cost efficiency but often causes phase separation and charge imbalance, degrading performance.

This study presents a dual-functional exciplex host integrating p-type and n-type motifs via a non-conjugated linker, enabling efficient exciplex formation while preserving photophysical properties. By forming a binary EML, this design eliminates donor-acceptor separation, simplifying fabrication. The host exhibits high thermal stability, and good film morphology, making it ideal for solution processing. Devices using this host with a TADF emitter achieved an  $\text{EQE}_{\text{max}}$  over 30%, attributed to its high PLQY (87%) and optimized charge balance. These findings highlight the potential of single-component exciplex hosts for high performance OLEDs.



**References:**

1. P. R. Bommireddy, C. S. Musalikunta, Y.-W. Lee, Y. Suh, M. Godumala, S.-H. Park, "Unveiling the potential of nonconjugate linkers (sp<sup>3</sup>-cores) in through-space charge transfer emitters and host materials for thermally activated delayed fluorescence organic light emitting diodes", *J. Mater. Chem. C*, **2024**, 12, 6743-6769.
2. M. J. Kang, S. Cho, N. Y. Kwon, S. H. Park, J. Y. Park, H. Kwak, C. Y. Park, H. Y. Kim, C. S. Hong, S. Park, M. J. Cho, D. H. Choi, "Effective exciplex host for solution-processed narrowband blue TADF-OLEDs using a 9-(dibenzo[b,d]thiophen-2-yl)-9H-carbazole analogue with an adamantane substituent", *Dyes Pigm.* **2024**, 226, 112118.
3. X. Ban, T. Zhou, K. Zhang, Q. Cao, F. Ge, D. Zhang, P. Zhu, Z. Liu, Z. Li, W. Jiang, "Developing homojunction exciplex for efficient multilayer solution-processed organic light emitting diodes", *Chem. Eng. J.* **2022**, 441, 135898.

**Presentation Title:** Conjugated Oligoelectrolyte-Driven Self-Assembled Monolayer for Bidirectional Interfacial Engineering in Sn–Pb Perovskite Solar Cells

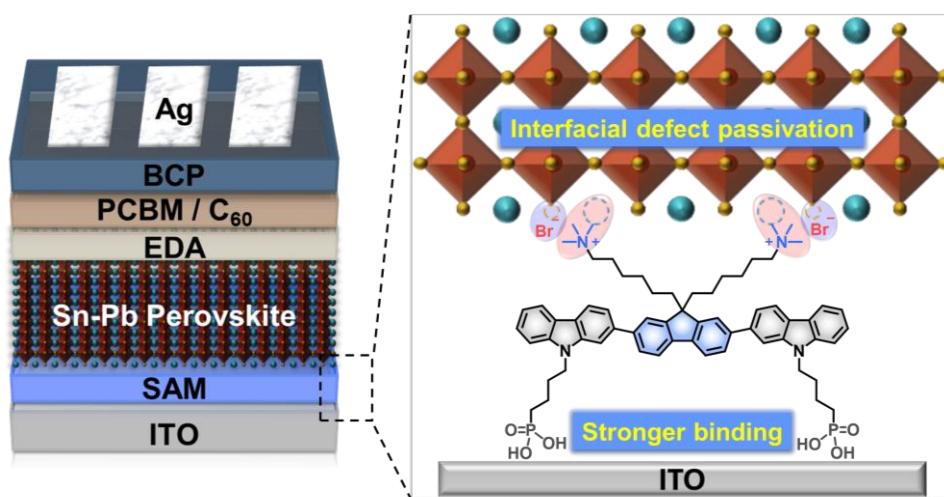
**Authors:** Jong Bin Park and Han Young Woo\*

**Affiliation:** Department of Chemistry, Korea University, Seoul, 02841, Republic of Korea

**Email:** pwj3466@korea.ac.kr

**Abstract:**

Tin–lead (Sn–Pb) mixed perovskites exhibit ideal bandgaps (1.21–1.25 eV) for high-efficiency single-junction and tandem solar cells, yet they suffer from interfacial instability arising from Sn vacancies, Sn oxidation, and poor film morphology. While self-assembled monolayers (SAMs) have emerged as promising hole-selective interlayers, conventional monophosphonate-based SAMs show weak interfacial binding and poor wettability, challenges that become more pronounced in scalable Sn–Pb perovskite solar cells (PSCs). Herein, a rationally designed SAM, 6,6'-(2,7-bis(9-(4-phosphonobutyl)-9H-carbazol-2-yl)-9H-fluorene-9,9-diyl)bis(N,N,N-trimethylhexan-1-ammonium bromide) (4PACz-TMABr), is developed, based on conjugated oligoelectrolytes featuring both phosphonic acid groups and ionic moieties. The dual phosphonic acid groups significantly improve interfacial coverage on indium tin oxide, while the quaternary ammonium bromide ionic moieties effectively suppress interfacial perovskite defects and  $\text{Sn}^{2+}$  oxidation. These dual interactions strongly promote the orderly alignment of the SAM and facilitate its function as a bidirectional interfacial linker. The formation of uniform, high-crystallinity Sn–Pb perovskite films is further supported by density functional theory calculations. Consequently, 4PACz-TMABr-based Sn–Pb PSCs achieve a champion power conversion efficiency of 22.67% in small-area devices and 17.61% in 1 cm<sup>2</sup> devices, along with markedly improved thermal stability. This work highlights a strategic molecular approach to SAM design, offering a pathway toward scalable, stable, and efficient Sn–Pb perovskite PSCs.



**Presentation Title:** Unveiling the Photoluminescence Mechanism of carbonized Polymer Dots: Evolution and Synergistic Photoluminescence of Multiple Molecular Fluorophores

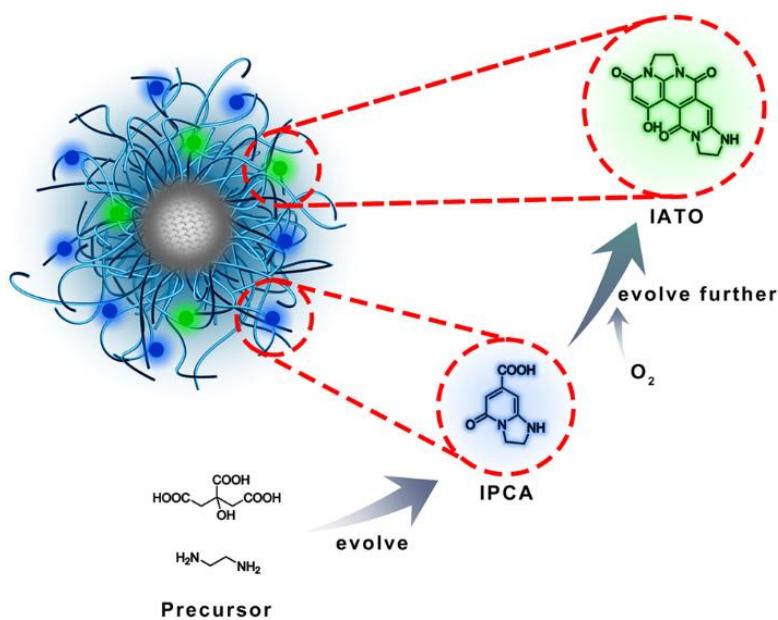
**Authors:** Xiao Han, Bai Yang\*

**Affiliation:** State Key Laboratory of Supramolecular Structure and Materials, College of Chemistry, Jilin University, Changchun 130012, China

**Email:** byangchem@jlu.edu.cn

**Abstract:**

Carbonized polymer dots (CPDs) are a class of exceptional fluorescent materials with diverse applications. However, their photoluminescence (PL) mechanism remained enigmatic and controversial, hindering further development and application. While molecular fluorophores explain primary fluorescence in some CPDs, the overall PL of CPDs still cannot be fully explained, such as their excitation-dependent behaviors, let alone the modulation of PL. Here, the emission around 510 nm of citric acid-ethylenediamine CPDs (CA-EDA CPDs) was proved to be contributed by a molecular fluorophore, which evolved from another molecular fluorophore following the quantum confinement effect. Further research revealed the whole PL mechanism of CA-EDA CPDs to be the evolution and synergistic PL of multiple molecular fluorophores linked on CPDs nanoparticle. This mechanism has been demonstrated to be universal, and a new approach for regulating the optical properties of CPDs was put forward based on it. This study not only refined the PL mechanism but also paved the way for future advancements of CPDs.



