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2021 충남대학교 소재화학연구소 국제학술대회

2021 Online

International Symposium on Materials Chemistry

November 11th (Thursday) 2021

Place: Zoom platform
https://cnu-ac-kr.zoom.us/j/85948816307
Meeting ID: 859 4881 6307

SCAN ME

| 주관 | 충남대학교 소재화학연구소
Research Institute of Materials Chemistry, Chungnam National University

| 후원 | 충남대 화학물질특성분석 핵심연구지원센터
CNU Chemistry Core Facility

Program

09:30 – 10:00 Registration

10:00 – 10:10 Opening Remarks :

Prof. Moon-Deock Kim *(Dean, CNS)*

Prof. Jeongkwon Kim *(Director, RIMC)*

【Session Ⅰ】

Chairperson : Prof. Kyung-sun Son
(Chungnam National University, Korea)

10:10 - 10:40 Hee Jung Koo *(Standigm UK, United Kingdom)*
"A journey to make a paradigm shift: facilitating early drug discovery using AI"

10:40 - 11:10 Yuhan Lee *(Harvard Medical School, USA)*
"Therapeutic luminal coating of the intestine for the treatment of type-2 diabetes"

11:10 - 11:40 Chang Woo Myung *(Chungnam National University, Korea)*
"Machine learning design of energy materials: challenges and opportunities"

11:40 – 11:50 Photo Time

11:50 – 13:10 Lunch Break

【Session Ⅱ】

Chairperson : Prof. Jaebeom Lee
(Chungnam National University, Korea)

13:10 - 13:40 Chenjie Xu *(City University of Hong Kong)*
"Nucleic acid-based functional nanoparticles for biosensing"

13:40 - 14:10 Jaheon Kim *(Soongsil University, Korea)*
"Design, synthesis, and gas adsorption applications of zeolitic imidazolate frameworks"

14:10 - 14:40 Dong-Myeong Shin *(University of Hong Kong)*
"Energy scavenging from the mechanical resource, and energy storage to high performing battery"

14:40 – 14:50 Photo Time

14:50 – 15:00 Closing

Session I 10:10 ~ 10:40

Speaker general information

Name: Hee Jung Koo
Email: heejung.koo@standigm.com
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Education

- 2011 ~ 2016 Ph.D. in Systems Biology at POSTECH
- 2009 ~ 2011 M.S. in Bioengineering at Seoul National University
- 2005 ~ 2009 B.S. in Chemical Engineering at POSTECH

Experience

- 2021 ~ Head of UK Office at Standigm (United Kingdom)
- 2016 ~ 2021 Senior Scientist/Biological Platform Team Leader at Standigm(Korea)

Representative publications

1. A Novel Target Identification Platform Utilizing a White-Box Deep Learning Model. *4th Global Pharma R&D AI, Data Science and Informatics Summit (PRADI 2020), Oral presentation.*
2. A Systems-Level Platform for Target Discovery and Its Application. *Discovery on Target 2020, Poster presentation.*
3. Standigm ASK™: Artificial intelligence-aided interactive platform for explainable disease target discovery. *24TH INTERNATIONAL CONFERENCE ON RESEARCH IN COMPUTATIONAL MOLECULAR BIOLOGY (RECOMB2020), Poster presentation.*
4. Standigm ASK™: A Novel Target Identification Platform Utilizing a White-box Deep Learning Model. *Milner Therapeutics Symposium 2020, Poster presentation.*
5. Introduction to AI-based drug discovery platform. *Korea Software Congress 2020, Oral presentation.*
6. iCLUE&ASK: An Artificial Intelligence-Aided Interactive Platform for Explainable Disease Target Identification. *AI Pharma Korea Conference 2020, Oral presentation.*
7. An artificial intelligence-aided interactive platform for explainable target identification. *2020 International Congress of Diabetes and Metabolism, Oral presentation.*

A journey to make a paradigm shift: facilitating early drug discovery using AI

Hee Jung Koo

Head of UK Office at Standigm (United Kingdom)

Prioritizing biological entities to target is an important challenge in developing therapeutics successfully. A vast amount of biomedical data and literature has been accumulated regarding this issue, and diverse approaches have also been developed to extract significant information from the comprehensive knowledge. Here, we constructed an AI-aided comprehensive platform, Standigm ASK™, covering novel target prioritization to target information enrichment.

