

# 2023

## 충남대학교 소재화학연구소 국내학술대회 및 대한화학회 대전충남세종지부 하계학술대회

| 일시 | 2023년 6월 30일(금)

| 장소 | 충남대학교 자연과학대학 4호관(W11-2) 109호

| 주관 | 충남대학교 소재화학연구소  
대한화학회 대전 · 충남 · 세종지부

| 후원 | 충남대학교 화학물질특성분석 핵심연구지원센터  
충남대학교 기초과학연구원  
충남대학교 화학과  
유전병 특이 점돌연변이 DNA 검출 비대칭 광학/질량센서 개발 기초연구실  
한국에너지기술원(N-LAB 연료전지 연구실)



충남대학교 소재화학연구소



## Program

10:00 ~ 10:20	등록 및 명찰 배부
10:20 ~ 10:30	축사 및 개회사 최 성 희 교수 (충남대학교 자연과학대학장) 김 정 권 교수 (충남대학교 소재화학연구소장)

### Section 1

좌 장 : 최진실 교수 (한밭대학교)

10:30 ~ 10:50	이 혁 진 교수 (공주대학교) “ Vitamins as Potent Matrix Metalloproteinase-2/9 Regulators ”
10:50 ~ 11:10	최 고 은 교수 (단국대학교) “ Artesunate drug-loaded 2D nano-shuttle landing on RBCs infected with malaria parasites ”
11:10 ~ 11:30	배 제 현 교수 (충남대학교) “ Nanoporous Electrochemistry for Better Electroanalysis ”
11:30 ~ 11:50	박 구 곤 박사 (한국에너지기술연구원) “Ultrastable Core-Shell Structured-Nanoparticles as active metals for the Oxygen Reduction Reaction of Fuel Cells”
12:00 ~ 13:50	점심식사
14:00 ~ 15:30	포스터 발표

### Section 2

좌 장 : 손영구 교수 (충남대학교)

15:30 ~ 15:50	이 승 호 교수 (한남대학교) “ Field-flow fractionation (FFF): a tool for separation of particles and macromolecules ”
15:50 ~ 16:10	김 환 규 교수 (고려대학교) “ Organic and Polymer Chemistry Toward Advanced Technology Era: Organic Semiconductor Materials ”
16:10 ~ 16:30	강 흥 석 교수 (전주대학교) “ Electronic Structure and CatalyticActivityof2D Materials ”
16:30 ~ 17:30	우수포스터 시상 및 폐회사 손 영 구 교수 (대한화학회 대전충남세종지부장)
17:30 ~	기념촬영 및 경품추첨

# 이혁진 Hyuck Jin Lee

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Kongju National University

Department of Chemistry Education



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## 학력

2007 – 2011 B.S. Catholic University of Daegu

2009 – 2011 B.S. Minnesota State University, Mankato

2011 – 2015 Ph.D. University of Michigan, Ann Arbor (Chemistry; Advisor: Prof. Mi Hee Lim)

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## 경력

2015. 12. – 2018. 02. Postdoctoral Researcher, UNIST (Advisor: Prof. Mi Hee Lim)

2018. 03. – 2019. 02. Postdoctoral Researcher, KAIST (Advisor: Prof. Mi Hee Lim)

2019. 03. – present Assistant / Associate Professor, Kongju National University

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## 수상 내역

2018 The Best Poster Award, *The 2018 KCS Inorganic Chemistry Division Summer Symposium*

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## 발표 논문

1. “Metal Complexes as Promising Matrix Metalloproteinases Regulators” Nguyen, Y. T., Kim, N., Lee, H. J.\* Int. J. Mol. Sci. 2023, 24, 1258.
2. “Potent Therapeutic Targets for Treatment of Alzheimer’s Disease: Amyloid Degrading Enzymes” Choi, H., Kim, E., Choi, J. Y., Park, E. Lee, H. J.\* Bull. Korean Chem. Soc., 2021, 42, 1419–1429. (Special Issue of “Bioinorganic Chemistry: Diverse Approaches to Elucidating the Roles of Metal Ions in Biology” in Bull. Korean Chem. Soc.)
3. “Redox Active Metal Ions and Amyloid Degrading Enzymes in Alzheimer’s Disease” Kim, N. and Lee, H. J.\* Int. J. Mol. Sci., 2021, 22, 7697.
4. “Target Enzymes Considered for the Treatment of Alzheimer’s Disease and Parkinson’s Disease” Kim, N. and Lee, H. J.\* BioMed Res. Int., 2020, 2020, 2010728.

# Vitamins as Potent Matrix Metalloproteinase-2/9 Regulators

Hyuck Jin Lee

*Department of Chemistry Education, Kongju National University, Gongju,  
Chungcheongnam-do 32588, Republic of Korea*

Over the past few decades, various studies have tried to find better strategies for the treatment of intractable diseases such as cancer. One potential target is Matrix metalloproteinases (MMPs), of which MMP-2 and MMP-9 play a crucial role in the onset and progression of cancer through multiple ways, including tumor cell invasion, angiogenesis, immune evasion, and metastasis. Therefore, several chemical agents have been developed to regulate the expression and activity of MMP-2/9 for treating cancer. Due to the dose limiting toxicity and biosafety, however, the chemicals need to be improved their biological properties. To reduce the risk of toxicity, we explored natural molecules, such as vitamins, as MMP-2/9 regulators. The abnormal amount of vitamins in the body have been linked to various diseases including multiple cancers; prostate, breast, brain, lung, and skin cancer. Therefore, we investigated the relationship between MMP-2/9 and vitamins to better understanding of the pathogenic mechanisms of cancers. In our study, we examined the effect of both fat- and water-soluble vitamins (vitamin A, B<sub>6</sub>, C, and D<sub>3</sub>) on the expression and activity of MMP-2/9 through biological and biochemical experiments, and identified the interactions between vitamins and MMP-2/9 through docking simulations. As a result, vitamin A significantly inhibited the activity and expression of MMP-2, while vitamin B<sub>6</sub> reduced the levels and actions of MMP-9. Vitamin C and D<sub>3</sub> slightly decreased the activity of MMP-2/9. This study could provide new insights into the regulation of MMP-2/9 by vitamins and contribute to the development of a new library for cancer therapy.

# 최고은 Goeun Choi

## 단국대학교

Department of Nanobiomedical Science,  
College of Science and Technology



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## 연구분야

Synthesis of bio-nanohybrid materials with heterostructure  
Exploration of 2-dimensional materials via intercalative soft chemistry  
Designing multimodal nanohybrid materials with theranostic functions

## 학력

Feb. 2016 **Ph. D.** Department of Chemistry and Nano Science, Ewha Womans University, Seoul, Korea  
Feb. 2010 **M. S.** Department of Chemistry and Nano Science, Ewha Womans University, Seoul, Korea  
Aug. 2007 **B. S.** Department of Chemistry, Sangmyung University, Seoul, Korea

## 경력

2020. Mar. – Present : **Assistant Professor**, Department of Nanobiomedical Science, Dankook University, Korea  
2018. Oct. – 2020. Feb. : **Invited Professor, NRF Research Fellow**, Dankook University, Korea  
2017. June. – 2018. Sep. : **Research Professor, NRF Research Fellow**, Center for Nano-Bio Materials (CINBM), Department of Chemistry and Nanosciences (BK21 PLUS), Ewha Womans University, Korea.  
2017. Mar. – 2017. May. : **Visiting Postdoctoral Fellow**, Future Industries Institute (FII), University of South Australia, SA, Australia.  
2016. Mar. – 2017. May. : **Research Associate**, Center for Nano-Bio Materials (CINBM), Department of Chemistry and Nano Sciences (BK21 PLUS), Ewha Womans University, Korea.  
2016 – Present : **Permanent member**, Korean Chemical Society, Korea.

## 수상 내역

2019.10. Best Oral Presentation Award, The 3rd A3 Foresight Symposium on Organic/Inorganic Nanohybrid Platforms for Precision Tumor Imaging and Therapy, Shanghai, China.  
2017.11. The Best Poster Presentation Award, The 9th Young Researcher's BNCT Meeting, Japan.  
2017. 8. IUMRS Research Encouragement Award, The 15th International Conference on Advanced Materials (IUMRS-ICAM 2017), Kyoto, Japan.  
2017. 2. Best Oral Presentation Award, Pure and Applied Chemistry International Conference 2017 (PACCON 2017), Bangkok, Thailand.  
2016. 10. A Prize for Excellent Ph. D. Thesis, Korean Chemical Society (KCS), Korea.

## 발표 논문

1. G. Choi<sup>‡</sup>, G.W. Jin<sup>‡</sup>, H. Piao, N.S. Rejinold, S. Asahina, S.J. Choi, H.J. Leeg, J.H. Choy\*, "NOAEL cancer therapy: a tumor targetable docetaxel-inorganic polymer nanohybrid prevents drug-induced neutropenia", Journal of Materials Chemistry B 11 (2023) 565. Cover Paper.
2. H. Piao, G. Choi, X. Jin, S.J. Hwang, Y.J. Song, S.P. Cho, J.H. Choy\*, "Monolayer graphitic carbon nitride as metal-free catalyst with enhanced performance in photo and electro-catalysis", Nano-Micro Letters 14 (2022) 55.
3. J.Y. Kim, H.I. Shin, S.E. Lee, H. Piao, N.S. Rejinold, G. Choi\*, J.H. Choy\*, "Artesunate drug-loaded 2D nano- shuttle landing on RBCs infected with malaria parasites", Biomaterials Science 10 (2022) 5980.

# Artesunate drug-loaded 2D nano-shuttle landing on RBCs infected with malaria parasites

Goeun Choi<sup>1,2,3</sup>

*1 Intelligent Nanohybrid Materials Laboratory (INML), Institute of Tissue Regeneration Engineering (ITREN), Dankook University, Cheonan 31116, Korea*

*2 Department of Nanobiomedical Science and BK21 PLUS NBM Global Research Center for Regenerative Medicine, Dankook University, Cheonan 31116, Korea*

*3 College of Science and Technology, Dankook University, Cheonan 31116, Korea*

Artesunic acid ( $AS^0$ ), a derivative of artemisinin, is recommended for the treatment of severe and complicated malaria, but its use is limited because of limitations such as a short half-life, non-specific targeting capability, low bioavailability, etc. To overcome these issues, a novel 2D inorganic delivery shuttle system for an  $AS^0$  drug to target the malarial host, red blood cells (RBCs), is explored by immobilizing  $AS^0$  into 2D metal hydroxides to form  $AS^-$  (artesunate, the deprotonated form of artesunic acid) nanohybrid drugs. Haemolysis assay showed that the  $AS^-$  nanohybrids not only are haemo-compatible but also target RBCs due to the electrostatic interaction and hydrogen bonding between RBCs and  $AS^-$  nanohybrids. As clearly demonstrated by the subsequent parasite lactate dehydrogenase assay, the antimalarial effect of the  $AS^-$  nanohybrids is determined to be 6 times more effective than that of intact  $AS^0$  against malaria. Therefore, the  $AS^-$  nanohybrids with haemocompatible 2D inorganic carriers could be the promising drug delivery systems for targeting the malarial host, RBCs.

# 배제현 Je Hyun Bae

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충남대학교 분석과학기술대학원



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## 학력

Sep. 2008 – Aug. 2013 **Ph.D.** in Chemistry, Seoul National University, Korea

Sep. 2006 – Feb. 2008 **M.S.** in Chemistry, Chung-Ang University, Korea

Mar. 2003 – Aug. 2006 **B.S.** in Chemistry, Chung-Ang University, Korea  
(summa cum laude)

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## 경력

Jul. 2020 – Present Visiting Professor, Division of Analytical Science, Korea Basic Science Institute, Republic of Korea

Mar. 2020 – Present Assistant Professor, Graduate School of Analytical Science and Technology, Chungnam National University, Republic of Korea

May 2019 – Jan. 2020 Senior Postdoctoral Associate, Queens College–The City University of New York, United States

Aug. 2018 – Dec. 2019 Adjunct Assistant Professor, Queens College–The City University of New York, United States

Mar. 2015 – Apr. 2019 Postdoctoral Associate, Queens College–The City University of New York, United States

Sep. 2013 – Feb. 2015 Postdoctoral Fellow, Seoul National University, Republic of Korea (Advisor: Prof. Taek Dong Chung).

Mar. 2008 – Aug. 2008 Researcher, Chung-Ang University, Republic of Korea.

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## 발표 논문

1. Electrochemistry at nanoporous interfaces: new opportunity for electrocatalysis, JH Bae, JH Han, TD Chung Physical Chemistry Chemical Physics 14 (2), 448-463
2. Effects of adsorption and confinement on nanoporous electrochemistry, JH Bae, JH Han, D Han, TD Chung Faraday discussions 164, 361-376
3. Diffuse layer effect on electron-transfer kinetics measured by scanning electrochemical microscopy (SECM), JH Bae, Y Yu, MV Mirkin The Journal of Physical Chemistry Letters 8 (7), 1338-1342



# Nanoporous Electrochemistry for Better Electroanalysis

Je Hyun Bae

*Graduate School of Analytical Science and Technology (GRAST), Chungnam National*

*University, Daejeon 34134, Republic of Korea*

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Electroanalytical methods are a class of analytical methods which study analytes by measuring the electrical properties in an electrochemical cell containing analytes. These methods have been widely used because of relatively simple and inexpensive techniques, low limit of detection, and measurement of electrically original signals. With the development of nanotechnology, electroanalysis has been advancing and offers new opportunities in analysis. Nanoporous electrodes are representative electrode materials for diverse applications, such as energy conversion devices and sensors. Our efforts for electroanalysis with enhanced sensitivity and selectivity based on nanoporous electrodes will be presented.



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## 연구분야

신재생에너지 (수소, 연료전지)

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## 학력

2004.4. ~ 2007.3. Kyoto 대학교, 물질에너지화학전공, 공학박사

1997.3. ~ 1999.2. 포항공과대학교, 화학공학과, 석사

1993.3. ~ 1997.2. 경희대학교, 화학공학과, 학사

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## 경력

1999 ~ 현재 한국에너지기술연구원, 책임연구원, 실장(2020년 ~현재)

2009 ~ 현재 한국과학기술연합대학원대학교 (UST), 소에너지공학, 전공책임교수

2009 ~ 현재 IEA(International Energy Agency) Advanced Fuel Cells Annex 31 : Polymer Electrolyte Fuel Cells, 한국대표

2014 ~ 2015 Brookhaven National Laboratory (BNL), Chemistry Dept., 방문연구원, 미국

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## 수상 내역

2019.04.22. 과학기술정보통신부 장관 표창

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## 발표 논문

1. Effect of PTFE contents in the gas diffusion media on the performance of PEMFC, GG Park, YJ Sohn, TH Yang, YG Yoon, WY Lee, CS Kim Journal of Power Sources 131 (1-2), 182-187
2. Development of microchannel methanol steam reformer, GG Park, DJ Seo, SH Park, YG Yoon, CS Kim, WL Yoon Chemical Engineering Journal 101 (1-3), 87-92
3. Pore size effect of the DMFC catalyst supported on porous materials, GG Park, TH Yang, YG Yoon, WY Lee, CS Kim International Journal of Hydrogen Energy 28 (6), 645-650

# Ultrastable Core–Shell Structured–Nanoparticles as active metals for the Oxygen Reduction Reaction of Fuel Cells

Eunjik Lee, Sung–Dae Yim, Tae–Hyun Yang, Gu–Gon Park\*

*Fuel Cell Laboratory, Korea Institute of Energy Research (KIER), 152, Gajeong-ro,  
Yuseong-gu, Daejeon 34129, South Korea*

Recently, R&D in the field of fuel cell vehicles is focused on heavy duty vehicles. It is analyzed that about 5 times more durability is required than conventional passenger cars, and the price ratio of electrocatalysts in fuel cell stacks reaches about 60%. As a result, there is a considerable demand for the development of novel electrocatalysts that satisfy high activity and durability requirements. By regulating the amount of nitrogen doped into the nanoparticles, we were able to increase the stability of Co@Pt core–shell nanoparticle catalysts in the previous study while retaining the electrochemical surface area even after a long-term durability evaluation of 1 million cycles. In comparison to commercial Pt/C, the high-pressure nitrogen-infused CoN@Pt/C catalyst demonstrated a two-fold increase in mass activity and a five-fold increase in durability. It retained 80% of its initial mass activity after 180k cycles and kept its core–shell structure even after 1000k cycles of accelerated stress tests. By adjusting the ambient pressure throughout the heat treatment process and regulating particle size and homogeneity in the nanoscale range, this work can also offer a practical and straightforward technique to create core–shell nanoparticles. Sizes of 3.1 to 4.2 nm for core–shell nanoparticles

# 이승호 Seungho Lee

한남대학교 화학과

대전시 유성구 유성대로 1646

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교수소개

## 연구분야

Implementation and application of field-flow fractionation (FFF), SPLITT Fractionation, SEC, Light Scattering and related techniques for separation and characterization of macromolecules and Nano to Micron-sized particles.