**References:**

1. S. Zhu, Q. Meng, L. Wang, J. Zhang, Y. Song, H. Jin, K. Zhang, H. Sun, H. Wang, B. Yang. "Highly Photoluminescent Carbon Dots for Multicolor Patterning, Sensors, and Bioimaging", *Angew. Chem. Int. Ed.* **2013**, 52 (14), 3953-3957.
2. Y. Song, S. Zhu, S. Zhang, Y. Fu, L. Wang, X. Zhao, B. Yang, "Investigation from Chemical Structure to Photoluminescent Mechanism: A Type of Carbon Dots from The Pyrolysis of Citric Acid and An Amine", *J. Mater. Chem. C* **2015**, 3 (23), 5976-5984.
3. J. Liu, R. Li, B. Yang, "Carbon Dots: A New Type of Carbon-Based Nanomaterial with Wide Applications", *ACS Cent. Sci.* **2020**, 6 (12), 2179-2195.

**Presentation Title:** Synthesis and Potential Application of the L/D-Cysteine-Induced Au 432 Helicoid I for Visible Light-Driven Asymmetric Reactions

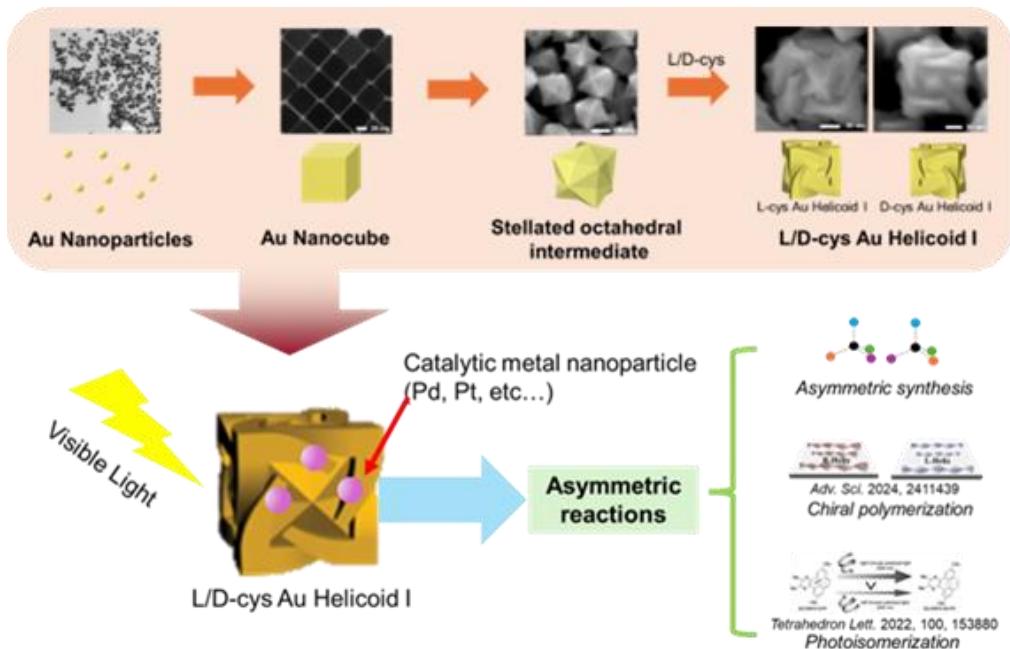
**Authors:** Joonwoo Seo<sup>1</sup>, Dong-Kwon Lim<sup>1,2\*</sup>

**Affiliation:** <sup>1</sup>KU-KIST Graduate School of Converging Science and Technology  
<sup>2</sup>Department of Integrative Energy Engineering, College of Engineering  
 Korea University, Seoul, Korea

**Email:** dklm@korea.ac.kr

**Abstract:**

The chiral plasmonic nanoparticles have recently garnered interest due to their potential in enantioselective applications, and in addition to this, the reaction based on visible light is considered an eco-friendly and sustainable strategy. In this study, to utilize it simultaneously, we synthesized enantiomeric 432 Au helicoid I nanostructures using the aqueous growth method guided by L/D-cysteine, following a previously reported protocol [1]. The resulting nanoparticles exhibited Absorption were observed on UV-Vis spectroscopy in a visible light range (about 500 nm  $\lambda$ ) and opposite handedness depending on the chiral ligand used, as confirmed by the field emission scanning electron microscopy (FE-SEM). The circular dichroism (CD) spectroscopy further verified the enantiomer-specific optical activity, with the two enantiomers displaying mirrored CD signals. The final 432 helicoid I structures are composed of nanogap that support strong electric field. [2] This nanostructure provides a foundation for future integration with catalytic metals to enhance asymmetric reactions under visible-light-driven conditions.



**References:**

1. Lee, HE., Ahn, HY., Mun, J. et al. "Amino-acid- and peptide-directed synthesis of chiral plasmonic gold nanoparticles" *Nature*. **2018**, *556*, 360–365
2. P. P. P. Kumar, M.-K Kim, and D.-K Lim "Amino Acid-Modulated Chirality Evolution and Highly Enantioselective Chiral Plasmonic Gold Nanoparticles" *Adv. Optical Mater.* **2023**, *11*, 2301503

**Presentation Title:** Deep learning model based on interpretable subgraph attention network

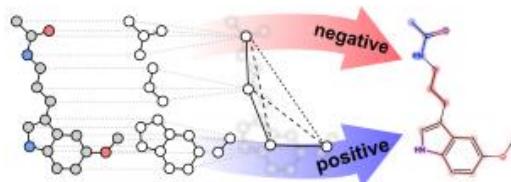
**Authors:** Jinyong Park and Sungnam Park\*

**Affiliation:** Department of Chemistry and Research Institute for Natural Science, Korea University, Seoul, Korea

**Email:** phillip1998@korea.ac.kr

**Abstract:**

Deep learning (DL) predictions of molecular properties can be effectively used to develop materials in various research fields. However, despite the remarkable performance achieved by DL models, interpretability remains a critical issue. For efficient molecular design, it is important to accurately predict molecular properties as well as to understand the underlying factors that determine molecular properties. Attention mechanisms have been employed in the DL models to account for the importance of the contributions of atoms and functional groups to the molecular properties, but the interpretability is still limited. In this study, we proposed a novel approach termed ‘interpretable subgraph attention network (ISAT)’, which includes subgroup-wise attentions to deduce a clearer correlation between molecular structures and properties. Specifically, we used a novel fragmentation algorithm and separate positive and negative attention layers to facilitate the implementation of the ISAT. Conventional attention methods primarily provide the importance of the moieties, which is not informative in regression task, without elucidating how individual moieties contribute to the molecular properties. In contrast, the ISAT allows for the quantification of the contributions of individual moieties, dividing the attention score into positive and negative contributions. Through comparative analysis with group contribution and conventional attention methods, we demonstrate that the interpretability of the ISAT is significantly enhanced while maintaining the comparable accuracy levels. The ISAT is found to provide meaningful insights into the contributions of individual moieties to the molecular properties, thereby advancing the interpretability of DL models for new material design.