Standigm ASK currently contains two different approaches for target prioritization. One is a recommender system on a knowledge graph, and the other is a random walk-based approach with transcriptome data on a warped protein-protein interaction network. Applying these two algorithms, Standigm ASK gives us new insights utilizing information with contrasting aspects: curated knowledge-level data and unbiased omics data. Additional approaches can be modularized and implemented in this platform.

The prioritized targets are further analyzed to enrich target-related information and reduced to a manageable number, considering experimental capabilities, competitiveness, and modalities to be developed in the next step. Natural language processing technologies are used to estimate what is known about the relationship between the target and queried disease. Pathway enrichment analysis is then performed to predict which pathways are affected by the target. Patient data are also considered if available. Additionally, the recommender system suggests important paths connecting disease-target pairs, and the information is used to provide explainability to users.

Standigm is currently utilizing this system to continuously provide novel targets to initiate new pipelines, minimizing the labor-intensive step.

Session I 10:40 ~ 11:10
Speaker general information
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Education
• 2004 ~ 2010 Korea Advanced Institute of Science & Technology (Daejeon, Republic of Korea) PhD Biology (Biomaterials) • 2000 ~ 2004 Korea Advanced Institute of Science & Technology (Daejeon, Republic of Korea) B.Sc. Biological Sciences
Experience
• 2021 ~ present Brigham and Women's Hospital, Harvard Medical School, Assistant Professor • 2016 ~ 2021 Brigham and Women's Hospital, Harvard Medical School, Instructor, Associate Biomedical Engineer • 2011 ~ 2016 Brigham and Women's Hospital, Harvard Medical School, Postdoctoral Research Fellow, Associate Biomedical Engineer • 2010 ~ 2011 Korea Advanced Institute of Science & Technology (Daejeon, Republic of Korea) Post-doc
Representative publications
1. G. M. Taboada, K. Yang, M. J. Pereira, S. S. Liu, Y. Hu, J. M. Karp*, N. Artzi*, Y. Lee*. Overcoming the translational barriers of tissue adhesives. Nature Reviews Materials, 5, 310-329, 2020 (*co-corresponding authors) 2. Y. Lee†*, T. E. Deelman†, K. Chen, D. S. Y. Lin, A. Tavakkoli*, J. M. Karp*, "Therapeutic Luminal Coating of the Intestine", Nature Materials, 17, 834-842, 2018 (†co-1st authors, *corresponding authors) 3. E. N. Feins*, Y. Lee*, E. D. O'Cearbhaill, S. Shimadaa, N. Vasilyev, I. Freihs, D. Perrin, P. Hammer, H. Yamauchi, A. Gosline, V. Arabagi, J. M. Karp, P. J. del Nido, "An Autonomously Growing Implantable Medical Device for Pediatric Applications", Nature Biomedical Engineering, 1, 818-825, 2017 (*co-first authors) 4. Y. Lee*, C. Xu*, M Sebastin, A. Lee, N. Holwell, C. Xu, D. Miranda Nieves, L. Mu, R. S. Langer, C. Lin, J. M. Karp, "Bioinspired nanoparticulate medical glues for minimally invasive tissue repair", Advanced Healthcare Materials, 4, 2587-2596, 2015. (selected as Inside Cover Article, VIP Article) (*co-first authors), also introduced in MIT Tech Review and Chosun News in Korea. 5. E. T. Roche*, A. Fabozzo*, Y. Lee**, P. Polygerinos**, I. Friehs, L. Schuster, W. Whyte, A. M. C. Berazaluce, A. Bueno, N. Lang, M. J. N. Pereira, E. Feins, S. Wasserman, E. D. O'Cearbhaill, N. V. Vasilyev, D. J. Mooney, J. M. Karp, P. J. del Nido, C. J. Walsh, "A Light-Reflecting Balloon Catheter for Atraumatic Tissue Defect Repair", Science Translational Medicine, 7, 306ra149, 2015. (*co-first authors, **co-second authors) 6. N. Lang*, M.J. Pereira*, Y. Lee**, I. Friehs**, N. Vasilyev, E. N. Feins, N. V. Vasilyev, K. Ablasser, E. O'Cearbhaill, C. Xu, A. Fabozzo, R. Padera, S. Wasserman, F. Freudenthal, L.S. Ferreira, R. Langer, J.M. Karp, P. J. del Nido, "A biocompatible light-activated adhesive for minimally invasive repair of cardiovascular defects", Science Translational Medicine 6, 218, 2014. (*co-first author, **co-second author), also introduced in NBC, Boston Globe, New York Time, and many other national and local media in USA and Korea)