## 학력

1980.2 연세대학교 화학과 학사 (화학 전공)

1982.2 연세대학교 화학과 석사 (분석화학 전공)

1988.8. 미국 Univ. of Utah 화학과 Ph.D. (물리-분석화학 전공)

## 경력

1989.7 – 1996. 8: 미국 3M 중앙연구원 Polymer characterization Lab, Group Leader

1996.9 – 현재: 한남대학교 화학과 교수

1999.1 – 2000.12: 대한화학회 상임편집위원

2002.3 – 2003.2: 스웨덴 Lund University 방문교수

2006.3 – 2020.8: 한남대 화학과 BK21 사업팀장 (바이오센서용 소재개발팀)

2008.3 – 2009.2: 한남대학교 대외협력처장

2009.2 – 2010.1: 미국 Cleveland Clinic 방문교수

2011.1 – 2015.12: 한국분석과학회지 편집위원장

2013.3 – 2016.2: 한남대학교 대외협력처장

2018.1 – 2018.12: 한국분석과학회 회장

2019.1-2022.12: 한국인그리에학회 회장

## 수상 내역

2014.12. 대한화학회 학술상

2014.6. 한국분석과학회 학술상

## 발표 논문

1. C. Fuentes, J. Choi, C. Zielke, J. M. penarrieta, S. Lee, L. Nilsson, "Comparison between conventional and frit-inlet channels in separation of biopolymers by asymmetric flow FFF", Analyst, 144, 4559-4568, 2019.
2. M. H. A. Elella, E. A. ElHafeez, E. S. Goda, S. Lee, K. R. Yoon, "Smart bactericidal filter containing biodegradable polymers for crystal violet dye adsorption", Cellulose, 25, 9179-9206, 2019.
3. C. Fuentes, H. Saari, J. Choi, S. Lee, M. Sjö, M. Wahlgren, L. Nilsson, "Characterization of non-solvent precipitated starch using asymmetrical flow FFF coupled with multiple detectors", Carbohydrate Polymers, 206, 21-28, 2019.

# Field-flow fractionation (FFF): a tool for separation of particles and macromolecules

Seungho Lee

*Department of Chemistry, Hannam University*

*slee@hnu.kr*

Field-flow fractionation (FFF) is a family of techniques that has been proven to be potentially useful for separation and characterization of various types of macromolecules and colloidal particles. FFF employs a thin ribbon-like open channel across which an external field is applied to interact with sample components. There are various subtechniques (or family members) of FFF depending upon the type of the external field employed, which includes thermal FFF (ThFFF), sedimentation FFF (SdFFF), and flow FFF (FIFFF). The principle and theory of FFF will be briefly introduced. Then some of detection methods (e.g., light scattering) suited for FFF will be discussed. Finally some of application examples of FFF for analysis of various types of particles and polymeric materials will be discussed.

Topics include:

- [1] Molecular Weight Characterization of Cationic Potato Amylopectin (CPAP) using flow FFF (AsFIFFF)–MALS.
- [2] Characterization of fluorescent pigment particles using FIFFF.
- [3] Capability of ThFFF for Analysis of Processed Natural Rubber.
- [4] Determination of gel content in polymers.

# 김환규 Hwan Kyu Kim

고려대학교(세종) 신소재화학과

글로벌 에너지미래선도 연구실



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## 연구분야

※ New Molecular Design & Synthesis of Organic and Polymeric Semiconductor Materials for Highly Efficient Dye-sensitized Solar Cells  
※ New Molecular Design & Synthesis of Organic Hole Transporting Materials for Highly Efficient Solid-state Dye-sensitized Solar Cells and Perovskite Solar Cells  
※ New Molecular Design & Synthesis of D-p-A Copolymers for Highly Efficient Perovskite Solar Cells and Organic Solar Cells  
※ Block Copolymers via Controlled Living Polymerization for Quasi-Solid-state Dyesensitized Solar Cells  
※ Copolymer-templated Carbon Nanomaterials for Next Generation Solar Energy Conversion and Storage Devices

## 학력

1980. 2. 울산공과대학 공업화학과 (현, 울산대 화학과) (공학사)  
1982. 2. 한국과학기술원(KAIST) 화학과 고분자화학 (이학석사)  
1990. 12. Carnegie-Mellon University 화학과 고분자화학 (이학박사) (지도교수: Prof. K. Matyjaszewski)

## 경력

2007. 3. - 현재 고려대학교 신소재화학과 교수(특별초빙)  
2007. 6 - 2007. 7 스위스연방공대(로잔) 화학과 방문교수 (Visiting Professor)  
2016. 12 - 2017. 2 미국 와싱턴대학교(시애틀) 재료공학과 방문학자 (Visiting Scholar)  
2017. 06 - 2017. 08 영국 옥스퍼드대학교 물리학과 방문석학 (Visiting Fellow)

## 수상 내역

1998. 4. 대한화학회 고분자화학분과회 학술진보상

## 발표 논문

1. "Effective Redox Shuttles for Polymer Gel Electrolytes-based Quasi-solid-state Dye-sensitized Solar Cells in Outdoor and Indoor Applications: Comprehensive Comparison and Guidelines", Masud, Haoran Zhou and Hwan Kyu Kim\*, *Materials Today Energy*, 34, 101299 (2023.06).
2. "Novel Trifluoropropoxy-Substituted Carbazole Asymmetric Derivatives as Efficient and Hydrophobic Hole Transporting Materials for High-Performance and Stable Perovskite Solar Cells", *Chemical Engineering Journal*, 428, 131108 (2022. 01).
3. "In-depth Understanding of the Energy Loss and Efficiency Limit of Dye-Sensitized Solar Cells Under Outdoor and Indoor Conditions", *J. Materials Chemistry A*, 9(44), 24715-25222 (2021. 11). (Perspective-Review Article) (Back Cover-Highlighted)

# Organic and Polymer Chemistry Toward Advanced Technology Era:

## Organic Semiconductor Materials

Hwan Kyu Kim (김 환규)

*Department of Advanced Materials Chemistry, Korea University*

*Sejong 339-700, Korea*

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Organic semiconducting materials have widely been used to many applications including displays, sensors, electronics, photonics and photovoltaics. By revisiting the lifetime research achievements, organic and polymer semiconducting materials for photonic and photovoltaic applications have been designed and synthesized within the past three decades. At the early stage, 1) a new class of silicon-based p-conjugated copolymers was synthesized by various C-C coupling reactions. The incorporation of organosilicon units into  $\pi$ -conjugated systems in the backbone improved their processability and interrupted the  $\pi$ -conjugation length to tune R/G/B EL colors for LED application. Also, 1) soluble polyimides having nonlinear optical (NLO) chromophores for photonic applications were synthesized by direct polycondensation without a curing step to ameliorate the optical property of NLO polymers. 3) Since 2001, Er(III)-cored supramolecular complexes—based on aryl-ether typed dendritic anthracene or porphyrin ligands were synthesized to exhibit strong near-IR emission bands via efficient energy transfer from the peripheral antenna to the  $\text{Er}^{3+}$  ions. 4) Very recently, organic and polymer semiconducting materials for dye-sensitized and perovskite solar cells were designed and synthesized in order to give right answers in overcoming the limitation of the existing technology for the practical use. In this presentation, organic and polymer semiconducting materials for photonic and photovoltaic applications and beyond their applications will be explored and the scientific lifetime career will be discussed with a thankful heart.

### References:

1. H. K. Kim and K. Matyjaszewski, *J. Am. Chem. Soc.*, 110, 3321 (1988).
2. S. J. Kang, C. S. Yoon and H. K. Kim, et.al., *Chem. Mater.*, 11, 779 (1999).
3. K. L. Paik, N. S. Baek, J. H. Lee and H. K. Kim, *Macromolecules*, 35, 6782 (2002).
4. N. S. Baek and H. K. Kim, et.al., *Advanced Functional Materials*, 16, 1873 (2006).
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## 연구분야

Using various first-principles methods, I have been involved in research for designing and understanding *electronic, optical, and chemical* properties of various low dimensional nanomaterials.

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## 발표 논문

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# Electronic Structure and Catalytic Activity of 2D Materials

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First, our first-principles calculation indicates that  $\text{TeSe}_2$  is the most stable among various  $\text{Te}_{1-x}\text{Se}_x$  compounds. Different from the case of bulk Te, its bulk can equally adopt three different crystal structures as well as their chiral images. Electronic band structure calculation shows that all three phases are semiconductors, where hidden spin texture or chiral spin texture is observed. Second, two non-Janus configurations of MXY (M = Mo, W; X = S/Se; Y = Se/Te) monolayers are shown to be considerably more stable than Janus configuration, displaying interesting physical properties such as giant in-plane electric polarization, giant spin splitting (160~480 meV) at the valence band maximum, and multiferroicity.<sup>2</sup> Furthermore, binary and ternary alloys of transition metal dichalcogenides have been extensively investigated in the whole composition range in collaboration with an experimental group. Typical examples are  $\text{Mo}_{1-x}\text{Nb}_x\text{Se}_2$ ,  $\text{Mo}_{1-x}\text{V}_x\text{Se}_2$ , and  $\text{Nb}_{1-x}\text{V}_x\text{Se}_2$ , and  $\text{Mo}_{1-(x+y)}\text{Nb}_x\text{V}_y\text{Se}_2$ . Detailed chemical structures of the alloys have been predicted at various compositions based on extensive spin-polarized DFT calculations. Experimental results can be understood in terms of alloy formation energy, phase transition, and Gibbs free energy change along the reaction path. Specifically, an excellent performance in the ternary alloy is due to a large number of active surface sites present even in the absence of defects. This is quite different from the cases of binary alloys which require defect sites such as Se vacancies for the activity.

## Poster Presentation

### 001 Interpenetrated 2D Cu(II) Coordination Networks and its applications

정은비, 이해리\*

한남대학교

We successfully formed Cu(II) complexes, which crystal structures were analyzed single crystal X-ray diffractometer. Notably, the coordination environment and counter anions surrounding the Cu(II) ion played a pivotal role in determining the overall skeletal structure of the complexes. Our ongoing research focuses on further exploring the structural effects and implications of Cu(II) networks. By gaining a deeper understanding of these factors, we aim to enhance our knowledge of the properties and potential applications of copper-based coordination compounds. The reversible oxidation-reduction behavior of copper metal ions is a fascinating phenomenon with wide applications in the fields of catalysts and sensors. In our study, we aimed to construct coordination networks incorporating Cu(II) by designing and synthesizing a bis(monodentate) N-donor ligand. The ligand was thoroughly characterized using advanced spectroscopic techniques, including  $^1\text{H}$ ,  $^{13}\text{C}$ , COSY NMR spectra, and mass spectrometry.

### 002 Imidazolyl-donor Ligand based Zn(II) Coordination Polymers

김현서, 이해리\*

한남대학교

Zn(II) coordination polymers allow to detect a toxic chemical 4-nitrophenol by electrochemical signals. The electrochemical measurement is a highly sensitive method providing evidence for chemical reactions on the surface of the electrode. Hereby, we designed and synthesized new coordination structures containing imidazolyl donor ligands and Zn(II). The presence of microcrystals on the working electrode enhanced the redox signals.

### 003 Self-assembly Mn(II)-imidazolyl Lignad Complexes

김현서, 신성민, 이해리\*

한남대학교

Recent research has shown that metal complexes containing imidazolyl group as electron donors have been formed rather rapidly and applied to various fields used as catalysts, containers for drug delivery systems. Imidazole donor groups have been found to be relatively stronger Lewis base compared to pyridyl donor groups.<sup>1</sup> In our research group, we aim to create new complex structures by binding imidazolyl ligands to transition metals using self-assembly, a well-known method that enables the formation of systematic structures through their internal and intermolecular interactions. The self-assembly method is highly productive and cost-effective, making it applicable to a wide range of fields. In this study, a new ligand was synthesized in two steps, and its characterization was analyzed using IR and  $^1\text{H}$  NMR spectroscopic techniques. Self-assembly of  $\text{MnX}_2$  ( $\text{X} = \text{Cl}, \text{Br}, \text{I}, \text{NO}_3, \text{ClO}_4$ ) and L gives rise to 1D and 2D structures. The physicochemical properties of Mn(II)

compounds were characterized using SC-XRD, PXRD, IR, and TGA analyses. The structure of  $[\text{MnL}_3]\text{Br}_2$  is 1D coordination polymers, with the Br ions and solvent molecules located outside the skeletal structure, not coordinating to metal centers. Therefore, both the choice of anion and solvent system play a key role in determining the skeletal structures of metal complexes with different sizes and spaces. This offers the potential for chemical storage and separation based on molecular size variations.

004 **MOF synthesis study: MOF-808 and ZIF-8**

김현서, 조유나, 이해리\*  
한남대학교

Metal-organic frameworks (MOFs) are a class of compounds that consist of metal ions (or metal clusters) bound to organic ligands, forming one-, two-, or three-dimensional structures. MOFs are well-known materials for their high surface area, tunable porosity, and diversity in metal and functional groups they possess. The stable pores are expected to adsorb guest molecules, which is often solvents or small molecules.[1] Small molecules or drugs can be adsorbed and stored in the voids for later use. The most common metal ions used in MOFs are Zn(II), Cu(II), Fe(III), and Zr(IV), while organic linkers such as terephthalic acid, trimesic acid, or 2-methylimidazole. [2] In this experiment, MOF-808 and ZIF-8 were synthesized following procedures.[3,4] The structures of the compounds were confirmed through the measurement of PXRD patterns.