**Interpretable Subgraph Attention**

**References:**

1. Jinyong Park, Minhi Han, Kiwoong Lee, and Sungnam Park “Hierarchical Graph Attention Network with Positive and Negative Attentions for Improved Interpretability: ISA-PN” *J. Chem. Inf. Model.*, **2025**, 65, 1115
2. Aouichaoui, A. R.; Fan, F.; Mansouri, S. S.; Abildskov, J.; Sin, G. “Combining Group-Contribution Concept and Graph Neural Networks Toward Interpretable Molecular Property Models.” *J. Chem. Inf. Model.*, **2023**, 63, 725
3. Xiong, Z.; Wang, D.; Liu, X.; Zhong, F.; Wan, X.; Li, X.; Li, Z.; Luo, X.; Chen, K.; Jiang, H.; Zheng, M. “Pushing the boundaries of molecular representation for drug discovery with the graph attention mechanism.” *J. Med. Chem.* **2019**, 63, 8749
4. Joonyoung F. Joung†, Minhi Han†, Minseok Jeong, and Sungnam Park\* “Beyond Woodward–Fieser Rules: Design Principles of Property-Oriented Chromophores Based on Explainable Deep Learning Optical Spectroscopy” *J. Chem. Inf. Model.*, **2022**, 62, 2933

**Presentation Title:** Sn Incorporation into Layered Octosilicates using Tin(IV) Chloride

**Authors:** Takeshi Iwakami<sup>1</sup>, Takamichi Matsuno<sup>1,2</sup>, and Atsushi Shimojima<sup>1,2,\*</sup>

**Affiliation:** <sup>1</sup>Department of Applied Chemistry, Faculty of Science and Engineering, Waseda University, 3-4-1 Okubo, Shinjuku-ku, Tokyo 169-8555, Japan

<sup>2</sup>Kagami Memorial Research Institute for Materials Science and Technology, Waseda University, 2-8-26 Nishiwaseda, Shinjuku-ku, Tokyo 169-0051, Japan

**Email:** shimojima@waseda.jp

**Abstract:**

Single-atom catalysts, which are materials consisting of catalytically active single atoms dispersed on bulk supports, have attracted considerable attention. Graphene, metal oxides, and silica are commonly used as supports, and the electronic structure of single atoms varies significantly depending on the type of support and the coordination environment, leading to diverse catalytic properties.<sup>1</sup> Given that metal species such as Al, Ti, and Sn exhibit stable coordination with silica, various catalysts have been synthesized by incorporating these metal species into silica frameworks such as zeolites and mesoporous silica.

Layered silicates, which have a stacked structure of crystalline silicate nanosheets, are considered promising catalyst supports. Their high specific surface area and regularly arranged SiOH groups are suitable for the preparation of high-density, well-defined metal sites. Previously reported systems are based on the single-atom organometallic catalyst approach, in which organic ligands are employed to stabilize the metal sites.<sup>2,3</sup> While this method enables precise control over the coordination environment, the presence of organic ligands can hinder access to the active site and limit the thermal and chemical stability of the catalyst. Therefore, developing a strategy to immobilize metal atoms directly onto the surface of layered silicates without the use of organic ligands is a crucial step toward designing more robust and accessible single-atom catalysts.

Here we report the introduction of Sn atoms into layered octosilicate using  $\text{SnCl}_4$  as the metal precursor. Ammonium-exchanged octosilicate prepared by the conventional method<sup>4</sup> was reacted with  $\text{SnCl}_4$  in dichloromethane at room temperature. However, the reaction did not proceed efficiently under these conditions, and the effect of adding various amines to scavenge HCl generating during the reaction was investigated. As a result, successful incorporation of Sn was confirmed by the solid-state  $^{29}\text{Si}$  NMR spectrum when diethylamine was added to the reaction mixture. Also, Sn 3d peaks of the XPS profile shown single binding energy with no shoulder, suggesting the presence of single-environment Sn atoms.

**References:**

1. L. Liu, A. Corma, *Chem. Rev.* **2018**, 118, 4981–5079.
2. N. Tsunooji, M. V. Opanasenko, M. Kubů, J. Čejka, H. Nishida, S. Hayakawa, Y. Ide, M. Sadakane, T. Sano, *ChemCatChem* **2018**, 10, 2536–2540.
3. M. Yatomi, T. Hikino, S. Yamazoe, K. Kuroda, A. Shimojima, *Dalton Trans.* **2023**, 52, 18158–18167.
4. D. Mochizuki, A. Shimojima, T. Imagawa, K. Kazuyuki, *J. Am. Chem. Soc.* **2005**, 127, 7183–7191.

**Presentation Title:** Size-dependent 2D materials: A comparative study on N<sub>2</sub> fixation activity via Gas Chromatography

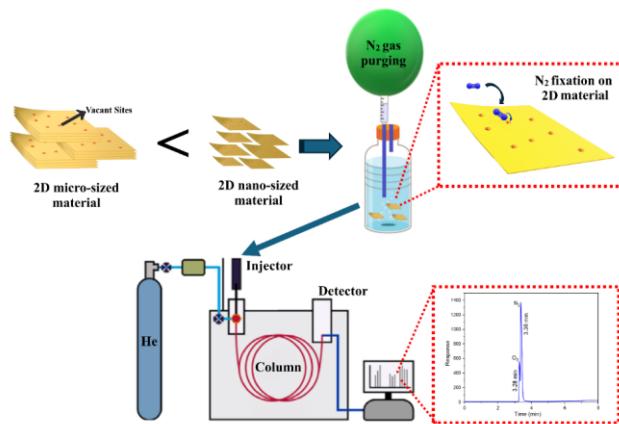
**Authors:** Jijoe Samuel Prabagar<sup>1</sup> and Dong-Kwon Lim<sup>1</sup>

**Affiliation:** <sup>1</sup> KU-KIST Graduate School of Converging Science and Technology, Korea University, 145 Anam-ro, Seongbuk-gu, Seoul 02841, Republic of Korea.

**Email:** joesam@korea.ac.kr

### Abstract:

2D materials have gained considerable attention for N<sub>2</sub> fixation, particularly in NH<sub>3</sub> synthesis, due to their unique features, such as active sites. While most studies emphasize NH<sub>3</sub> production, direct assessment of N<sub>2</sub> fixation remains limited. This work investigates widely reported 2D materials, synthesized, characterized, and tested, for their N<sub>2</sub> fixation potential using thermal conductivity-based gas chromatography, a rarely applied method. All samples showed fixation activity, with nano-sized variants produced via sonication demonstrating superior performance. Specifically, nano g-C<sub>3</sub>N<sub>4</sub> containing nitrogen vacancies reached ~1.28 μL of fixed N<sub>2</sub>. Similarly, Ti<sub>2</sub>C<sub>3</sub> MXene and Bi<sub>2</sub>O<sub>3</sub> showed promising results, likely due to oxygen vacancies performing as active sites. Even under ambient air conditions, fixation was achieved, suggesting broader applicability. Overall, the findings highlight the potential of nanoscale 2D catalysts for effective N<sub>2</sub> fixation. Notably, NH<sub>3</sub> production through photocatalysis aligned closely with N<sub>2</sub> fixation results, supporting the relevance of these materials for scalable and practical applications. These findings confirm that nanoscale 2D materials exhibit high efficiency in N<sub>2</sub> fixation, offering substantial promise for scalable, real-world applications.



### References:

1. J.S. Prabagar, K.L. Reddy, D. K. Lim, Visible-Light Responsive Gold Nanoparticle and Nano-sized Bi<sub>2</sub>O<sub>3</sub>-x Sheet Heterozygote Structure for Efficient Photocatalytic Conversion of N<sub>2</sub> to NH<sub>3</sub>. Chinese Journal of Structural Chemistry. 100564 (2025).
2. H.H. Shin, W. Yang, D.K. Lim, Gold and nano-sized titanium carbide MXene heterozygotes as highly efficient visible-light responsive photocatalysts for ammonia synthesis. Carbon N Y. 214, 118359 (2023).
3. G. Dong, W. Ho, C. Wang, Selective photocatalytic N<sub>2</sub> fixation dependent on g-C<sub>3</sub>N<sub>4</sub> induced by nitrogen vacancies. J Mater Chem A Mater. 3, 23435–23441 (2015).
4. J. Qin, B. Liu, K.H. Lam, S. Song, X. Li et al., 0D/2D MXene Quantum Dot/Ni-MOF Ultrathin Nanosheets for Enhanced N<sub>2</sub> Photoreduction. ACS Sustain Chem Eng. 8, 17791–17799 (2020).
5. S.S. Xia, L. Li, C. Bao, C. Li, J. Wu et al., Constructing 2D MOF/In<sub>2</sub>S<sub>3</sub> heterojunctions for efficient solar-driven H<sub>2</sub>O<sub>2</sub> synthesis in pure water. Inorg Chem Front. 11, 6605–6615 (2024).
6. H.M. Lu, Q. Jiang, Size-dependent surface energies of nanocrystals. Journal of Physical Chemistry B. 108, 5617–5619 (2004).

**Presentation Title:** Bipolar Redox-active molecules for organic aqueous redox flow batteries

**Authors:** Hyeong hui Kim and Han young Woo\*

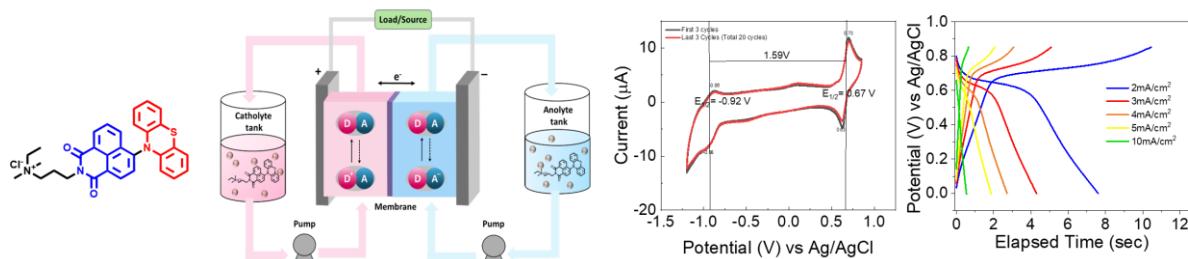
**Affiliation:** Department of Chemistry and Organic Optoelectronic Materials Laboratory, Korea University, Seoul, 02841, Korea

**Email:** taus2001@korea.ac.kr

**Abstract:**

Organic redox flow batteries (ORFBs) offer key advantages over inorganic systems, such as tunable molecular structures, sustainability, and cost-effective materials.<sup>1</sup> Among them, aqueous ORFBs (AORFB) provide improved safety, higher ionic conductivity, and affordability compared to nonaqueous systems.<sup>2</sup> However, crossover of redox-active species across membranes remains a major challenge, leading to capacity loss and reduced efficiency. To address this, bipolar redox-active molecules—capable of acting as both anolyte and catholyte—are gaining attention as a strategy to suppress crossover and enhance long-term stability.<sup>3</sup>

In this study, a bipolar AORFB was developed using phenothiazine as the catholyte and naphthalimide as the anolyte. Cyclic voltammetry (CV) measurements confirmed that both redox-active materials exhibit reversible redox behavior, with half-potentials ( $E_{1/2}$ ) of +0.67 V and -0.92 V respectively, resulting in an open-circuit voltage (OCV) of 1.59 V. This lies well within the electrochemical stability window of water, thereby contributing to an enhanced energy density. To enable stable symmetric cell operation, various conditions including pH, electrolytes and membrane were optimized. Among the tested conditions, 0.5 M  $\text{Na}_2\text{SO}_4$  was selected as the optimal supporting electrolyte, offering the highest cell stability. Under this condition, the solubility of the bipolar molecule reached 170 g/L, corresponding to a theoretical capacity of 8.37 Ah/L. However, long-term cycling stability tests revealed a gradual decrease in coulombic efficiency (QE), which is presumed to originate from radical-radical dimerization and degradation of the phenothiazine. To overcome this issue, molecular engineering is currently underway to introduce substituents at the para-position of the donor unit, thereby providing steric hindrance and improving cycling stability.



**References:**

1. Winsberg, J.; Hagemann, T.; Janoschka, T.; Hager, M.D.; Ulrich S. Schubert, U.S. Redox-Flow Batteries: From Metals to Organic Redox-Active Materials. *Angew. Chem. Int. Ed.*, 2017, 56, 686–711.
2. Raihan, M.A.; Dyker, C.A. Status and prospects for symmetric organic redox flow batteries. *Journal of Energy Chem.*, 2025, 125–143.
3. Liu, Y.; Dai, G.; Chen, Y.; Wang, R.; Li, H.; Shi, X.; Zhang, S.; Xu, Y.; Zhao, Y.; Effective Design Strategy of Small Bipolar Molecules through Fused Conjugation toward 2.5V Based Redox Flow Batteries. *ACS Energy Lett.* 2022, 7, 1274–1283.

**Presentation Title:** Sulfur-Locked Multiple Resonance Emitters for High Performance Orange-Red/Deep-Red OLEDs

**Authors:** Yexuan Pu, Yue Wang\*

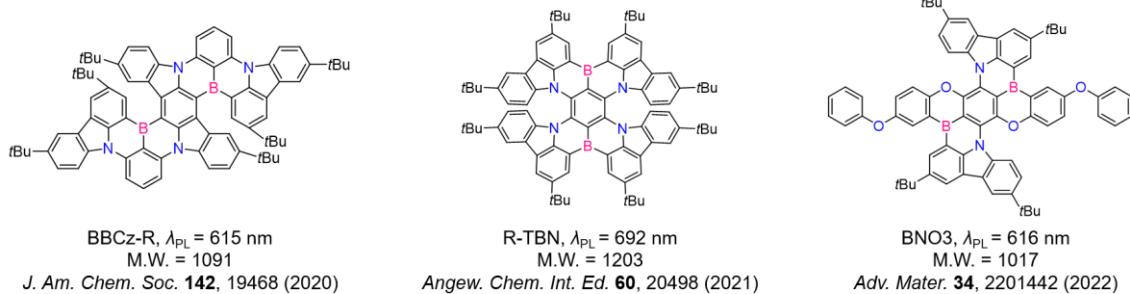
**Affiliation:** State Key Laboratory of Supramolecular Structure and Materials, College of Chemistry, Jilin University, Changchun 130012, P. R. China.