005 **Co(II) Coordination Polymers consisting of naphthalene-2,6-diylbis(methylene)-dinicotinate**

정은비, 이민정, 이해리\*  
한남대학교

Cobalt has been used as a raw pigment for glass coloring since the 19th century due to the excellent stability. The color cobalt blue, cobalt green, and cobalt violet are attributed to specific oxidation states of cobalt. Naphthalene exhibits a high quantum yield and excellent photostability due to its conjugated  $\pi$ -electron system and a rigid plane shape. In this research, L (L = naphthalene-2,6-diylbis(methylene)dinicotinate) was synthesized by the reaction of 2,6-bis(hydroxymethyl)-naphthalene and nicotinoyl chloride hydrochloride in chloroform. Self-assembly of  $\text{CoX}_2$  (X= Br,  $\text{NO}_3$ ) and L gives rise to 1D coordination polymers. Crystal structures of each complex were analyzed by single crystal X-ray diffraction. In this presentation, we will present the results of our structural study, including the geometry of metal centers. In the future, we will study thermal stabilities of each complex and obtain the crystal structures containing different type of anions.

006 **Discrete Zn(II) Complexes and its Catalytic Effects**

권소현, 정은비, 이해리\*  
한남대학교

Catalysts play a crucial role in enhancing the efficiency of chemical reactions in a field of environmental, industrial, and biological applications. In particular, heterogeneous catalysts provide the advantage of easy separation from the reaction solution. Polymeric

metal compounds, which have less solubility in organic solvents, are applied as heterogeneous catalysts to initiate organic reactions. With the increasing focus on environmental concerns, sustainable and alternative energy sources like biodiesel derived from fats and soybean oils have gained prominence over fossil fuels. Biodiesel production involves a transesterification process, which requires specific catalysts, sensitive to moisture and pressure conditions. In our research, we synthesized discrete Zn(II)-based complexes and used them as catalysts in the transesterification reaction. The ligand and metal complexes were analyzed by spectroscopic techniques and characterized their crystal structures by X-ray diffraction method. Subsequently, the catalytic activities of these complexes in the transesterification reaction were examined.

007 **CRISPR/Cas12a-based SERS Sensor for Detection of SARS-CoV-2**

Minkyu Kim, Hongki Kim\*

*Kongju National University*

To effectively diagnose and control the spread of coronavirus disease 2019 (COVID-19) caused by the severe acute respiratory syndrome coronavirus-2 (SARS-CoV-2), it is crucial to develop fast and reliable diagnostic tools. In this study, we report a Clustered Regularly Interspaced Short Palindromic Repeats (CRISPR)/Cas (associated protein) system-based Au nanowire (NW) surface-enhanced Raman scattering (SERS) sensor that can detect SARS-CoV-2 by adopting the Hairpin Probe-Mediated Isothermal Amplification (HIamp) method. When the target RNA is present, the HIamp reaction generates a large amount of double-stranded DNA products (FPs). Subsequently, the Cas12a/crRNA complex specifically recognizes the FPs and cleaves the Cy5-labeled single-stranded DNA attached to the Au nanowire, which leads to a decrease in SERS intensity. We believe that this novel CRISPR/Cas12a-based SERS sensing method will significantly contribute to the accurate diagnosis of SARS-CoV-2 and broaden the application of the CRISPR/Cas detection system.

008 **Metal-Organic Framework Coating for the Preservation of Ag Nanowire SERS Platform**

YunJi Cho, Hongki Kim\*

*Kongju National University*

Ag nanostructures have been intensively studied as one of the most promising surface enhanced Raman scattering (SERS) platform due to their superior optical properties. However, the susceptibility of Ag surfaces to corrosion from oxygen or sulfur in the atmosphere can significantly impact their optical characteristics, thereby limiting the stable performance of Ag SERS platforms. In this study, we report a corrosion-resistant Ag nanowire (NW) SERS platform with an metal-organic framework (MOF) coating. A single Ag NW on a film (Ag-NOF) is coated with the zeolitic imidazolate framework-8, and then the corrosion resistance of the Ag-NOF structures is tested under various harsh environmental conditions. Interestingly, the MOF-coated Ag-NOF platforms exhibited outstanding resistance to oxidation and sulfidation. The SERS signals of the Ag-NOF structures were well-preserved under harsh conditions when coated with the MOF, whereas the signals diminished without the MOF coating. Importantly, the MOF coating also maintained the

DNA sensing capability of the Ag-NOF platform, even after exposure to different environmental conditions. Based on these findings, we anticipate that MOF-coated Ag-NOF structures will bring us one step closer to the practical application of Ag-based plasmonic nanostructures in a variety of research fields.

009 **Regulating MMP-2 and MMP-9 by Vitamins: Implications for Cancer Therapy**

박수민, 이혁진\*

공주대학교

Over the decades, extensive research efforts have been dedicated to uncover novel treatment of cancer. Matrix metalloproteinases (MMPs), particularly MMP-2 and MMP-9, have emerged as potential targets, due to their pivotal roles in cancer pathogenesis encompassing tumor cell invasion, angiogenesis, immune evasion, and metastasis. To regulate the expression and activity of MMP-2/9 for effective cancer treatment, several chemical agents have been developed. Due to the dose limiting toxicity and biosafety, however, the improvement of biological properties of those chemical agents is required. To reduce the risk of toxicity, we explored natural molecules, such as vitamins, as MMP-2/9 regulators. Aberrant vitamin levels have been associated with various diseases, including prostate, breast, brain, lung, and skin cancers. Therefore, this study aims to understand the pathogenic mechanisms based on the relationship between MMP-2/9 and vitamins. Through biological and biochemical experiments, we examined the impact of both fat- and water-soluble vitamins on the expression and activity of MMP-2/9. Fat-soluble vitamins could inhibit (i) the activity of MMP-2/9 possibly locating at the active site and (ii) the expression of MMP-2/9 through inactivation of ERK-1/2 and JNK-1/2, while water-soluble vitamins could not regulate either the activity or expression of MMP-2/9. This study could provide new insights into the regulation of MMP-2/9 by vitamins and contribute to the development of a new library for cancer therapy.

010 **Fluorescence Imaging-Guided Photothermal Therapy of Cancers using Polydopamine Nanoparticle-Incorporated Fluorescent Hydrogel**

Daehyeon Kim, Hongki Kim\*

Kongju National University

Polydopamine (PDA)-based photothermal agents (PTAs) used in photothermal therapy (PTT) for cancer treatment have emerged as potential alternatives to conventional PTAs containing molecules or dyes. However, the preparation of these agents as hydrogels has not been investigated. In this study, we report the development and characterization of a fluorescent PDA nanoparticle (FPNP)-incorporated hydrogel (FPNP-hydrogel) for fluorescence imaging-guided photothermal cancer therapy. The FPNP-hydrogel was prepared by incorporating fluorescent FPNPs into polyvinyl alcohol (PVA) using a simple method. The FPNP-hydrogel demonstrated excellent biocompatibility, strong fluorescence, and high photostability, all of which reflect its potential applications in fluorescence imaging. Moreover, the FPNP-hydrogel showed excellent photothermal conversion effects. When combined with near-infrared laser irradiation, the FPNP-hydrogel successfully reduced tumor volumes in 4T1 tumor-bearing mice within 14 d without inducing the

inflammatory response in major organs. These results suggest that multifunctional hydrogels with excellent fluorescence properties and high photothermal conversion efficiency could be useful for designing novel therapeutic methods for cancer treatment.

011 **CRISPR/Cas12a-based Au Nanowire SERS sensor for detection of ATP**

Toeun Kim, Hongki Kim\*

*Kongju National University*

The clustered regularly interspaced short palindromic repeats (CRISPR)-Cas12a system has attracted significant attention in the field of molecular diagnostics due to its simplicity, sensitivity, specificity, and wide range of applications. In this study, we report the CRISPR/Cas12a-assisted Au nanowire surface-enhanced Raman scattering (SERS) sensor for detection of adenosine triphosphate (ATP). When ATP is present, the locked activators, which consist of an ATP aptamer and a DNA activator, induce the release of the DNA activator. Subsequently, the released DNA activator is specifically recognized by the Cas12a/crRNA complex, initiating cleavage of the Cy5-labeled single-stranded DNA that is attached to the Au nanowire. Consequently, this cleavage event leads to a reduction in SERS intensity. By employing this approach, we effectively convert the recognition of ATP into a detectable SERS signal. This research expands the scope of applications for the CRISPR-Cas detection system and offers a practical method for analyzing non-nucleic acid targets.

012 **천연계면활성제를 이용한 태양광 패널 세척용 생분해성 세척제에 관한 연구**

이선아, 김운중\*

*한남대학교*

현재 산업에서 사용하고 있는 산업용 세척제는 합성계면활성제를 기반으로 제조한다. 합성계면활성제는 석유로부터 화학적으로 합성되어 진다. 이러한 합성계면활성제는 생물독성이 강하며, 생분해가 잘 이루어지지 않아 환경오염의 원인이 된다. 린스공정 과정에서 오염수가 발생하여 수질 오염으로 연결된다. 합성계면활성제에 장기노출된 작업자의 경우에는 피부, 호흡기 면역저하로 인해 비염, 천식, 아토피 등이 유발될 수 있다. 따라서 본 연구에서는 합성계면활성제로 인한 환경오염 발생을 해결하기 위해 sodium Methyl cocoylTaurate 라는 천연계면활성제를 사용하여 세척제를 제조하였다. 천연 계면활성제로 사용한 sodium Methyl cocoylTaurate 는 코코넛 오일에서 추출한 음이온성 계면활성제로 미국 EWG 측정 안전위험도 1등급의 친환경적인 클렌징 소재로 잘 알려져있다. 일반 계면활성제보다 생분해도가 우수하여 자연분해 속도가 빠르고 친환경적이라는 장점이 있다. sodium Methyl cocoylTaurate 를 이용하여 세척제를 제조하여 세척력 및 안정성 테스트를 진행하였고 태양광 패널에 적용 가능성을 확인하였다. 세척제는 Distilled water, sodium carbonate, citric acid, sodium Methyl cocoyl Taurate, EDTA·2Na, propylene glycol, ethanol, Urea 성분으로 NCC-1~6 의 세척제를 제조하였다. 제조 후 pH, Conductivity 및 IR 분석을 통해 세척제의 물성을 분석하였다. 세척력 분석을 위해 slide glass 에 Flux 를 이용하여 오염시킨 후 10% reference, 10% sample 을 사용하여 sonicator 로 5분간 세척하였다. 또한, 60°C에서 열 안정성을 확인하였고 중금속과 VOC 분석을 진행하였다. 태양광 패널에 적용성을 확인하기 위하여 경량 인공지능을 탑재하여 태양광 패널에서의 오염원 세척 실험을 진행하였다. 본 연구 결과, 제조한 세척제 중 pH 가 reference 와 비슷한 NCC-4~6 의 세척제를 이용하여 세척력 실험을 진행하였다. 세척력 실험 결과, NCC-4 의 세척력이 가장 우수한

것을 확인하였고 NCC-4 를 최종 세척제로 선정하였다. 또한, 안정성 분석을 통해 NCC-4 가 60°C에서 안정한 것을 확인하였고, 휘발성 유기화합물(VOC) 및 중금속 분석 결과 기준치에 적합한 것을 확인하였다. 경량 인공지능을 탑재하여 태양광 패널을 세척한 결과, 태양광 패널 세척제로서의 활용 가능성이 있음을 확인하였다.

013 **양쪽성 Copolymer 분산제를 이용한 반도체 CMP용 세리아 슬러리의 AMP 함량에 따른 pH 안정성 연구**

임진아, 김운중\*

한남대학교

CMP(Chemical Mechanical Polishing) 공정은 반도체 웨이퍼의 박막 표면을 화학적/기계적 요소를 통해 연마하여 평탄화하는 공정이다. 그 중 슬러리는 반도체 공정중 제품의 품질을 결정하는 연마 과정 수행시 사용한다. 슬러리의 구성 성분인 분산제는 연마를 하는 과정에서 불량이 생길 수 있기 때문에 거품이 생성되거나, 층분리가 나타나면 품질에 결정적인 문제가 발생된다. 또한 슬러리 분산제중 양쪽성 Copolymer 분산제는 사용시 높은 산화막 연마량과 Uniformity를 나타내지만, 시간이 경과함에 따라 슬러리의 pH가 감소하여, 세리아 입자간 응집을 발생시키는 단점이 있다. 본 연구에서는 이러한 단점을 해결하기 위해 pH 완충제로 AMP(2-Amino-2-methyl-1-propanol)를 함량별로 첨가한 후 안정성을 평가하였고, 기준 슬러리와 함량별로 첨가한 AMP를 60°C와 실온에서 6주 동안 pH 안정성을 확인하기 위해 물성 분석을 진행하였다. 물성은 pH, Conductivity, OM(Optical microscope), DLS(Dynamic light scattering), Viscosity를 통해 분석을 진행하였다. pH 와 Conductivity 분석결과, AMP 첨가제의 함량이 증가할수록 pH는 점점 감소하였고, Conductivity는 증가하는 경향을 나타내었다. 이것은 세리아 표면에 분산제 또는 분산제에 포함된 이온의 영향으로 예측된다. 그러나, AMP 첨가제가 포함된 슬러리는 첨가하지않은 슬러리에 비해, 실온과 고온(60 °C)에서 모두 입자간 응집이 발생되지않고 안정적인 분산상태를 DLS와 OM분석을 통해 확인하였다. 또한 Viscosity 분석결과, AMP 첨가에 의해, 실온과 60 °C에서 모두 장기간 안정적인 분산상태를 유지하였다.

014 **Synthesis of Oxidized High-Order Securinega Alkaloids**

강규민, 한순규\*

한국과학기술원

Securinega alkaloids have captivated the synthetic community due to their remarkable structural diversity and bioactivities. Oligomerizations and oxidative transformations are major pathways for biosynthetic diversification based on their structural phenotype. An emerging subclass of Securinega alkaloids, termed “oxidized high-order Securinega alkaloids,” comprises eight natural products. These alkaloids undergo both dimerization and oxidation events during their biogenesis. However, their intricate structural complexity poses significant challenges in synthetic access, resulting in the synthesis of only two members to date, while the majority of the biosynthetic pathway for this subclass remains elusive. In this poster, we present our syntheses of oxidized high-order Securinega alkaloids and monomeric high-oxidation state Securinega alkaloids. Our strategies involve both exploring the potential biosynthetic pathway and utilizing cutting-edge C-C forming reactivity. Additionally, we propose alternative biosynthetic pathways of high-oxidation state Securinega alkaloids based on the chemical insights gained through our synthetic investigations.

015 **Dynamics of Photoinduced Electron Transfers in Ir(III)–Re(I) Photocatalysts**

김수환, 신재윤\*

고려대학교 세종캠퍼스

The conversion of CO<sub>2</sub> to energy-rich compounds using electrons from photocatalysts, after absorbing light, is a promising technology for effectively reducing atmospheric CO<sub>2</sub> and achieving sustainable energy production. In these systems, intramolecular electron transfer (IET) or intermolecular ET between photosensitizer and catalysts are precondition steps for photocatalytic CO<sub>2</sub> reduction. They are crucial for the formation of one-electron-reduced-species (OERS) and for understanding the overall reaction mechanism of CO<sub>2</sub> reduction. Therefore, we have studied the electron transfer (ET) dynamics in a series of Ir(III)–Re(I) photocatalysts, where two bipyridyl ligands of Ir and Re moieties are conjugated at the meta(m) – or para(p) – position of each side. The femtosecond transient absorption (TA) measurements identified the intramolecular electron transfer (IET) dynamics from the Ir to Re moiety, followed by the formation of one-electron-reduced species (OERS) through the intermolecular ET with a sacrificial electron donor (SED). The IET rate depends on the bridging ligand structure, while the formation of OERS occurs on a time scale near 1.4ns. Connecting the Re moiety at the meta-position of the bipyridyl ligands of the Ir moiety induce steric hindrances by restricting the rotational motion around a covalent bond between two bipyridyl ligands. These findings highlight the importance of bridging ligand structures on the ET dynamics in photocatalysts.

016 **Unveiling Fast Electron Transfer Dynamics in Photosensitization Reactions of Zinc Porphyrin Derivatives**

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In this study, we have investigated the electron transfer (ET) process of the photosensitization system to understand the complicated multi-electron transfer processes in the photocatalytic system. The Photosensitization ET process occurs in a wide time range, spanning picoseconds to minutes. Although the diffusion rate and slow quenching processes of a series of zinc porphyrin derivatives (ZnPs), which serve as a photosensitizer in the binary hybrid system with a heterogeneous TiO<sub>2</sub>/Re(I) for photocatalytic CO<sub>2</sub> reduction, were previously reported, there are not many studies about their fast dynamics. Therefore, we employed picosecond time-resolved fluorescence spectroscopy and femtosecond transient absorption (TA) to investigate the fast ET dynamics under the presence of BIH, the sacrificial electron donor (SED), and TiO<sub>2</sub>. As a result, the global analysis of the TA spectra reveals the ET dynamics of the one electron reduced species (OERS) formed at adjacent TiO<sub>2</sub> without involving diffusion. In addition, we found that the quenching process of the ZnPs induced by SED not only occurs via dynamic quenching but also through static quenching as evidenced by the Stern–Volmer analysis of fluorescence lifetimes. In conclusion, designing more efficient photosensitizers for CO<sub>2</sub> conversion requires an accurate understanding of ET mechanisms in the photosensitization reaction. Particularly, for the understanding of these ET mechanisms, ultrafast time-resolved



spectroscopy is necessary to unveil the reaction dynamics concealed in steady-state or slow time-resolved measurements.

017 **산화철 나노클러스터의 크기에 따른 나노자임 효과**

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한밭대학교

나노자임은 효소와 유사한 활성을 가진 나노물질로 인공 효소로써 사용되어 왔다. 천연효소는 우수한 촉매 활성을 나타내며 다양한 분야에서 사용되고 있다. 그러나 높은 비용과 보관이 어렵고 특정 환경에서만 활성을 나타낸다는 단점이 있다. 산화철 나노입자를 기반으로 한 나노자임은 높은 안정성을 가지며 환경에 따라 특성이 조정 가능하다. 산화철 나노입자는 저비용으로 쉽게 합성할 수 있다. 생체 적합성이 높고 자기성을 갖는 입자의 특성으로 인해 효소 대체재뿐만 아니라 진단 및 치료 등 생체의학 분야에서 잠재적인 응용 가능성이 있다. 산화철 나노자임은 사용되는 조건에 따라 다양한 요인이 영향을 미친다. 입자의 크기는 촉매 특성에 큰 영향을 미칠 수 있으며 최적의 크기는 응용 분야나 환경 조건에 따라 달라질 수 있다. 본 연구에서는 산화철 나노클러스터 크기 제어에 영향을 주는 요인에 대한 이해를 제시하며 합성 요인들은 변경하여 다양한 크기의 입자를 합성하였다. 크기별로 합성된 산화철 나노입자로 나노자임 효과의 차이를 확인하고, 천연효소 중 하나인 HRP와 효과를 비교함으로써 산화철 나노입자의 효소 대체재로써의 가능성을 제시한다.

018 **CRISPR/Cas12a-based Nanoneedle sensors for intracellular ATP detection**

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Besides gene-editing, the clustered regularly interspaced short palindromic repeats (CRISPR)-associated protein (Cas) (CRISPR/Cas) system has also widespread attention in the field of in vitro molecular diagnostic because it offers unique collateral cleavage activity that can provide enormously amplified signals in response to target analytes. Nevertheless, its applications in live cell biosensing are still challenging due to the difficulty of co-delivery of multiple components, performing the amplification reactions in living cells, and risks indiscriminate off-target cleavage of nucleic acids essential to cell function. In this study, we report a CRISPR/Cas-assisted nanoneedle sensor, namely nanoCRISPR, for intracellular molecule detection. As a proof of concept, adenosine triphosphate (ATP) was selected as a model target. With the synergistic combination of the non-perturbing intracellular access granted by nanoneedle array and the amplifying capacity of the CRISPR system, nanoCRISPR sensor can quantitatively detect ATP with a LOD of 246 nM and a dynamic range from 1.56  $\mu$ M to 50  $\mu$ M. We believe that our study makes a significant contribution to the literature because this new approach opens the way to noninvasive longitudinal monitoring of cell viability for long-term culture and promotes the applications of CRISPR/Cas systems in living cells.

019 **Control of Iron Oxide Nanocluster Size Using Solvothermal Method**

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Iron oxide nanoclusters are aggregates of single iron oxide particles and exhibit unique behavior compared to single iron oxide nanoparticles. Due to its similar size to bacteria, high saturation magnetization, superparamagnetism, and low toxicity. Also it is widely utilized in various industries such as bioimaging, biosensors, and magnetic separation based on its distinctive magnetic properties that vary with size. However, there are limitations in controlling the size of iron oxide nanoclusters, such as a narrow size control range and a complicated synthesis process. To overcome this, it is necessary to study the size-controlled synthesis of iron oxide nanoclusters in a simple and wide range. In this study, the method and principle of synthesis of iron oxide nanoclusters of various sizes are presented using the solvent thermal synthesis method. By changing the synthesis factors such as synthesis time, temperature, precursor concentration, reducing agent type and concentration, the size of the iron oxide nanocluster is finely controlled between 90 and 420 nm. The size of the synthesized iron oxide nanocluster was analyzed by dynamic light scattering (DLS) and Scanning Electron Microscope (SEM) and confirmed that the particles synthesized by X-ray diffraction analysis (XRD) were  $\text{Fe}_3\text{O}_4$ . Through this study, we present an understanding of the synthesis factors such as reducing agent type and concentration, precursor concentration. Synthesized iron oxide nanocluster shows applicability in various fields depending on size.

020 **탄소점(Carbon dots)에서 Mn 도핑과 촉매 효과에 대한 금속염의 영향**

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나노자임(Nanozyme)은 효소 모방 활동을 나타내는 나노 물질 기반 인공 효소이다. 천연효소는 인공효소와 비교하여 보관이 어렵고 비싸다는 단점이 있다. 나노자임은 이런 천연효소의 단점을 보완하는 대체재로 주목받고 있다. Carbon Dots (CDs)는 나노자임의 한 종류이다. CDs는 높은 안정성, 높은 수용성, 높은 생체 적합성 등의 장점이 있다. 본 연구에서 CDs는 효소모방활성을 나타내는 촉매로 사용되었다. CDs를 합성할 때 다양한 Manganese source를 사용하여 Mn을 도핑하고 효소모방활성을 제어하며 질병 진단에 중요한 ascorbic acid 검출에 적용했다. CDs는 Citric acid, Ethylenediamine을 각각 carbon source, nitrogen source로 Manganese Chloride(II), Manganese Nitrate(II) 및 Manganese Sulfate(II)를 망간 도핑원으로 했다. 그리고 Manganese salt source에 따른 Mn의 도핑 정도, 조성 및 화학 작용기를 비교했다. 또한, 산화된 TMB(3,3',5,5'-Tetramethylbenzidine)의 흡광도 측정을 통해 Mn 도핑 CDs의 효소모방활성을 비교하고 Ascorbic acid 검출에 사용했다. Mn 도핑 CDs는 바이오 센서 감지, 이미징 등에 추가로 적용될 것으로 기대하고 있다.

021 **Center for Nanotectonics**

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KAIST

Center for nanotectonics is a research group in KAIST chemistry department taking Prof. Sang Woo Han as a supervisor. Our research aim is to implement an unprecedented

multidimensional hybrid nanostructure through hierarchical assembly between nanostructures. To this end, we are intended to find factors that control the shape and composition of nanostructures and the binding between nanostructures. Through this, the unique physicochemical properties of newly implemented hybrid nanostructures are identified. Moreover, their applications to various research areas, especially photocatalysis, electrocatalysis, heterogeneous catalysis and plasmonics, are explored.

022 **Exploring Solid-Gas and Solid-Liquid Interfaces using Environmentally Controlled Atomic Force Microscopy (UHV to 1 bar to Liquid Phase)**

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In past decades, importance of surface characterization has been emerged because most of chemical reactions occur on surfaces. To investigate surface properties, atomic force microscope (AFM) has been used to investigate various surface properties, including topography, friction, adhesion, conductance, and surface potential. In our lab, there are ambient-condition AFM, which also can be used as an electrochemical AFM, and variable-pressure AFM. With ambient-condition AFM, we have investigated phase-dependence on the friction of exfoliated MoS<sub>2</sub> and MoTe<sub>2</sub>. These transition metal dichalcogenides(TMDCs) are 2D materials and have been widely studied because of its semiconducting nature.[1] Especially, for MoS<sub>2</sub> is getting attention as an anode for Li-ion batteries, because it can intercalate between MoS<sub>2</sub> layers. TMDCs have several phases. Among them, we have investigated 2H and 1T phase. As Li ion intercalate between layers, phase of 2H-MoS<sub>2</sub> turns into 1T-MoS<sub>2</sub>. We have observed that as phase changes, friction of MoS<sub>2</sub> increased significantly with the phase transition of 2H to 1T. We can explain this with DFT calculation, and this higher friction comes from an overlap of phonon density of states with mica substrate, as well as the higher potential energy surface of 1T-MoS<sub>2</sub>. [2] We have also constructed electrochemical AFM(EC-AFM), which can measure various surface properties in liquid environment. The electrochemical cell is specialized to allow the application of a voltage to the sample's surface, enabling the measurement of its electrochemical properties. To investigate how this AFM works, we conducted experiment of deposition of Cu on Au(111) surface and observed its process. We could distinguish between gold and copper with friction difference. In addition, we introduce ambient-pressure AFM, which enables precise control of gas and pressure from UHV to ambient pressure with simultaneous AFM measurement.[3] With this AFM setup, we have investigated stability and degradation of MAPbBr<sub>3</sub> perovskite.[4] This provides the direct observation of the clean and unmodified structure of single-crystal MAPbBr<sub>3</sub> and its surface degradation at room temperature. And we found out surface termination-dependent nanotribological properties of MAPbBr<sub>3</sub> surface.[5] When surface is MABr-terminated, it exhibits high friction relative to PbBr<sub>2</sub>-terminated surface. With this AFM, we conducted load-dependent friction on Au(111) surface in variable water pressure environment. At high load, Au(111) surface undergoes plastic deformation, which can be directly observed by AFM. However, when water molecules exist between tip and surface, they reduce contact

stress applied to gold atoms. So as in low-load case, only elastic deformation occurs, so no severe surface deformation is observed.

023 **Synthesis and control of iron oxide nanoparticles using 3D-printed microfluidic chip**

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한밭대학교

In recent decades, various studies have been conducted on the production and application of iron oxide nanoparticles. Due to their low toxicity and unique magnetic properties, iron oxide nanoparticles are utilized in various biochemical applications and can be synthesized using methods such as thermal decomposition, microwave-assisted growth, and co-precipitation. However, commonly used co-precipitation synthesis has several limitations such as long synthesis time and complex processes. To overcome these limitations, a technology for synthesizing nanoparticles in microfluidic chips has been developed. Microfluidic chips are a technology for controlling the flow, mixing, and separation of fluids on a small scale, providing the advantages of fast reaction time, low experimental error, and high reproducibility. Microfluidic chips made of PDMS have the disadvantage of requiring a complex manufacturing process and long production time. 3D printing has a single manufacturing process and a short production time, with properties similar to PDMS. In this study, iron oxide nanoparticles were synthesized by precisely controlling various conditions such as flow rate and precursor concentration using microfluidic chips made by 3D printing. The synthesized iron oxide nanoparticles are expected to be utilized in coating, conjugation, and other applications using microfluidic chips.

024 **Operando Surface-Sensitive Characterization Techniques for Probing Metal-Support Interaction in Heterogeneous Catalysts**

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한국과학기술원

Heterogeneous catalysts are one of the most widely used catalysts due to their advantageous features, such as easy separation, high stability, and efficient metal utilization. Metal-support interaction (MSI), the interaction between a metal nanoparticle (NP) and reducible metal oxide, plays a central part in the catalytic behavior of the heterogeneous catalyst, including supported metal NPs and bimetallic alloy NPs due to the synergistic effect on the catalytic activity at the metal-oxide interface. [1-3] Thus, a fundamental understanding of MSI is crucial for the development of high-performance heterogeneous catalysts. Surface-sensitive characterization techniques under a realistic environment are necessary to investigate the MSI effect, because the difference in Gibbs free energy between an ultrahigh vacuum (UHV) and an ambient-pressure environment is enough to cause unexpected surface changes. [4] Recently developed in situ/operando techniques, such as ambient pressure X-ray photoelectron spectroscopy (AP-XPS), diffuse reflection infrared Fourier-Transform (DRIFT) spectroscopy, and environmental transmission electron microscopy (E-TEM), enable the observation of the surface restructuring induced by the interaction between reactant gas molecules and the surface of

catalysts under a catalytic environment. [5] Herein, we investigated the MSI phenomenon at the metal–oxide interface from oxide supported NPs to bimetallic alloy NP, utilizing in situ/operando techniques. Especially, facet–controlled cubic and octahedral Cu<sub>2</sub>O supports are employed to study the facet–dependent MSI, which advantages by reducing the structural complexity. [6] The catalytic measurement revealed facet–dependent CO oxidation activity for Cu<sub>2</sub>O supported Pt NPs. The results of in situ AP–XPS and DRIFT measurements indicate that the surface changes during the reaction depends on the facet of the support, resulting in different catalytic performance. Furthermore, we observed classical strong metal–support interaction (SMSI) using Co<sub>3</sub>O<sub>4</sub> supported Pt NPs, where metal encapsulation by oxide overlayer was demonstrated through a combination of AP–XPS and DRIFT and density functional theory calculation. [7] The encapsulation of Pt NPs proved to be a key factor in driving catalytic enhancement to the CO oxidation reaction. Additionally, bimetallic AuCu NP catalysts exhibited MSI by forming a metal–oxide interface under an oxidative environment due to restructuring to metal and oxide interfacial heterostructure. [8] The oxygen–induced restructuring of bimetallic AuCu alloy NPs into a CuO<sub>x</sub>/Au heterostructure was investigated using combined operando spectroscopic and microscopic techniques, including AP–XPS, DRIFT, and E–TEM. The formation of the CuO<sub>x</sub>/Au heterostructure gives rise to the enhancement of catalytic activity for CO oxidation. Conclusively, we revealed direct evidence of the MSI using various metal–oxide interfaces and employing in situ/operando techniques.