**Email:** yuewang@jlu.edu.cn

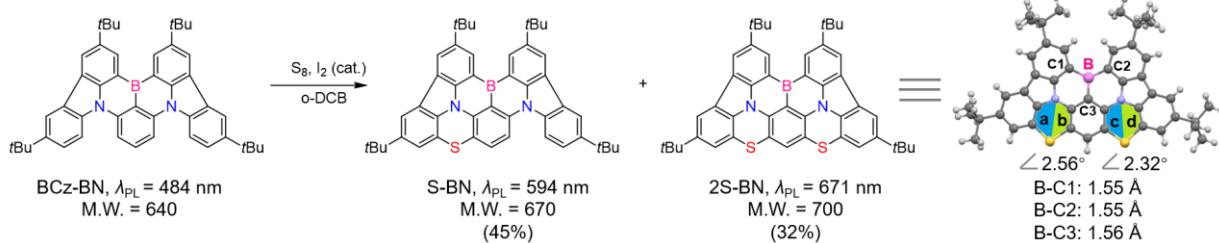
**Abstract:**

Multiple resonance thermally activated delayed fluorescence (MR-TADF) materials are preferred for their high efficiency and high color purity in organic light-emitting diodes (OLEDs). However, the design strategies of MR-TADF emitters in the red region are very limited. Herein, we propose a concept for a paradigm shift in orange-red/deep-red MR emitters by linking the outer phenyl groups in a classical MR framework through intramolecular sulfur (S) locks. Endowed with the planar architectural feature of the MR mother core, the proof-of-concept S-embedded emitters S-BN and 2S-BN also exhibit considerable flatness, which proves critical in avoiding the direct establishment of potent charge transfer states and inhibiting the non-radiative decay process. The emission maxima of S-BN and 2S-BN are 594 nm and 671 nm, respectively, and both have a high PLQY of ~100%, a rapid radiative decay rate of around  $10^7 \text{ s}^{-1}$ , and a remarkably high reverse intersystem crossing rate of about  $10^5 \text{ s}^{-1}$ . Notably, maximum external quantum efficiencies of 39.9% (S-BN, orange-red) and 29.3% (2S-BN, deep-red) were also achieved in typical planar OLED structures with ameliorated efficiency roll-offs.

**a: Previous Work**



**b: This Work**



**References:**

1. M. Mamada, M. Hayakawa, J. Ochi, T. Hatakeyama, “Organoboron-Based Multiple-Resonance Emitters: Synthesis, Structure–Property Correlations, and Prospects”, *Chem. Soc. Rev.* **2024**, 53, 1624.
2. Y. Pu, Q. Jin, Y. Zhang, C. Li, L. Duan, Y. Wang, “Sulfur-Locked Multiple Resonance Emitters for High Performance Orange-Red/Deep-Red OLEDs”, *Nat. Commun.* **2025**, 16, 332.

**Presentation Title:** Enhanced dispersibility and prodrug conversion rate of Sulfasalazine by UV irradiation

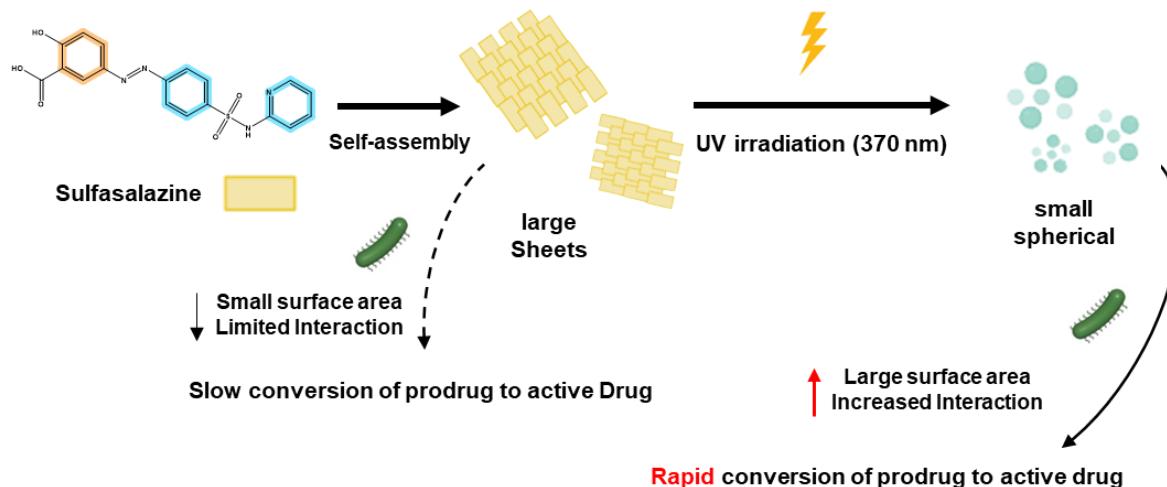
**Authors:** Sungchan Choi, Yongju Kim

**Affiliation:** KU-KIST Graduate School of Converging Science and Technology  
Korea University, Seoul, Korea

**Email:** zzgzzg12@korea.ac.kr

**Abstract:**

Sulfasalazine is a pharmaceutical used to treat inflammatory diseases such as rheumatoid arthritis, ulcerative colitis, and Crohn's disease. However, sulfasalazine has poor solubility in water, and enhancing its solubility is crucial for efficient drug delivery. Previous studies have attempted to increase the solubility of sulfasalazine by attaching hydrophilic functional groups or utilizing specific nanostructures. However, these methods are difficult to use and take up a lot of time. Therefore, we aimed to investigate the increased solubility of sulfasalazine through photoisomerization induced by UV irradiation, leveraging the fact that sulfasalazine is a drug based on the azo-benzene structure. We also investigated whether the increased solubility has a positive impact on the degradation rate of the sulfasalazine drug through bacterial experiments. Finally, through mouse model experiments, we confirmed that the photoisomerized sulfasalazine exhibited faster therapeutic onset and improved anti-inflammatory efficacy compared to the untreated drug, demonstrating the practical potential of this method for efficient drug delivery.



**Presentation Title:** Machine Learning Prediction of Optical Properties of Coumarin Derivatives

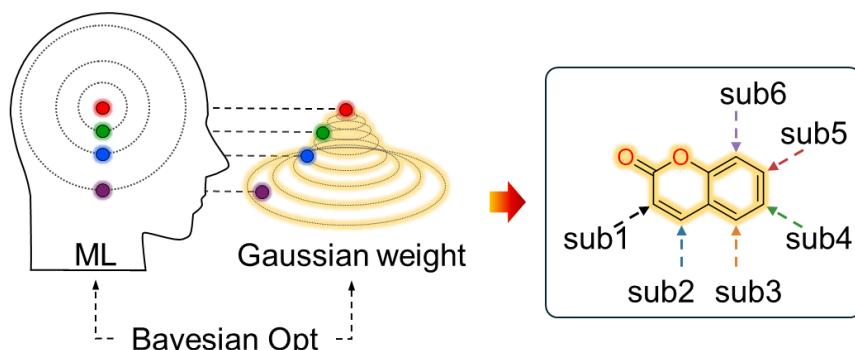
**Authors:** Seokwoo Kim and Sungnam Park\*

**Affiliation:** Department of Chemistry and Center for Advanced Molecular Science, Korea University, Seoul, 02841, Korea

**Email:** seokwookorea@korea.ac.kr

**Abstract:**

Machine learning (ML) and deep learning (DL) methods in chemistry have been applied to predict various molecular properties including optical and electrochemical properties<sup>1</sup> as well as to design new molecules with target properties.<sup>2</sup> Within these areas, predicting optical properties is essential for developing new chromophores and fluorophores, which are central to materials science, sensing, and bioimaging. Coumarin-based compounds serve as important chromophores and fluorophores, finding broad application across diverse areas of research. Here, we present a new machine learning (ML) framework for predicting absorption and emission wavelengths of coumarin derivatives.<sup>3</sup> We built an experimental dataset of optical properties and introduced two novel concepts for molecular representation: Gaussian-weighted graph convolution (GWGC) and subgraph modular input (SMI). GWGC enables the ML model to capture interatomic interactions by applying a Gaussian weighting scheme in the graph convolution process. Meanwhile, the SMI approach represents each molecule as a composite of a coumarin core and six distinct substituents, providing separate and positional encoding of the substituent effects. This modularization enhances interpretability, enabling insight into how substituent structure and location impact coumarin's photophysical behavior. Our models utilizing GWGC and SMI outperform traditional models based on RDKit descriptors or Morgan fingerprints, and the GWGC-SMI framework can be readily extended to other core–substituent systems for molecular property prediction.