## 025 **Scanning tunneling microscopy under chemical reaction at solid–liquid and solid–gas interfaces**

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Understanding chemical reactions occurring on the surface of heterogeneous catalysts is crucial for advancing energy conversion and environmental remediation processes. However, uncovering the reaction mechanisms and synergetic chemistry of catalytic systems had been a challenge because of differences between confined model catalyst systems and real catalytic conditions, such as a pressure gap. In modern surface chemistry, many attempts and developments of in situ/operando characterization techniques have emerged to bridge the gap by investigating the chemical properties of heterogeneous catalytic surfaces. Scanning tunneling microscopy (STM) has been an exceptional technique for probing surface structure changes and dynamics of molecular interaction at the atomic scale. The previous approaches to employing STM in surface chemistry were predominantly conducted under ultra–high vacuum (UHV) and low temperature (LT) conditions. The UHV and LT conditions of STM measurements offer valuable insights into atomic–resolution imaging of the surface and the initial stages of surface–molecule interactions. However, although these well–defined approaches have provided a fundamental understanding of surface chemistry and heterogeneous catalysis, we need more information to explain industrial catalytic processes occurring under the gas or liquid environments. Consequently, it is crucial to integrate STM techniques and the relevant fundamental surface chemistry with the catalytic reaction conditions. SCALE lab has gone

one step further in industrial catalysis by bridging the gap with ambient-pressure STM (AP-STM) and electrochemical STM (EC-STM) under the reactive environments. AP-STM and EC-STM explore a solid-gas interface at reactive temperature and a solid-liquid interface with electrochemical circuits, respectively. AP-STM measurements can observe atomic-resolved interactions of gaseous molecules and surfaces, revealing effects of defective sites (e.g., steps and kinks), catalytic activation sites, ordering or diffusion of adsorbed reactants, and reaction intermediates.<sup>1-3</sup> In addition, the surface reconstruction processes can be investigated by AP-STM to explain the reaction mechanism and the importance of catalytic surface by combining AP-STM with other operando surface analysis techniques.<sup>4</sup> The electrochemical solid-liquid interface has a more complicated system influenced by many factors, such as the electrical double layer induced by solvent molecules and adsorbed ions. EC-STM offers comprehensive investigations into complex electrochemical interactions in real-time and with atomic resolution observations.<sup>5</sup> Notably, EC-STM is powerful for studying the dynamics of charge transfer during electrochemical processes on the liquid-solid interface and the following surface reconstructions.<sup>6</sup> In this presentation, we show the recent achievements of the SCALE lab in employing AP-STM and EC-STM, emphasizing the importance of catalytic interfaces and their complex interactions in understanding the surface chemistry of heterogeneous catalysis. The knowledge gained from these studies will advance our fundamental understanding of catalytic processes and facilitate the rational design and optimization of heterogeneous catalysts.

026 **Hot Carrier Chemistry for Photodiodes, Catalytic Sensors, and Plasmonic Photoelectrochemical Devices**

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KAIST

Hot electrons, a fascinating phenomenon in nanoscience and nanotechnology, have attracted considerable attention for their potential in diverse applications. We explore different categories of research on hot electrons and their implications for renewable energy technologies and catalysis. The first category focuses on hot electrons in photodiodes, where the generation and detection of hot carriers play a crucial role in optoelectronic devices. We highlight the enhancement of hot electron generation by employing perovskite-modified plasmonic metal nanodiodes, resulting in improved solar-to-electrical conversion performance and suggesting the potential for sensitive hot-electron-based photovoltaics.<sup>1,2</sup> The second category delves into plasmonic photocatalysis, where hot electrons are utilized in catalytic systems for efficient solar energy conversion. We elucidate the intrinsic relationship between surface plasmon-driven hot electrons and catalytic activity. This study utilizes catalytic Schottky nanodiodes to reveal how plasmonic effects amplify the flow of reaction-induced hot electrons, leading to enhanced catalytic performance.<sup>3</sup> The third category explores the utilization of hot electrons in photoelectrochemical water splitting, a promising approach for renewable hydrogen production. We investigate the injection of plasmonic hot holes and their size dependence using Au/p-GaN nanostructures, demonstrating enhanced photoelectrochemical reactions

and improved energy transfer efficiency.<sup>4</sup> Also, the synthesis of Au/Ni<sub>2</sub>P heterostructures is presented, enabling precise control of hot electron transfer during surface plasmon decay.<sup>5</sup> The fourth category investigates chemically induced-hot electrons (chemicurrent) and their influence on reactivity and selectivity in catalytic reactions. We present a comparative study of electronically nonadiabatic interactions at solid-gas and solid-liquid interfaces, highlighting the remarkable increase in the efficiency of reaction-induced hot electron excitation at the solid-liquid interface.<sup>6</sup> Additionally, we explore the influence of metal-oxide interfaces on catalytic selectivity and hot electron excitation in methanol oxidation.<sup>7</sup> Each category represents a unique research field, showcasing the wide range of possibilities offered by hot electrons in the realm of sustainable energy solutions and chemical reactions. This categorization framework underscores the significant contributions in harnessing hot electrons for various applications and paves the way for further exploration and development in this exciting field.

027 **Synthesis and Optimization of Small Molecule JAK1 Inhibitors for Autoimmune Disease Treatment**

SANTOSH SHIVANAND RAIKAR, PILHO KIM\*

UST

JAK inhibitors have revolutionized the treatment of autoimmune diseases, offering significant benefits to patients with conditions such as rheumatoid arthritis and psoriasis. However, concerns over the safety and selectivity of these drugs have been raised. While non-selective JAK inhibitors could lead to off-target effects and potential toxicity, selective inhibitors could offer greater specificity and reduce side effects. Filgotinib, a promising JAK1 selective inhibitor, has shown encouraging results in early clinical trials and may offer more safe and effective alternative to the regimens including JAK inhibitors. To discover JAK1-selective inhibitors, we designed novel compounds derived from filgotinib. Our optimization process, biological activities and ADME/Tox profiles of selected compounds will be discussed.

028 **Discovery of novel small molecule inhibitors targeting TRIB2 for the treatment of TNBC**

Hoyeong Park, PILHO KIM\*

UST

Triple-Negative Breast Cancer (TNBC) is one of the most challenging breast cancers to overcome. In general, aiming at three well-validated targets, such as estrogen receptor (ER), progesterone receptor (PR), and human epidermal growth factor receptor 2 (HER2), could be typical strategies to discover small molecule drugs for the treatment of breast cancers. In contrast, TNBC lacks these three receptors. In addition, TNBC has a poor prognosis due to few treatment options. Nevertheless, TNBC is composed of more than 10 % of total breast cancer patients. Tribbles homolog 2 (TRIB2) is a pseudo serine/threonine kinase without a catalytic function expressing multifunctional oncogenic roles. It has been known that TRIB2 is involved in survival and drug resistance in solid and hematologic cancers. TRIB2 is considered a direct target of Notch1, which is related to a hallmark for

TNBC. Thus, inhibition of TRIB2 could be an effective strategy to overcome TNBC. With a view to developing an anti-TNBC drug candidate, we launched our campaign to discover TRIB2 inhibitors by high-throughput screening of a virtual library from the Korea Chemical Bank. In this work, we will discuss our strategies to discover TRIB2 inhibitors. In addition, biological data profiles of some of selected TRIB2 inhibitors will be presented, such as TRIB2 enzyme activity and in vitro anti-cancer activity against TNBC cell line MDA-MB 231.

029 **Functional Surfaces with Zwitterionic Carboxybetaine L-3,4-dihydroxyphenylalanine: Synthesis, Coating, and Antifouling Applications**

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KAIST

In this work, we present synthesis of a novel carboxybetaine L-3,4-dihydroxyphenylalanine derivative (CB-DOPA) and its excellent antifouling properties to inhibit bacterial adhesion. We optimized the coating efficiency by controlling oxidation-induced polymerization with various oxidants in an alkaline environment. The surface coating was investigated by UV-vis spectroscopy, water contact angle goniometry, X-ray photoelectron spectroscopy, atomic force microscopy, and FT-IR spectroscopy. Among the conditions examined, the optimal condition was the sodium periodate-mediated oxidation, which achieved the highest CB-DOPA coating efficiency. The optimized CB-DOPA coating was applied to a variety of substrates, including gold, titanium dioxide, stainless steel, poly(tetrafluoroethylene), and polyurethane. Compared with bare controls, CB-DOPA-coated substrates showed high resistance to the adhesion of Escherichia coli.

030 **Synthesis and interfacial properties of fluorine-containing PEG and sulfonamide-based surfactants**

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The reaction mixture ( $\text{CF}_3(\text{CF}_2)_5\text{CH}_2\text{CH}_2(\text{EO})_n\text{OH}$ ) prepared from the reaction of perfluorohexylethanol with *n* ethylene oxide (EO,  $n = 1 \sim 15$ ) was fractionated by silica gel column chromatography (MPLC) to provide perfluorohexylethanol EO ethers. And Fluorine-containing sulfonamide-based succinates moiety were synthesized from *N,N*-(3-hydroxypropyl)-propyl-perfluoroalkyl sulfonylamides followed by esterification with succinic anhydride. The structure of each purified and synthesized surfactant was unambiguously characterized by using spectroscopic methods including 1D and 2D NMR (proton, carbon, fluorine, COSY, HSQC, and HMBC) spectroscopy. The surface tension and interfacial tension of each synthesized surfactants were measured and compared with regard to structural variation.



031 **Characterization of protein encapsulated lipid vesicle by asymmetrical flow field-flow fractionation (AF<sub>4</sub>) coupled with multiple detectors**

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한남대학교

Lipid vesicles are used for drug delivery materials (DDMs), encapsulating drugs and proteins. Knowing their size and encapsulation efficiency is important because they are related to the dosage of the drug or protein. Therefore, we observed the effect of the protein and lipid concentration on encapsulation efficiency by asymmetrical flow field-flow fractionation (AF<sub>4</sub>) coupled with multiple detectors. Lipid vesicles were prepared by extrusion method with 25 mM phosphate buffer at pH 7.4 and 100 nm nominal pore polycarbonate membrane. The quantitative analysis was performed after separating encapsulated proteins and protein-encapsulated lipid vesicles. As a result, the protein encapsulation efficiency increased from 3% to 12%, with the lipid concentration increasing from 1 mg/mL to 5 mg/mL. However, contrary to expectations, in the protein concentration case, maximum encapsulation efficiency of 5% was shown at 2 mg/mL of protein.

032 **Electroreductive formylation of activated alcohols via radical-polar crossover**

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한국과학기술원

The direct synthesis of sterically hindered aldehydes is highly challenging. Herein, we report a direct approach to generate such compounds via electroreductive cleavage of the C(sp<sup>3</sup>)-O bond of activated alcohols. Under the established reaction conditions, benzylic radical intermediates were efficiently generated. A subsequent radical-polar crossover generated carbanions that further reacted with N,N-dimethylformamide to form various aldehydes with tertiary or quaternary benzylic carbon centers. The feasibility of a gram-scale synthesis was also demonstrated. This reaction is also operated in a simple undivided cell, which avoids the use of any transition metal catalysts, toxic gas, and reductants.

033 **양쪽성 계면활성제 분산제가 함유된 반도체 CMP 세리아 슬러리의 TEA 함량에 따른 안정성 연구**

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CMP(Chemical Mechanical Polishing)는 화학 반응과 물리적 에칭(etching) 반응을 통해 웨이퍼를 평탄화하는 폴리싱 공정이다. 과거에는 보조 공정이라는 인식이 많았으나, 최근에는 신뢰성 높은 반도체를 만들기 위한 핵심 공정으로 인식되고 있다. CMP 공정에 사용되는 슬러리는 케미컬과 연마 입자로 구성되어 있는데 화학적 반응을 일으켜 CMP 공정 중 기계적 연마를 도와주는 역할을 한다. 양쪽성 계면활성제 구조를 가진 분산제는 CMP 공정 중 중앙(center) 부분과 모서리(edge)의 연마율에 큰 변화가 없으나 경시적으로 pH 감소가 나타나며 입자들의 응집으로 인해 CMP 연마 시 스크레치가 발생하는 문제점이 있다. 따라서 슬러리의 pH가 산성화되는 것을 방지할 수 있으며 분산 안정성을 높일 수 있는 pH 완충제로 유기화합물인 TEA(Triethanolamine)를 사용하여 연구를 진행하였다. 양쪽성 계면활성제 분산제가 4.5 wt% 첨가된 슬러리에 pH 완충제인 TEA 를 단계적으로 첨가하여 실온과 60°C에서 6주 동안 분산

안정성을 확인하였다. 물성은 pH, Conductivity, OM(optical Microscope), DLS(Dynamic Light Scattering), Viscosity 및 Zeta potential 을 이용하여 분석하였다. pH 는 TEA 함량이 증가할수록 pH 가 8.46에서 9.67, 9.98, 10.1로 증가하였다. 또한 Conductivity 도 336.0에서 412.7, 423.7, 417.5로 증가하였다. OM 은 시간이 경과됨에 따라 Original 슬러리는 응집이 발생했으나, TEA 가 첨가된 슬러리는 응집이 발생하지 않았다. DLS 역시 Original 슬러리는 입자 크기가 대폭 증가하였지만, TEA 가 첨가된 슬러리는 큰 변화가 나타나지 않았다. Viscosity 는 실온과 60°C 모두에서 큰 변화가 없었으나, 60°C에 보관한 Original 슬러리에서만 재응집구조가 형성되었다. Zeta potential은 Original 슬러리에 비해 TEA 첨가 슬러리는 초기와 큰 변화 없이 안정적인 분산 상태를 나타냈다.

#### 034 산화철 나노클러스터의 크기에 따른 나노자임 효과

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나노자임은 효소와 유사한 활성을 가진 나노물질로 인공 효소로써 사용되어 왔다. 천연효소는 우수한 촉매 활성을 나타내며 다양한 분야에서 사용되고 있다. 그러나 높은 비용과 보관이 어렵고 특정 환경에서만 활성을 나타낸다는 단점이 있다. 산화철 나노입자를 기반으로 한 나노자임은 높은 안정성을 가지며 환경에 따라 특성이 조정 가능하다. 산화철 나노입자는 저비용으로 쉽게 합성할 수 있다. 생체 적합성이 높고 자기성을 갖는 입자의 특성으로 인해 효소 대체재뿐만 아니라 진단 및 치료 등 생체의학 분야에서 잠재적인 응용 가능성이 있다. 산화철 나노자임은 사용되는 조건에 따라 다양한 요인이 영향을 미친다. 입자의 크기는 촉매 특성에 큰 영향을 미칠 수 있으며 최적의 크기는 응용 분야나 환경 조건에 따라 달라질 수 있다. 본 연구에서는 산화철 나노클러스터 크기 제어에 영향을 주는 요인에 대한 이해를 제시하며 합성 요인들은 변경하여 다양한 크기의 입자를 합성하였다. 크기별로 합성된 산화철 나노입자로 나노자임 효과의 차이를 확인하고, 천연효소 중 하나인 HRP와 효과를 비교함으로써 산화철 나노입자의 효소 대체재로써의 가능성을 제시한다.

#### 035 초음파 추출공법을 이용한 편백 잎 오일 추출물의 화장품 소재 가능성에 관한 연구

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편백은 측백나무 과에 속하는 상록교목으로, 편백 잎에 함유된 피톤치드의 주성분인 Terpene 류는 휘발성 유기화합물로 삼림향을 내어 사람의 심신 안정과 스트레스 완화 작용에 도움을 주며, 편백 정유의 주성분인 Monoterpene 류와 Sesquiterpene 류는 박테리아와 진균에 대한 항균작용이 있어 약용으로도 이용되고 있다. 그러나 편백 추출물에 대한 선행연구에서는 특정 소취 및 화장품으로서 활용 가능성에 대한 보고가 부족한 실정으로, 본 연구에서는 편백잎 오일의 초음파 추출을 통해 노인냄새 제거 효과, 항균 효과, 미백 및 주름개선 효과에 대한 실험을 진행하고 편백잎 오일 추출물의 천연 화장품 소재로서의 다양한 활용 가능성을 확인하였다. 편백잎 오일은 40% 에탄올 조건에서 초음파추출장비로 추출하였으며, 추출 후 분액깔때기를 이용하여 상층부와 하층부로 분리하였다. 또한 감압여과 및 농축 후 효능 분석을 진행하였다. 추출물의 조성 성분은 GC-MS로 분석하였고, S.aureus, C.albicans, E.coli 총 3종의 균주에 대해 디스크 확산검사법(paper disk diffusion assay)으로 항균력을 평가하였다. 노인냄새 제거 효과는 노인냄새의 원인 물질인 trans-2-nonenal 의 농도 감소에 따른 흡광도 감소를 비교하여 확인하였다. 미백 효과는 Tyrosinase 효소에 대한 대조군과 추출물의 저해율을 비교하였으며, 주름개선 효과는 Collagenase 효소에 대한 대조군과 추출물 간의 저해율을 비교하였다. 본 연구 결과, 편백잎 오일 원액과 상층부에서는 Terpinen-4-ol, alpha-Terpineol, gamma-terpinene,

D-Limonene, Sabinene 이 검출되었고 하층부에서는 Terpinen-4-ol 및 alpha-Terpineol 성분이 검출되었다. 또한, 상층부에서 S.aureus, C.albicans, E.coli 에 대한 항균 효과가 확인되었으며 편백잎 오일 추출물에서 노네랄 감소 효과가 85.0%이상으로 확인되어 노인냄새 제거 효과가 있음을 확인하였다. 미백 효과는 상층부에서 63.1% 로 가장 높은 효과를 나타내었다. 또한 주름 개선 효과도 상층부에서 85.1% 의 높은 효과가 확인되었다. 따라서, 편백잎 오일의 상, 하층 초음파 추출물은 각기 다른 효과가 나타났으며, 선택적으로 천연 기능성 화장품 소재로서의 적용이 가능할 것으로 기대된다.

036 **Chemical Control of Flavonoid-Fe<sup>3+</sup> Self-Assembly in Biphasic Oil-Water Systems for Surface Functionalization**

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Self-assembly of metal-organic complexes is a powerful strategy for functionalizing microparticles and living cells. However, its application has been limited to homogeneous systems. Here, we demonstrated that simple vortexing of a biphasic water-oil system of Fe<sup>3+</sup> ions and flavonoids rapidly formed nanoshells on microparticles. This approach enables simultaneous use of water-insoluble ligands and water-soluble metal ions as coating materials in a one-step, one-pot manner. Mechanistic studies revealed that the shell formation is governed by mass-transfer equilibrium of flavonoid-Fe<sup>3+</sup> species across the water-oil interface, with the oil phase acting as a reservoir of coating precursors for continuous shell formation.

037 **Total Synthesis of Dimeric Epoxyquinoids.**

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In 2019, Gao, Lei, and their coworkers reported the isolation of herpotrichones A and B, two dimeric epoxyquinoids presumed to be biosynthesized through intermolecular [4+2] cycloaddition reactions. These natural compounds exhibited potent anti-neuroinflammatory activity in lipopolysaccharide (LPS)-induced BV-2 microglial cells, with half maximal inhibitory concentration (IC50) values of 0.41 and 0.11 μM, respectively. Their intriguing molecular structures, particularly the plausibility and stereoselectivity of the key Diels-Alder reaction, alongside their promising biological profiles, prompted us to initiate a synthetic program targeting these secondary metabolites. In this report, we will share the details of our journey towards successfully obtaining the first synthetic samples of herpotrichones A and B.

038 **Re-examining the structure of stereochemically-dense polycyclic suffruticosine via TDDFT calculations, ECD spectroscopy, and chemical synthesis**

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The elucidation of complex natural product structures involves two steps: determining atom connectivity and assigning stereochemistry. While the former step is now routinely performed with <sup>1</sup>H, <sup>13</sup>C NMR data aided with various 2D NMR experiments, a complex

natural product's relative and absolute stereochemical assignment is often more challenging. Herein, we deconvoluted electronic circular dichroism (ECD) spectra by performing time-dependent density functional theory (TDDFT) computations to revise the structure of stereochemically-dense polycyclic suffruticosine. The TDDFT-assisted ECD spectral assignment, along with the acquisition of experimental ECD spectra from the eastern fragment (allosecurinine and securinine) and the chemically synthesized western segment of suffruticosine, provided evidence indicating that the actual structure of natural suffruticosine is the enantiomer of the initially assigned structure from the isolation paper.

039  **$\alpha/\gamma$ -Hybrid Peptide Resistant to Screw-Sense Induction**

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A series of  $\alpha/\gamma$ -hybrid peptides were designed and synthesized. X-ray diffraction analysis revealed the coexistence of left- and right-handedness in both molecular and macroscopic level. We believe these peptides having chiral residue but helically pseudo-achiral suggests the novel design principle of artificial peptide in the fields of peptide drug design, metalloprotein, and peptide catalyst.

040 **분자합성생물학 및 단백질화학 연구실 소개**

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한국과학기술원 (KAIST) 화학과 소속 분자합성생물학 및 단백질화학 연구실에서는 박희성 교수님의 지도 하에 새로운 기능이나 성질을 갖는 단백질을 설계, 개량, 생산, 분석하는 연구가 이루어지고 있다. 박희성 교수님은 KAIST 생명과학과 김학성 교수님 연구실에서 효소 디자인 및 진화 관련 연구로 박사 학위를 받으셨고, 이후 Yale 대학교 화학과 Dieter Söhl 교수님 연구실에서 인산화세린 (O-phosphoserine)을 유전암호확장 (genetic code expansion) 기술을 통해 단백질의 원하는 위치에 도입하는 기술을 개발하신 바 있다. 본 연구실에서는 세포 내에서 단백질이 만들어지는 번역 (translation) 과정에 관여하는 여러 구성 요소들 (아미노아실-tRNA 합성효소 (aaRS), 전달RNA (tRNA), 신장인자 (elongation factor) 등)의 기능을 탐구하고, 그 성능을 개량하여 비천연아미노산 (unnatural amino acid)이 도입된 맞춤형 단백질을 생산하고, 생직교적 반응 (bioorthogonal reaction)을 이용하여 위치특이적인 단백질 변형을 도입하는 연구가 이루어지고 있다. 이번 학술대회를 통해 본 연구실에서 이루어지는 연구 내용들을 더 많은 사람들에게 소개하고자 한다.

041 **Compositional Change of  $\text{Fe}^{3+}$ -BTC to  $\text{Fe}^{3+}$ -Phosphate Complexes in Phosphate-Containing Medium**

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KAIST

Cell-in-shell nanobiohybrids represent a promising technology that combines living cells with synthetic materials to safeguard them against harsh environmental conditions. However, the current artificial shells are static and have a predetermined form and composition. The next step in shell design is to create transformable shells that can detect and respond to sudden environmental changes by changing their form and composition. In

this study, we report on the transformation of a  $\text{Fe}^{3+}$ -trimesic acid complex nanoshell into an iron phosphate shell in media containing phosphate. The shell-forming and transformation processes are highly compatible with living cells, and the transformed iron-phosphate shells retain the ability to protect the nanoencapsulated cells from various lethal stresses. Our work will advance the development of cell-in-shell nanobiohybrids that can actively and adaptively interact with their surroundings.

042 **Comparative Analysis of Physiological Activities of 3 Seaweed Species in Korea and Exploration of active compounds through UPLC-MS.**

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Seaweeds are nutritional ingredients that can serve as alternatives to high-fat foods and can also be utilized as materials to reduce carbon emissions in the era of climate change, contributing to the steady growth of domestic and international consumption trends(The Top Superfoods of 2023). Among these, brown algae easily found in Korea, particularly exhibit high average polyphenol content, resulting in excellent antioxidant activities. In this study, we compared the in vitro physiological activities of 70% ethanol extracts from three brown algae species (*Petalonia binghamiae* (P. binghamiae), *Dictyota coriacea* (D. coriacea), *Ishige okamurae* Yendo (I. okamurae)) harvested offshore of Jeju island. The total polyphenol content was highest in I. okamurae ( $49.8 \pm 1.6 \mu\text{g GAE/mg}$ ), which was approximately 10 times higher than the lowest content found in D. coriacea ( $5.5 \pm 0.5 \mu\text{g GAE/mg}$ ). Increasing polyphenol content correlated with enhanced DPPH/ABTS radical scavenging activity. The tyrosinase and elastase inhibitory effects of 70% ethanol extract of I.okamurae were measured to have IC50 values of  $0.408 \pm 0.03 \text{ mg/mL}$  and  $0.906 \pm 0.01 \text{ mg/mL}$ , respectively. Bioactive compounds such as pachymic acid, retinol and puerarol were identified in the I. okamurae extract which exhibited relatively high physiological activities, through UPLC-MS analysis. Therefore, our results suggest that the 70% ethanol extract of I. okamurae could be a potential ingredient for cosmeceuticals and functional foods.

043 **Manipulation of Chemotactic Behaviors of Immune Cells via Single-Cell Nanoencapsulation**

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Chemotaxis, a phenomenon where cells migrate in response to chemical signals, remains a largely uncharted field, despite its potential applications in numerous areas, including biosensors and targeted cell therapy. Herein our study examined the movement of biohybrid structures in D-glucose gradients by attaching glucose oxidase ( $\text{GO}_x$ )-tethered liposomes to Jurkat cells. As a result of the decoration of the cells, we found that the  $\text{GO}_x$ -decorated cells migrated toward the lower concentrations of D-glucose, while unmodified Jurkat cells showed the opposite chemotaxis toward the gradient. In the field of single-cell nanoencapsulation, this research provides an advanced tool for controlling and

manipulating cellular chemotaxis at the single-cell level and maintaining cellular metabolism.

044 **Electrical and optical properties of catalysts in solutions**

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Catalysis is of prime importance owing to its versatility in chemistry. To disclose the underlying mechanism of catalytic chemical reactions, it is inevitable to figure out their electronic structures and optical properties, which mainly determine chemophysical phenomena, including light absorption, charge transfers, and, ultimately, chemical reactions. Despite its fundamentality, the experimental observations or measurements can sometimes be unintentionally affected by the interaction between catalysts and solvent molecules when chemical compounds are submerged in solvents like water. To resolve this issue at the subatomic scale, we have developed a new methodology by combining the GW approximation with the generalized Poisson equation, named GW-GPE. In this scheme, the polarization-field effect (PFE) and environmental screening effect (ESE) play important roles in describing the solvent effect on catalysts. With this many-body perturbation theory, we have tested various catalysts and have been able to unveil the structure-property relationship. Additionally, a harmony between PFE and ESE makes the band edge positions in solutions distinguishable from those in vacuum. Based on the reestablished band theory, we can accurately reproduce experimentally observed energy levels. Furthermore, we have extended our new method to explain the optical properties of catalysts by combining the Bethe-Salpeter equation (BSE) with GW-GPE, leading to GW/BSE-GPE. Using this extended methodology, we have successfully reproduced the first bright peak. Moreover, we discovered the universality of the excitonic behavior in solutions. These results suggest that our new methodology, GW/BSE-GPE, can be an effective theory for unlocking the hidden chemistry in catalysis.

045 **Comparison of Polymer-based Enrichment Methods for Human Saliva Exosomes**

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Exosomes are one of extracellular vesicles that play an important role in various biological processes and intercellular communication. Recently, exosomes are being studied as potential biomarkers for disease. For enriching exosomes from human fluids, various methods have been reported including size-based isolation, ultracentrifugation, synthetic polymer-based precipitation, immunoaffinity chromatography, ultrafiltration, and microfluidic technologies. Commercial kits (e.g. ExoQuick) that use polymer-based enrichment methods have also been developed and are available on the market. In this study, we compared the efficiency of exosome enrichment from human saliva using polymer-based enrichment methods. Specifically, we compared the efficiency of commercially available ExoQuick kit and PEG polymers (PEG 8000, PEG 10000, PEG 12000, PEG 20000, PEG 35000) after multiple rounds of enrichment cycles. The results obtained from each method were then analyzed and compared using size exclusion chromatography.

The results showed that after three rounds of enrichment, most of the protein peaks disappeared in all samples, while the loss of exosome peaks tended to decrease as the molar mass of PEG increased. These findings demonstrate that PEG molecular weight affects the efficiency of exosome concentration. Specifically, PEG 20000 and PEG 35000 showed higher exosome recovery yields. Although the recovery yields were slightly lower than those of ExoQuick, the difference was small enough to demonstrate the potential use of PEG polymers as a substitute for ExoQuick. These results indicate that high molar mass of PEG has important potential applications in the research and diagnosis of exosomes.

046 **Effectiveness Comparison of Polarity-Based Extraction Methods for Salivary Metabolites**

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Saliva, one of the biofluids, contains several biologically important molecules, including enzymes, proteins, metabolites, nucleic acids, peptides and lipids, which are clinically informative. Since these molecules are transferred from blood to saliva through transcellular or paracellular routes, saliva provides a reflection of the physiological status of the body, similar to blood and urine. Therefore, saliva can be utilized for diagnosing, monitoring, and predicting disease status, and for developing biomarkers due to its non-invasive collection. To simplify the analysis of complex biological samples, polar and nonpolar solvents are commonly used to extract analytes based on their polarity. In this study, the extraction process involved using two different mixtures: one mixture containing 2-methoxy-2-methylpropane (MTBE), methanol, and H<sub>2</sub>O, and the other mixture containing chloroform, methanol, and H<sub>2</sub>O. Each mixture was vortexed and centrifuged, and the upper and lower layers were transferred into four separate tubes. Next, the samples were dried using a speed vacuum concentrator and derivatized with 2 ppm of methoxyamine hydrochloride in pyridine (2 h, 37 °C) and 2,2,2-trifluoro-N-methyl-N-trimethylsilylacetyl amide (MSTFA) with 1% chloro(trimethyl)silane (TMCS) (1 h, 37 °C) before GC-MS analysis. For comparison, we also prepared derivatized mixtures of upper and lower layers and derivatized saliva for GC-MS. Similar GC-MS chromatograms were observed for the CHCl<sub>3</sub> layer mixture, the MTBE layer mixture, and the derivatized saliva.

047 **Quantitative and qualitative analysis of extracellular vesicles isolated from human urine**

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This study aimed to develop a reliable and efficient method for the isolation and analysis of extracellular vesicles (EVs) from human urine using size exclusion chromatography (SEC). The optimal conditions for separating pure EVs from urine were determined, and the amount of pure EVs was quantified using liquid chromatography and BCA protein assay. The results demonstrated that the intensity of the SEC chromatogram of EVs increased as the number of concentration steps through centrifuge increased, while the intensity of the protein peak decreased. Furthermore, the amount of protein in urine decreased as the number of

concentration steps increased. Western blot was used to confirm the specificity of the separation method, with CD63 as a positive marker for EVs and calnexin and calreticulin as negative controls. The results showed that the pure EVs were properly separated, and the negative controls did not show any detectable signals in the EVs, confirming the specificity of the separation method. Overall, this study provides a reliable and efficient method for the isolation and analysis of pure EVs from urine using SEC. This method has potential applications in biomarker discovery and disease diagnosis in the field of EVs research.