**References:**

1. Joung, J. F.; Han, M.; Hwang, J.; Jeong, M.; Choi, D. H.; Park, S. Deep Learning Optical Spectroscopy Based on Experimental Database: Potential Applications to Molecular Design. *JACS Au*, **2021**, *1*, 427-438.
2. Han, M.; Joung, J. F.; Jeong, M.; Choi, D. H.; Park, S. Generative Deep Learning-Based Efficient Design of Organic Molecules with Tailored Properties. *ACS Cent. Sci.*, **2025**, *11*, 219.
3. Kim, S.; Han, M.; Park, J.; Lee, K.; Park, S. Machine Learning Prediction of Optical Properties of Coumarin Derivatives Using Gaussian-Weighted Graph Convolution and Subgraph Modular Input. *J. Chem. Inf. Model.*, **2025**, *65*, 4889-4897.

**Presentation Title:** Development of Poly(phenylene sulfide)-Based Charge-Transfer Complexes for Solid polymer electrolyte with high electrochemical stability

**Authors:** Toshinori Kozakai, Kenichi Oyaizu

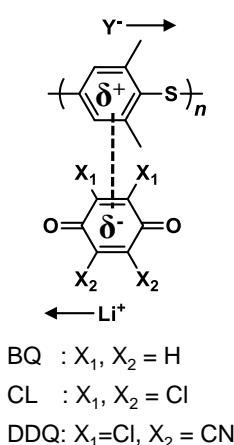
**Affiliation:** Department of Applied Chemistry, Waseda University, Tokyo, 169-8555, Japan

**Email:** kozatoshinori@toki.waseda.jp

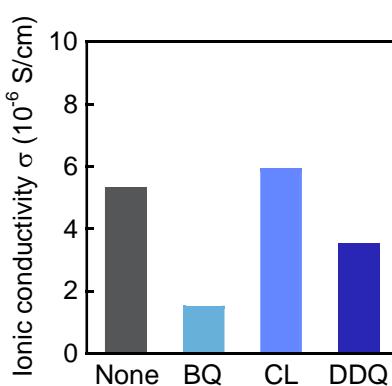
**Abstract:**

In the conventional poly(ethylene oxide)-based solid polymer electrolyte, ions are transported by the segmental motion of the polymer chain which limits the ionic conductivity. This limitation could be overcome in solid polymer electrolytes based on charge-transfer (CT) complexes consisting of aromatic polymers and electron acceptors<sup>1)</sup>. The polarized structure derived from the CT complexes seemed to facilitate salt dissociation, giving rise to the ion transport properties<sup>2)</sup>. Preliminary reports on the CT-complex-based ionic conductors suggested the possibility of enhancing the conductivity through an unconventional approach (Fig. 1)<sup>3,4)</sup>. However, the specific conditions required to achieve high ionic conductivity and the detailed mechanisms of the ion transport still needed to be elucidated.

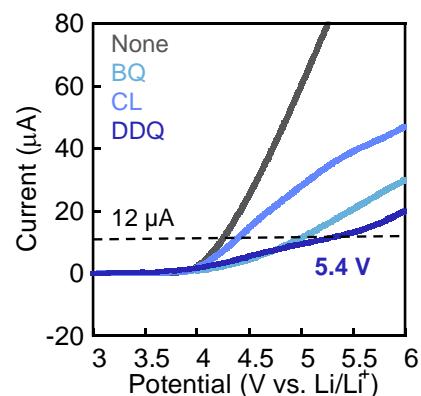
In this study, solid polymer electrolytes with CT complexes based on poly (phenylene sulfide) derivatives were prepared by mixing the CT complexes, a lithium salt, and trace amounts of additives such as water as a plasticizer. High ionic conductivity exceeding  $10^{-6}$  S/cm at room temperature was achieved, maintaining the oxidative stability (Fig. 2, 3). Based on this result, solid polymer electrolytes without the low molecular weight additives were prepared by incorporating the function of the additive into the polymer. Through optimizing the combination of the electron donor and the acceptor, electrochemical stability was improved while maintaining high ionic conductivity.



**Fig. 1** Ion conduction mechanism of charge-transfer complexes-based solid electrolytes.



**Fig. 2** Ionic conductivities of solid polymer electrolytes at 25 °C.



**Fig. 3** LSV curves of solid polymer electrolytes at 25 °C (0.5 mV/sec, Li||SUS cell).

**References:**

1. M. A. Zimmerman, U.S. Patent 20170005356A1.
2. K. Hatakeyama-Sato, M. Umeki, T. Tezuka, K. Oyaizu, *ACS Appl. Electron. Mater.* **2020**, 2, 2211-2217.
3. L. Yang, J. L. Schaefer, *ACS Energy Lett.* **2023**, 8, 2426-2431.
4. P. Bonnick, M. Redko, C. Wang, M. Frey, M. Jones, S. Wang, G. Allred, C. Ling, R. Sugiura, J. Muldoon, *ACS Energy Lett.* **2023**, 8, 4251-4258.

**Presentation Title:** Exploring Chiral Nanostructures via Self-Assembly of Pagoda[4]arene Derivatives

**Authors:** Wonpyo Rhee, Yongju Kim

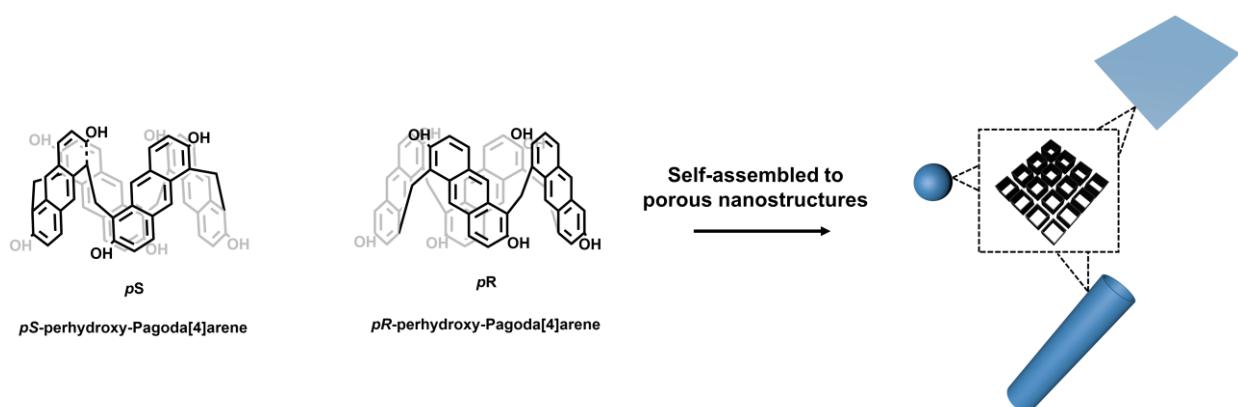
**Affiliation:** KU-KIST Graduate School of Converging Science and Technology  
Korea University, Seoul, Korea