048 **광감응형 전기변색소자 특성과 리간드 변화**

홍석천, 강효민, 김영준\*

충남대학교

광감응형 전기변색 소자는 빛에 의해 자동으로 색이 변하여 투과율을 조절할 수 있는 특성이 있어, 건물이나 자동차의 유리에 적용하면 에너지 효율을 향상시킬 수 있다는 장점이 있다. 광감응형 전기변색 소자는 다층 구조로 이루어져 있고 빛에 의해 개시되어 여러 단계의 산화환원 반응이 일어난다. 그 중에서 유기물질인 리간드에서  $\text{TiO}_2$  층으로 전하가 이동하는 단계가 소자의 성능을 결정하는 중요한 단계 중 하나인데 리간드에 따른 소자 특성의 변화에 대한 연구는 아직 체계적이지 못하였다. 본 연구에서는  $\text{TiO}_2$ 에 쉽게 부착 가능한 카복실산기를 가지는 다양한 종류의 리간드를 광감응형 전기변색 소자에 적용시켜 보았다. 리간드가 소자 특성에 미치는 기초적인 실험을 진행하였으며 이에 대한 초기단계 결과를 보고하고자 한다.

049 **Synthesis and characterization of FeSe nanomaterials in a two-dimensional cluster configuration**

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Chungnam National University

Renewed interest has been sparked in recent years regarding transition metal chalcogenides, owing to their distinctive properties and broad array of potential applications as nanomaterials. Among them, FeSe has garnered significant attention as a two-dimensional layered structure, with exceptional performance as both a superconductor and a thermoelectric material. Moreover, it presents a promising avenue for the development of next-generation electronic devices. In this research, we present our recent endeavors in exploring the optical and optoelectronic properties of FeSe nanoplates synthesized through hydrothermal methodologies. To comprehensively analyze the samples, a range of characterization techniques were employed, including power X-ray diffraction (XRD), transmission electron microscopy (TEM), scanning electron microscopy (SEM), atomic force microscopy (AFM), and ultraviolet-visible (UV-Vis) spectroscopy. The creation of novel two-dimensional nanocrystals and the discovery of their extraordinary properties offer an effective pathway towards unraveling the intrinsic relation between conventional superconductivity and Mott physics states.



050 **One-pot scalable synthesis of FeSe quantum dots in aqueous and organic phases**

강효진, 이재범\*

충남대학교

Colloidal quantum dots (QDs) are nanoscale particles with a typical diameter size of 2–10nm, and they represent a significant breakthrough in the field of nanoscience. These QDs possess unique chemical and physical properties, including diverse emission colors and bandgaps that depend on their size. As a result, they have found successful applications in various fields such as optics, electronics, and biology. One specific type of QDs, known as FeSe QDs, belongs to the category of layered transition metal chalcogenide nanomaterials. These QDs exhibit a remarkable property called multicolored excitation-dependent emission (MEDE). Additionally, FeSe QDs have low toxicity and display unique optical properties, making them particularly attractive for biological imaging applications that utilize two- and three-photon absorption. In our research, we have developed a scalable synthesis protocol for FeSe QDs, optimizing various synthetic parameters in both organic and aqueous phases with diverse synthesis method. The QDs synthesized using the optimized protocol exhibit intense light blue fluorescence when exposed to 365nm light. Furthermore, they demonstrate strong photoluminescence and relatively high quantum yield, reaching approximately 20%, in an aqueous system.

051 **Photocatalytic degradation of bisphenol and photoluminescence properties of Eu(III)-doped CaTiO<sub>3</sub>, BaTiO<sub>3</sub> and SrTiO<sub>3</sub> nanoparticles**

김소영, 손영구\*

충남대학교

In this study, we synthesized Eu(III)-doped perovskite CaTiO<sub>3</sub>, BaTiO<sub>3</sub>, and SrTiO<sub>3</sub> nanoparticles (NPs) through solvent evaporation followed by thermal treatment. A photoluminescence analysis revealed that CaTiO<sub>3</sub> exhibited the highest red emission intensity, attributed to the transition of Eu(III) ions. Under UVB and UVC irradiation, photocatalytic CO<sub>2</sub> reduction led to the production of primarily CO and CH<sub>4</sub>. Notably, SrTiO<sub>3</sub> and BaTiO<sub>3</sub> nanoparticles demonstrated high efficiency as catalysts under UVB and UVC, respectively. We investigated the photocatalytic degradation of bisphenol AF and bisphenol S in this work, presenting the corresponding kinetics and proposing simple mechanisms for their removal.

052 **Aerobic Decarbonylative Liebeskind–Srogl Reaction to Produce Biaryls**

진영화, 이지홍, 손정훈\*

충남대학교

An aerobic decarbonylative Liebeskind–Srogl reaction of S-pyrimidinyl thioesters with arylboronic acids to yield biaryl compounds is presented. It is likely that the reaction proceeds by cleavage of the thioester S–C(O) bond and subsequent release of CO, rather than by cleavage of the S–C(pyrimidine) bond and release of SCO. Investigation of the reaction scope with various electrophilic and nucleophilic coupling partners revealed that the chelatable ortho substituent of the thioester enhances reaction efficiency.

053 **Synergistic Effect of Thermal-Treated Brass and Silver in CO<sub>2</sub> Reduction**

윤가은, 손영구\*

충남대학교

Scientists are investigating the potential of CO<sub>2</sub> recycling as a solution to address concerns related to rising CO<sub>2</sub> levels and diminishing fossil fuel resources. In this research, a novel approach involving a thermal-treated Ag/Brass electrode for electrochemical CO<sub>2</sub> reduction was introduced. The electrode demonstrated the ability to generate a variety of gas and liquid products. The study revealed that the efficiency of the products generated was influenced by the experimental conditions, and the incorporation of thermal-treated Brass with Ag significantly enhanced the production of CH<sub>4</sub>. Surface elemental oxidation states were analyzed using X-ray photoelectron spectroscopy, providing valuable insights into the conversion of CO<sub>2</sub> to CH<sub>4</sub> through electrochemical CO<sub>2</sub> reduction. These findings carry significant implications for energy and environmental sustainability.

054 **Electrochemical reduction of CO<sub>2</sub> utilizing Ag, Au, and Cu-Modified bronze electrocatalysts**

권윤지, 손영구\*

충남대학교

Bronze has been widely acknowledged for its exceptional electrochemical efficiency and selectivity in the reduction of CO<sub>2</sub>. In this study, we conducted experiments by incorporating Ag, Au, and Cu metals onto bronze electrodes to investigate their electrochemical properties in CO<sub>2</sub> reduction. Gas chromatography and nuclear magnetic resonance spectroscopy were employed to confirm the primary reduction products, which were identified as CO, CH<sub>4</sub>, ethanol, and formate. The Faraday efficiency was utilized as a quantitative measure of selectivity. To evaluate the oxidation states of the electrodes, X-ray photoelectron spectroscopy and scanning electron microscopy analyses were performed before and after the CO<sub>2</sub> reduction process.

055 **Enhanced Electrochemical Reduction of CO<sub>2</sub> to CO via Galvanic Substitution of Ag in Cu-Mesh Electrodes**

배수연, 손영구\*

충남대학교

By employing Copper (Cu) electrodes in the electrochemical reduction of CO<sub>2</sub>, various products such as CH<sub>4</sub> and C<sub>2</sub> compounds can be generated. This research aimed to stimulate the production of CO by carrying out galvanic substitution of Silver (Ag) in the Cu-mesh. To investigate the influence of galvanic substitution time on the thickness of the substituted Ag, we conducted a comparative analysis. The electrochemical reduction products of CO<sub>2</sub> were analyzed using gas chromatography and nuclear magnetic resonance spectroscopy. Additionally, we examined the fundamental characteristics of the electrode through scanning electron microscopy, X-ray photoelectron spectroscopy, and energy dispersive X-ray spectroscopy. The results revealed that as the thickness of the substituted Ag increased, the Faradaic efficiency of CO also increased. Furthermore, we discussed the correlation between Faradaic efficiency and the characteristics of the developed electrode.

056 **Understanding Photo-Cycloaddition Reactions in Metal-Organic Frameworks: Synthesis, Characterization, and Influence of Guest Molecules**

오지혜, 박인혁\*

충남대학교

Metal-organic frameworks (MOFs) are popular crystalline materials that form a structure through coordination bonds between metal salts and organic ligands.<sup>1</sup> They have a significant advantage in controlling their properties by utilizing different combinations of metal salts and ligands, leading to extensive application research in various fields. In this study, we investigated the [2+2] cycloaddition reaction by synthesizing MOFs using the olefin ligand 1,4-bis[2-(4'-pyridyl)ethenyl]benzene (bpeb). The [2+2] cycloaddition reaction is a photochemical process that forms cyclobutane rings when the double bond of the olefin ligand is positioned within a specific range (3.5 – 4.1 Å) in the MOF structure through self-assembly upon UV irradiation.<sup>2</sup> bpeb exhibits diverse arrangements within the MOF structure and possesses two photoreaction sites, allowing for the formation of various photoreaction products. [Zn(bpeb)(m-bdc)]·DMA (1) and [Zn(bpeb)(m-bdc)]·DMF (2) were synthesized under solvent heat reaction conditions with DMA and DMF, respectively, using Zn(II) metal salt, 1,3-benzenedicarboxylic acid (m-H<sub>2</sub>bdc) and bpeb. Interestingly, the crystal containing bpeb exhibits a two-dimensional (2D) layer structure with flexible spaces between the layers, which can be influenced by guest molecules, thereby affecting the photo-reactivity. When the solvent within the lattice was replaced or exchanged with alternative guest molecules, it led to the formation of different photoreaction products. In the MOFs 1 and 2, upon UV irradiation, in-phase double photo-reaction products were formed between neighboring bpeb ligands within each layer. Additionally, upon UV irradiation after removing guest molecules from the lattice using methanol, out-of-phase single photo-reactions occurred involving bpeb ligands from other adjacent layers. When xylene was introduced as a guest molecule into a crystal from which the guest molecules in the lattice had been removed, it led to the formation of an in-phase single photo-reaction product. This observation was confirmed through analysis using Nuclear Magnetic Resonance (NMR) and Single-Crystal X-ray Diffraction (SC-XRD).

057 **Formation of Concentration-Dependent Zn(II) Metal-Organic Frameworks with Photoreactive 4-Styrylpyridine**

안재욱, 박인혁\*

충남대학교

We report two Zn(II) metal-organic frameworks (MOFs) controlled by the concentration of reaction solvents. [Zn<sub>2</sub>(spy)<sub>2</sub>(tdc)<sub>2</sub>] (1) and [Zn(spy)<sub>2</sub>(tdc)(H<sub>2</sub>O)]·1.3DMA (2) from Zn(NO<sub>3</sub>)<sub>2</sub>·6H<sub>2</sub>O, 4-styrylpyridine (spy), and 2,5-thiophenedicarboxylic acid (H<sub>2</sub>tdc) were synthesized by a solvothermal reaction with different concentration. A low concentration of solvent is the condition for the synthesis of 1, which is yellow plate shaped crystals. A high concentration of solvent is the condition for the synthesis of 2, which is pale yellow block shaped crystals. Single Crystal X-ray diffraction (SC-XRD) analysis reveals that the single crystals of 2 crystallize in the space group Pna21 and is one-dimensional (1D) coordination polymer. Zn(II) atom of 2 is octahedrally coordinated by three O atoms from two tdc ligands

and one O atoms from H<sub>2</sub>O in the equatorial plane, and by two N atoms from two spy ligands at the axial pillar. The olefins of spy ligands in 1 are parallelly aligned to each other at a distance of 3.8 Å. The alignment of the C=C bonds between the spy ligands in a head to tail fashion is of interest as this arrangement follows Schmidt's Criteria[1] for the [2+2] cycloaddition reaction. Photoreactive in 1 was confirmed by <sup>1</sup>H nuclear magnetic resonance (NMR) analysis. When UV is irradiated to 1, the olefins of spy in 1 completely undergo the [2+2] cycloaddition reaction. Unlike 1, in 2, olefins are not only aligned, but phenyl-olefin are also aligned. while UV is irradiated to 2, <sup>1</sup>H NMR confirmed that most olefin-olefin undergo the [2+2] cycloaddition reaction, but some reactions undergo the [2+2] cycloaddition reaction between phenyl-olefin.

058 **Synergistic strategy of europium-doped magnetoplasmonic nanoparticles for aqueous copper(II) sensing**

원미지, 이재범\*  
충남대학교

Luminescent lanthanide compounds are of interest in imaging, sensing, and catalysis applications owing to their sharp emission and high resistance to photobleaching. Here, europium ion was doped into hybrid magnetoplasmonic nanoparticles which inherit high photoluminescence efficiency and strong magnetic characteristic. The incorporation of fluorescent lanthanide and Ag@Fe<sub>3</sub>O<sub>4</sub> nanoparticles has effectively boosted photoluminescence, attributed to the existence of core-shell structure and plasmon silver core. The as-synthesized NPs exhibit as a sensing probe in environmental technology because photoluminescence is selectively and sensitively quenched when encountering copper (II). This heavy metal ion can be possibly removed by intrinsic magnetic NPs. These results suggest that the complex of Eu-doped magnetoplasmonic NPs can be assigned to be an effective sensing material for aqueous copper(II).

059 **Inorganic Nanowire/Titania Hydrogel Composite with Microscopic Helical Chirality**

원유광, 이재범\*  
충남대학교

Hydrogel is a type of soft material formed by the coordinated networking of organic or inorganic matters, which results in an open and highly porous structure. When the solvents are removed, hydrogels could be converted to xerogels or aerogels depending on the preparation method. In this study, ultralight, magnetic translucent aerogel monoliths were fabricated from trizma-functionalized anatase (TiO<sub>2</sub>) and magnetoplasmonic core/shell gold-magnetite composite nanowires (Au@FexOy MagPlas NWs). The resulting aerogel weighs only 0.13 grams per cubic centimeter and possess UV-visible broad absorption, which were modulated by the amount of doped MagPlas NWs. The combination between highly UV-absorbing TiO<sub>2</sub> anatase and magnetoplasmonic core-shell nanowires allows utilization of both UV- and visible spectrum range of light, which potentially enhances the light-harvesting efficiency and photocatalysis applications. Furthermore, the magnetic susceptibility of the gold-magnetite nanowires also allows unique arrangements in TiO<sub>2</sub>

hydrogels, which opens up possibilities for self-assembly into unique linear and helical superstructures.

060 **Regioselective Photo-Cycloaddition Reaction of Supramolecular Isomers  
Triggered by Guest Exchange**

오지혜, 박인혁\*

충남대학교

We report the two-dimensional(2D) Zn(II) supramolecular isomers showing different photo-reactivity depending on guest molecules. The two Zn(II)-based metal-organic frameworks (MOFs, 1 and 2) derived from an olefinic dipyrindyl ligand, 1,4-bis[2-(4'-pyridyl)ethenyl]benzene (bpeb) and 1,3-benzenedicarboxylic acid (m-H<sub>2</sub>bdc) have been synthesized by solvothermal with a mixture of different solvent conditions. The orange block-shaped crystals of [Zn(bpeb)(m-bdc)]·DMA (1) and brown block-shaped crystals of [Zn(bpeb)(m-bdc)]·DMF (2) contain guest molecules used in the synthetic procedure (dimethylacetamide=DMA; dimethylformamide=DMF). The bpeb molecules as a diolefinic ligand aligned in an in-phase manner in the isomers 1 and 2 undergo [2+2] photo-cycloaddition reaction in a single-crystal-to-single-crystal (SCSC) fashion to the doubly dimerized MOFs 3 and 4. In MeOH, the guest molecules in 1 and 2 were removed to yield [Zn(bpeb)(m-bdc)]·xH<sub>2</sub>O (5). Xylene molecules were present in 5 through guest exchange of xylene isomers (o-xylene, m-xylene and, p-xylene), thereby controlling the photoreactivity. More details will be presented at the symposium.

061 **Time-dependent Oxidative Poly(Pyrogallol/Amine) Coating:  
Formulation for Black Hair-Dyeing**

김나윤, 조우경\*

충남대학교

Gray hair dye shampoos have been developed by applying the natural antioxidative principle of the browning phenomenon found in fruits and plants, using plant-derived polyphenolic compounds. The major component reported in the well-known gray hair dye shampoos, 1,2,4-trihydroxybenzene (THB), still raises concerns about its safety, and the need for fundamental chemical research in related industries has received great attention. In this regard, we explored the possibility of utilizing readily available polyphenolic molecules for oxidation-based coating formation and hair dyeing. Among the polyphenolic substances present in plants, pyrogallol was considered suitable for surface coating and dyeing due to its high oxidative power and biocompatibility. Pyrogallol has a similar chemical structure to THB, except for the location of a single hydroxyl group. It can undergo oxidation under ambient conditions, resulting in brownish color. Based on previous studies where we demonstrated that a polyphenol, quercetin can coat various organic and inorganic substrates through oxidation and subsequent cross-linking reactions with amines, we conducted research on oxidation-induced pyrogallol coating with amine cross-linkers and optimized the formulation for hair dyeing. In this study, ethylenediamine (EDA), diethylenetriamine (DETA), triethylenetetramine (TETA), and tetraethylenepentamine (TEPA) were used as amine compounds. The coating efficiency was investigated over time

using silicon as a model substrate. The oxidation-induced surface coating was analyzed by ellipsometer, surface profiler, contact angle goniometer, UV-Vis spectroscopy, and scanning electron microscope. The optimal coating condition was employed to dye hair and color maintenance was examined after shampooing in daily life. Our study is significant in that it suggests a polyphenolic compound for hair dyeing application and serves as a basis to understand polyphenol-based chemistry.

062 **Catechol-Amine Coating Formation and its Application in Hair Dyeing**

박혜림, 조우경\*

충남대학교

When an apple is sliced, polyphenol oxidase is triggered upon exposure to oxygen in air, and polyphenolic compounds present in the apple are oxidized to form o-quinones. The generated o-quinones then react with amino acids to produce brown-colored pigments. This sequence of events is known as enzymatic browning. Inspired by this phenomenon, a new dyeing shampoo was recently developed. It is known that polyphenolic molecules and 1,2,4-trihydroxybenzene (THB) are crosslinked in the shampoo to increase hydrophilicity and facilitate easy color change to brown. Alongside the hair dyeing shampoo, the polyphenol chemistry has recently received great attention. In this study, catechol, which acts as a monomeric compound capable of crosslinking through polyphenol oxidase, was used as an alternative to THB. Catechol is found in various plants, including strawberries and grapes, and it can undergo crosslinking reactions through interaction with polyphenol oxidase. We investigated oxidation-induced catechol coatings by using amine cross-linkers. Ethylenediamine (EDA), diethylenetriamine (DETA), triethylenetetramine (TETA), and tetraethylenepentamine (TEPA) were used as the crosslinking agents. The surface coating was performed in a solution containing catechol and each amine in tris buffer (pH=8.5), and silicon was used as a model substrate. All coatings were characterized using spectroscopic ellipsometry, contact angle goniometry, and UV-vis spectroscopy. The optimal surface coatings and the potential application to hair dyeing will be discussed in this presentation. We believe that this study will broaden the potential applications of polyphenol chemistry and contribute to evaluating its practical applicability in various industries such as cosmetics and pharmaceuticals.

063 **Au-Cu oxide nanowires rapid thermal annealing for C<sub>2</sub> hydrocarbons by electrocatalytic CO<sub>2</sub> reduction**

양호성, 손영구\*

충남대학교

In this study, we investigated the improved activity of copper oxide nanowires deposited with gold (Au) for the electrochemical CO<sub>2</sub> reduction reaction. Although copper oxide nanowires are widely used for electrochemical CO<sub>2</sub> reduction reaction due to their high conductivity, stability, and catalytic activity, their efficiency still needs improvement. We confirmed the synthesis and characteristics of Au-deposited copper oxide nanowires through SEM, XRD, and XPS analysis, and measured their activity for CO<sub>2</sub> reduction reaction using electrochemical and photocatalytic methods. As a result, we found that Au-deposited

copper oxide nanowires showed significantly enhanced activity for electrochemical CO<sub>2</sub> reduction reaction compared to normal copper oxide nanowires. Products were measured using gas chromatography, and the main products include carbon oxide and hydrogen.

064 **Effects of Ionic Size on Formation of Electrical Double Layer at Microporous Pt Electrodes**

Jinju Kim, Je Hyun Bae\*

*Chungnam National University*

Nanoporous electrodes with extremely small pores have been developed for improved supercapacitors and electroanalysis. Ion transport into nanoconfined spaces has been studied using nanoporous carbon. Herein, we explore the effect of ionic size on the charging dynamics using microporous Pt by cyclic voltammetry and electrochemical impedance spectroscopy. As the size of the effective hydrated ions decreased, the capacitance increased, and the movement of ions into and within the nanopores was less restricted. The effect of ionic size was more pronounced for hydrophobic organic cations than for hydrophilic alkali cations in microporous Pt. These findings provide insight into the formation of an electrical double layer at microporous metal electrodes and their applications in supercapacitors, electrocatalysts, and electroanalysis.

065 **Dual-functional solar-to-steam generation and SERS detection substrate based on plasmonic nanostructure**

Ba Thong Trinh, Ilsun Yoon\*

*충남대학교*

Solar-to-steam generation based on plasmonic material has attracted extensive attention as a green method to provide the fresh water. Herein, we introduce a simple fabrication heating method to in-situ fabricate Au nanoparticles (AuNPs) on cellulose filter paper as a dual-function “Solar-to-steam” and “Surface-enhance Raman Scattering” substrate. The substrates showed broadband absorption ability of 90% in the range of solar spectrum (350~1800 nm), with maximum absorption of 95% in the visible region, and the minimum absorption of 78% in the NIR region. The substrates provided an evaporation rate of 1.0 kg.m<sup>-2</sup>.h<sup>-1</sup> under 1-Sun illumination and the room condition of 20 °C and RH 40%. Also, the enriched SERS hot spot between AuNPs gave the substrates potential to detect the chemical contamination in water with the limit of detection of R6G dye down to ppb level, and can detect melamine in water with the ppm level within one minute processing. The enhancement factor of the substrate reached the maximum value of 8.5 × 10<sup>5</sup>. After the examine by SERS function, the contaminated water purification by the Solar-to-steam generation process, then collected purified water was again examined check the dual-function properties of substrate in the real application. The substrate also showed strong stability when working under 1 Sun illumination, with no decay in evaporation rate, making this substrate having strong potential to be used as efficient solar-to-steam and SERS system.

066 **Transparent high-refractive-index  $\text{ZrO}_2\text{@SiO}_2\text{-PDMS}$  nanocomposite film**

조한준, 윤일선\*

충남대학교

Transparent high-refractive-index materials can effectively manipulate light. Therefore, these materials can play an essential role in developing compact lenses, optical fibers, and high-efficiency mobile displays by enhancing light extraction. Nanocomposite is one of the methods that can realize transparent high refractive material, and it can be fabricated by dispersing a nanometer-sized high refractive index material in a matrix. To realize a transparent nanocomposite with a high-refractive index, the following criteria must be satisfied: First, there is no absorption light in the visible range. Next, the size of the high refractive index materials should be negligibly small compared to the wavelength of light to prevent a reduction in light transmission and an increase in haze due to scattering. Thus, it is crucial to strengthen the chemical affinity or conform a stable chemical bond between the high refractive index materials and matrix to avoid agglomeration. This presentation will introduce a transparent, high-refractive-index, nanocomposite film fabrication method with  $\text{ZrO}_2$  nanoparticles ( $n=2.16$ ) and polydimethylsiloxane (PDMS) ( $n=1.42$ ).  $\text{ZrO}_2$  nanoparticles were synthesized with a size of 13.7 nm using conventional hydrothermal synthesis. Then, to prevent agglomeration, surface-modification of  $\text{ZrO}_2$  nanoparticles was done with  $\text{SiO}_2$  ( $n=1.46$ ) using the Stöber method ( $\text{ZrO}_2\text{@SiO}_2$ ). For uniform dispersion in PDMS while maintaining the high refractive index of nanoparticles, in this process, by controlling the reaction time, the appropriate thickness (1.3 nm) of the  $\text{SiO}_2$  layer was found. Finally, dispersion of  $\text{ZrO}_2\text{@SiO}_2$  nanoparticle and PDMS resin by curing after the spin-coating process, a  $\text{ZrO}_2\text{@SiO}_2\text{-PDMS}$  nanocomposite was fabricated. The thickness of  $\text{ZrO}_2\text{@SiO}_2\text{-PDMS}$  nanocomposite film was 100 nm. It exhibited excellent optical transparency ( $T_{\text{average}}=91.1\%$ ), comparable to the transparency of the coverslip ( $T_{\text{average}}=91.4\%$ ) in the visible range. Furthermore, the refractive index of  $\text{ZrO}_2\text{@SiO}_2\text{-PDMS}$  was able to adjust from  $n=1.42$  to  $n=1.60$  with different nanoparticle contents (0.0–50.0 wt%) in the visible range

067 **bandgap determination of beta-FeSe**

류하은, 이재범\*

충남대학교

In the field of electrochemistry, increasing selectivity is a very important research topic when using electrodes as catalysts or sensors. nanoporous Pt electrodes are representative electrode materials for diverse applications, such as catalysts and sensors. Selectivity arising from a nanoporous structure has been applied to systems using non-faradaic reactions such as capacitive deionization, electrochemical supercapacitors, and conductometry. Cases applied to Faradaic reactions have been studied mainly based on reactivity and molecular size. Here, we suggest the surface adsorption of reactant molecules as another important factor for selectivity. We observed that a non-adsorption reaction was selectively enhanced more than that of an adsorption reaction at a nanoporous Pt electrode due to the nanoconfinement effect. This finding may provide insights into the effective utilization of a nanoporous Pt electrodes as catalysts or sensors.



068 **Selectivity of electrochemical reactions based on adsorption in nanoporous electrodes**

양현주, 김진주, 배제현\*  
충남대학교

In the field of electrochemistry, increasing selectivity is a very important research topic when using electrodes as catalysts or sensors. nanoporous Pt electrodes are representative electrode materials for diverse applications, such as catalysts and sensors. Selectivity arising from a nanoporous structure has been applied to systems using non-faradaic reactions such as capacitive deionization, electrochemical supercapacitors, and conductometry. Cases applied to Faradaic reactions have been studied mainly based on reactivity and molecular size. Here, we suggest the surface adsorption of reactant molecules as another important factor for selectivity. We observed that a non-adsorption reaction was selectively enhanced more than that of an adsorption reaction at a nanoporous Pt electrode due to the nanoconfinement effect. This finding may provide insights into the effective utilization of a nanoporous Pt electrodes as catalysts or sensors.

069 **Green and blue emissive Cs<sub>4</sub>PbBr<sub>6</sub> perovskites single crystals**

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We report on the optical properties of non-emissive, blue-emissive, and green-emissive Cs<sub>4</sub>PbBr<sub>6</sub> perovskite single crystals. Crystals of different colors were obtained depending on the solvent and growth conditions. It is confirmed by XRD patterns that all crystals have same lattice symmetry. When synthesized in water and DMSO solvent, non-emissive crystals (WN416) and green emissive crystals (DG416), respectively, were grown. By changing the growth time in DMF solvent, we grew non-emissive (FN416), blue-emissive (FB416), and green-emissive (FG416) crystals. The band gap energies of FN416, FB416 and FG416 were measured 3.06 eV, 3.02 eV, and 2.73 eV, respectively. The PL spectrum peaks of FB416, and FG416 were observed at 497nm and 510nm, respectively.

070 **Synthesis of Inorganic Lead Halide Perovskites in UiO-66 MOF Composite**

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We synthesized inorganic perovskite quantum dots (IPQDs) in UiO-66, a zirconium-based MOF. UiO-66 has a white powder, which is suitable for observing the emission color of QDs. We impregnated a polar organic solution of PbX<sub>2</sub> (X = Cl, Br, I) into the pores of the MOF to prepare PbX<sub>2</sub>@UiO-66, which was then reacted with cesium halide (CsX) dissolved in methanol. We confirmed that CsPbBr<sub>3</sub> and CsPbClBr<sub>2</sub> perovskites in UiO-66 still exhibit PL after two month. The compositions of the halogen anions in the perovskites can be modulated with various halide precursors, leading to CsPbX<sub>3</sub>@UiO-66 composites that exhibit gradual variation of band gap energies and tuned emission wavelengths from 400 to 700nm.

071 **Green-emissive copper-based perovskite quantum dots in UiO-66(Zr)**

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We synthesized green-emissive copper-based perovskite quantum dots (PQDs) in UiO-66(Zr). Lead-based PQDs are efficient optoelectronic materials, but they have the disadvantage of being toxic. Recently, copper-based perovskite materials have been proposed as an alternative light-emitting material. By using metal-organic frameworks (MOFs) as a template, we synthesized stably emitting Cu-based perovskite QDs. Green-emissive PQDs@MOFs were prepared using a precursor solution in which alkali iodide and copper (I) iodide were dissolved in DMF solvent. After the precursor solution was impregnated into the MOF pores and washed with toluene solvent, yellow emission at about 600 nm was observed. When alkali iodide was added, yellow PQDs changed to PQDs@MOF with a green photoluminescence (PL) of 530 nm.

072 **Synthesis of Blue Emissive Cs<sub>3</sub>Cu<sub>2</sub>I<sub>5</sub> Perovskite Single Crystals**

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We successfully grew high-quality single crystals of Cs<sub>3</sub>Cu<sub>2</sub>I<sub>5</sub> using an antisolvent vapor-assisted crystallization (AVC) method. Millimeter-sized crystals were obtained without the need for crystal-seeding in the dimethylformamide (DMF) solvent. Cs<sub>3</sub>Cu<sub>2</sub>I<sub>5</sub> single crystals were obtained at 40°C growing temperature, and polycrystals were grown at 0°C and -20°C under ambient atmosphere. Copper-based halide perovskite crystals grown in N-methyl-2-pyrrolidone (NMP) as the solvent resulted with mixed phase and small sized polycrystals. The phase purity and emission properties of the Cs<sub>3</sub>Cu<sub>2</sub>I<sub>5</sub> perovskite single crystals were characterized by using X-ray diffraction (XRD) and photoluminescence (PL) measurements.