**Email:** wonpyo97@korea.ac.kr

**Abstract:**

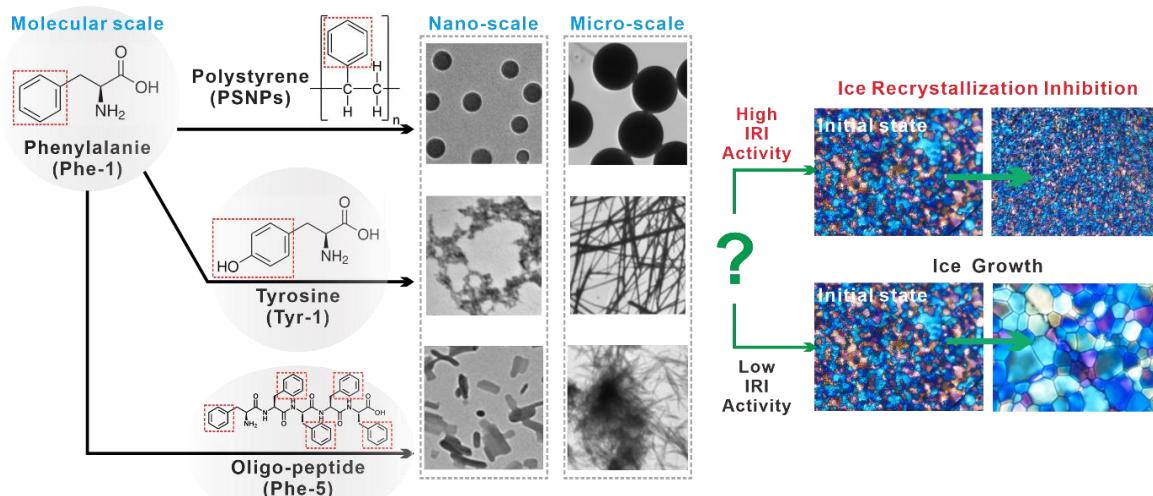
Chirality plays a crucial role in various biological processes, including the function of cell membranes, which are primarily composed of nucleotides, sugars, lipids, and amino acids. These molecules contribute to the chirality of cell membranes, influencing the recognition and interaction with chiral drug molecules. In drug delivery systems, leveraging the chirality of cell membranes to design chiral drug carriers can enhance the targeting and efficacy of therapeutics. To this end, we have designed chiral drug delivery vehicles using chiral Pagoda[4]arene derivatives.

Pagoda[4]arene, composed of 2,6-dimethoxyanthracene units, possesses a fixed conformation due to steric hindrance, enabling a stable self-assembled structure. Furthermore, by demethylating Pagoda[4]arene, we have synthesized amphiphilic molecules that can self-assemble into diverse nanostructures, which was achieved through simple manipulation of the solvent composition, eliminating the need for complex synthetic processes. This approach highlights the potential of chiral Pagoda[4]arene derivatives in the development of innovative drug delivery systems.



**Presentation Title:** Tyrosine Nanoassembly as a Potent Ice Recrystallization Inhibition Activity**Authors:** Yong Duk Kim<sup>†</sup>, Yedam Lee<sup>‡</sup>, Dong June Ahn<sup>†, ‡, \*, and Dong-Kwon Lim<sup>†, §, \*</sup></sup>**Affiliation:** <sup>†</sup> KU-KIST Graduate School of Converging Science and Technology, Korea University, 145 Anam-ro, Seongbuk-gu, Seoul 02841, Republic of Korea<sup>‡</sup> Department of Chemical and Biological Engineering, Korea University, Seoul, Republic of Korea<sup>§</sup> Department of Integrative Energy Engineering, Korea University, 145 Anam-ro, Seongbuk-gu, Seoul 02841, Korea.**Email:** selapin@korea.ac.kr (Yong Duk Kim), yedam96@korea.ac.kr (Yedam Lee), ahn@korea.ac.kr (Dong June Ahn), dklm@korea.ac.kr (Dong-Kwon Lim)**Abstract:**

The inhibition of ice growth and recrystallization plays a role in cryo-technology. Ice formation during freeze-thaw cycles causes irreversible chemical and physical damage to biosamples. Among various approaches to overcome such challenges, an effective strategy is to search for and utilize materials with potential ice recrystallization inhibition (IRI) activity. Previously, we demonstrated the formation of self-assembled nanostructures from homo-oligopeptides, which act as effective ice growth inhibitors. Herein, we investigate the effect of particle size and functional groups on IRI activity. Polystyrene nanoparticles (PSNPs) can form size-tunable assemblies, but their hydrophobic groups alone were insufficient to induce IRI activity. Although Phe-5 (pentamer of phenylalanine) is capable of self-assembly, its nanostructures are unstable under saline conditions, leading to aggregation. As a result, the concentration of dispersed structures in the unfrozen aqueous phase decreases, no enhancement in IRI activity. Compared to the IRI activity of amino acids (L-Phenylalanine, L-Tyrosine, 3,4-Dihydroxy-L-phenylalanine), tyrosine showed the strongest IRI activity. Notably, tyrosine exhibits potent IRI activity both intracellularly and extracellularly. These results suggest that IRI activity depends not only on structure formation, but also on structural stability, functional groups. Tyrosine exhibits excellent biocompatibility and can be used in various fields such as biomedicine and cryobiology.

**References:**

1. Kim, Y. D. et al. "Self-Assembled Nanostructures of Homo-Oligopeptide as a Potent Ice Growth Inhibitor" *Nano Lett.* **2023**, 23, 20, 9500–9507.
2. Warren, M. T. et al. "Minimalistic ice recrystallisation inhibitors based on phenylalanine" *Chemical Communications* **2022**, 58, (55), 7658-7661.
3. Lee, C, Lee, Y et al. "Peptide-DNA origami as a cryoprotectant for cell preservation" *Sci. Adv.* **2022**, 8, eadd0185.

**Presentation Title:** Poly(p-phenylene sulfide)-based Block Copolymers for PPS/Hydrophilic Interface Adhesion

**Authors:** Yugo Tosaki, Yuki Yoshida, Seigo Watanabe, Kenichi Oyaizu

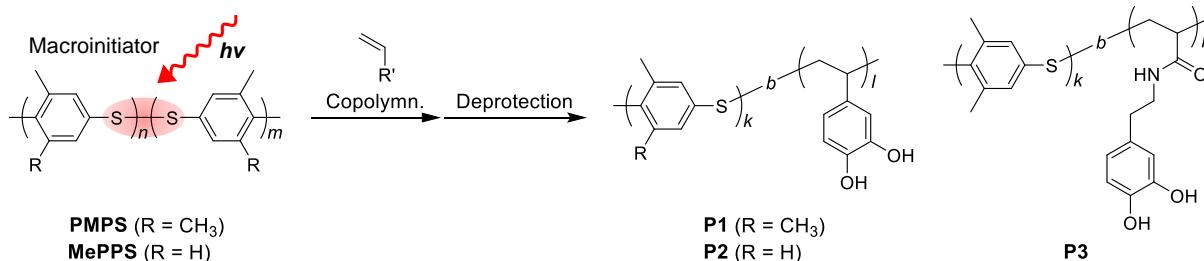
**Affiliation:** Department of Applied Chemistry and Research Institute for Science and Engineering, Waseda University, 3-4-1 Okubo, Shinjuku-ku, Tokyo 169-8555, Japan

**Email:** y.tosaki@fuji.waseda.jp

**Abstract:**

Poly(*p*-phenylene sulfide) (PPS) is an engineering plastic with outstanding high thermostability and mechanical properties, although PPS exhibits poor adhesiveness to other materials/substrates because of its low surface energy. Therefore, a high-cost and cumbersome surface modification process of PPS via chemical etching is required to achieve dissimilar material bonding of PPS<sup>1</sup>.

In this context, we herein synthesized the PPS-based block copolymers **P1-P3** as adhesives for dissimilar material bonding of PPS, which requires high affinity with both PPS and hydrophilic surfaces. **P1-P3** are composed of the methyl-substituted PPS segment (**PMPS** or **MePPS**) and the catechol-containing polymer segment (poly(4-vinylcatechol): **PVCA**<sup>2</sup> or poly(dopamine acrylamide): **PDA**<sup>3</sup>). These copolymers were synthesized via photo-radical polymerization using the corresponding PPS derivative as a macroinitiator, followed by deprotection of the catechol groups<sup>4</sup> (Fig. 1). The resulting copolymers displayed microphase-separated morphologies and demonstrated strong adhesion to both PPS and hydrophilic surfaces. Furthermore, the adhesion strength is precisely controllable by the segment ratio, following that the methyl-substituted PPS segment facilitates adhesion to PPS surfaces, whereas the catechol-containing segment enhances adhesion to hydrophilic surfaces.



**Fig. 1** Synthesis of the block copolymers.

**References:**

1. Y. I. Hsu, H. Uyama *et al.*, *Polym. J.* **2021**, *53*, 1231-1239.
2. K. Satoh, A. Takahara *et al.*, *ACS Appl. Polym. Mater.* **2022**, *4*, 3687–3696.
3. D. S. Seferos *et al.*, *Macromolecules* **2022**, *55*, 10167–10175.
4. S. Watanabe, K. Oyaizu, *ACS Appl. Polym. Mater.* **2021**, *3*, 4495-4503.

**Presentation Title:** Assembly-driven enhanced anticancer effect of berberine by guaiazulene sulfonate

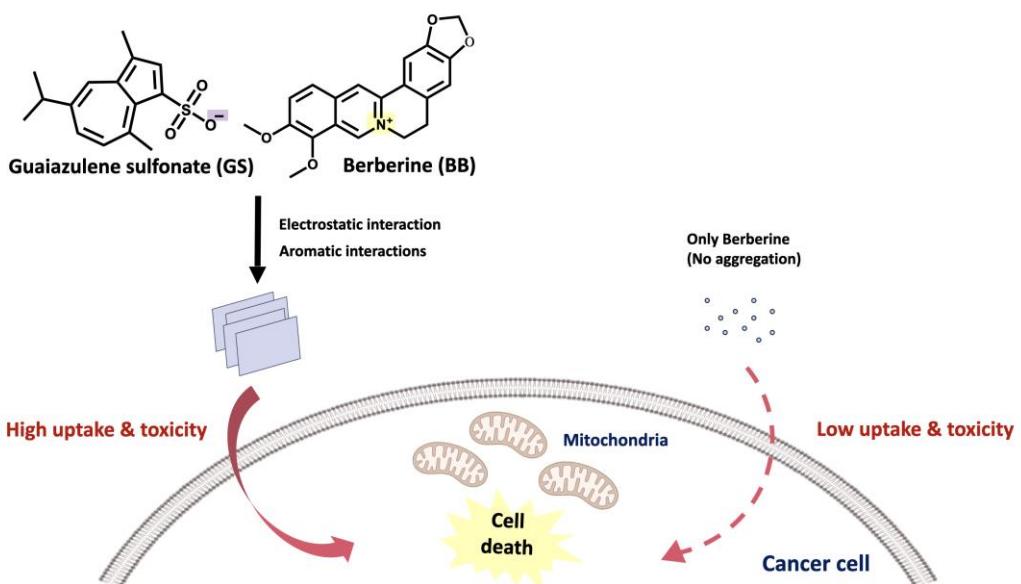
**Authors:** Yeojin Choi, Yongju Kim

**Affiliation:** KU-KIST Graduate School of Converging Science and Technology  
Korea University, Seoul, Korea

**Email:** yongjukim@korea.ac.kr

**Abstract:**

Berberine is a versatile natural compound with the potential to treat various pathological conditions. Recently, there has been widespread interest in the anticancer effects of berberine. However, due to the instability of berberine as a drug, there is a limitation in its direct effect on cancer cells, which is relatively weak. To increase stability and enhance efficacy, we present the development of supramolecular anticancer materials based on berberine. Supramolecules were constructed using berberine and sodium guaiazulene sulfonate, a biocompatible natural compound, through ionic bonds and aromatic interactions. The resulting supramolecular anticancer materials induced greater toxicity in Hela cells compared to a single molecule. This supramolecular approach not only provides insights into the assembly of next-generation anticancer agents at the molecular level but also offers a strategy for producing well-defined supramolecular anticancer drugs.



**Presentation Title:** Differential Regulation of Glucose Transporter 1 (GLUT1) Expression and Antioxidant Activity by Micelle and Chiral Sheet Structures

**Authors:** Yerim Kim, Yongju Kim

**Affiliation:** KU-KIST Graduate School of Converging Science and Technology  
Korea University, Seoul, Korea

**Email:** yerimm30@gmail.com

**Abstract:**

Supramolecular structures are formed through noncovalent interactions, such as hydrogen bonds and  $\pi$ - $\pi$  interactions, and can be assembled into various forms, including micelles, sheets, and fibers. Depending on their shape, these structures serve different functions within cells, with the ability to either stimulate the cell exterior or be absorbed into the cell to produce various biological effects such as anticancer and antioxidant activities. Micelles interaction have been extensively studied due to its excellent intracellular uptake, in contrast, studies about its interaction with cell membrane remains limited. In this study, we reported the interaction of micelles and chiral 2D sheet with cell membrane, using chiral glucose derivatives.

Through a comparative analysis of the interaction with glucose transporter 1 (GLUT1), we confirmed that the 2D sheet significantly increased GLUT1 expression and glucose uptake, better than micelle. Moreover, it exhibited antioxidant effect as well. These findings demonstrated that glucose-based chiral sheets have the potential to influence cellular responses and biological functions by selectively binding with specific proteins

**References:**

1. T. Kim, J. Y. Park, J. Hwang, G. Seo, **Y. Kim\*** “Supramolecular Two-dimensional Systems and their Biological Applications” *Adv. Mater.* **2020**, 32, 2002405.
2. G. Seo, T. Kim, B. Shen, J. Kim, **Y. Kim\*** “Transformation of Supramolecular Membranes to Vesicles driven by Spontaneous Gradual Deprotonation on Membrane Surfaces” *J. Am. Chem. Soc.* **2022**, 144, 17341.
3. T. Kim, J. Hong, J. Kim, J. Cho, **Y. Kim\*** “Two-dimensional peptide assembly via arene–perfluoroarene interactions for proliferation and differentiation of myoblasts” *J. Am. Chem. Soc.* **2023**, 145, 1793.

**Memo**

**Memo**