Therapeutic luminal coating of the intestine for the treatment of type-2 diabetes

Yuhan Lee

Brigham and Women's Hospital, Harvard Medical School

The worsening type-2 diabetes (T2D) epidemic will affect over 600 million people worldwide by 2035. Recently, bariatric surgery has been shown in multiple randomized clinical trials to be superior to traditional pharmaceuticals in managing T2D. However, the risks of surgery along with permanent changes to gastrointestinal anatomy have hampered widespread acceptance. As a less invasive alternative, the duodeno-jejunal endoscopic sleeve was developed to prevent contact between food and duodenal mucosa, and has shown promising results in remitting T2D in patients. However, its pivotal FDA trial was recently halted due to serious complications. There is thus an urgent need for a safe, non-invasive and effective treatment with broad applicability for diabetic patients. Here we aim to develop an orally administered gut-coating formulation that forms a transient physical barrier to nutrient exposure through coating of the luminal surface of proximal intestine, and in essence emulates a critical part of the RYGB non-invasively. Through an in vitro screening study, we identified sucralfate, an orally administrated FDA-approved material, and further engineered sucralfate that can form a thin paste barrier coating on healthy gastrointestinal mucosa. We expect that the orally administered intestine barrier coater that can transiently reduce the postprandial glucose response, could be a new therapeutic approach that is safer, associated with significantly less complications, and thus can potentially help a wide T2D patient population.

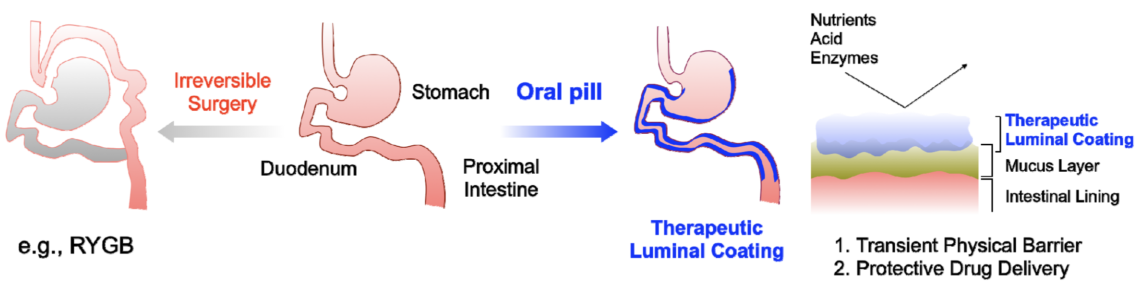

Figure 1. Representative cartoon demonstrating the oral administration luminal coating of intestine as an alternative of highly invasive and irreversible bariatric surgeries. The coating is designed to form a transient physical barrier on mucosa against substances such as nutrients, acids, and enzymes, and a drug delivery platform that can deliver therapeutics (e.g., protein) protected from stomach acid and digestive enzymes.

Session I 11:10 ~ 11:40

Speaker general information

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ORCID:	0000-0002-9480-6982
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Education

- 2014.09 ~ 2019.02 Ph.D., Department of Chemistry, Ulsan National Institute of Sci. and Tech.(UNIST) Supervisor: Prof. Kwang S. Kim
- 2012.09 ~ 2014.08 M.S., Pohang Univ. of Sci. and Tech. (POSTECH)
- 2007.03 ~ 2012.08 B.S., Pohang Univ. of Sci. and Tech. (POSTECH)

Experience

- 2021.09 ~ present Assistant Professor, Department of Chemistry, Chungnam National University (충남대학교), Korea
- 2020.12 ~ 2021.08 Postdoctoral Fellow of National Research Foundation of Korea, Yusuf Hamied Department of Chemistry, University of Cambridge, United Kingdom Research Group: Prof. Angelos Michaelides
- 2019.12 ~ 2020.11 Postdoctoral Researcher, ETH Zürich & Università della Svizzera italiana (USI), Switzerland Research Group: Prof. Michele Parrinello
- 2019.02 ~ 2019.11 Postdoctoral Researcher, Ulsan National Institute of Sci. and Tech. (UNIST), Korea Research Group: Prof. Kwang S. Kim

Representative publications

1. C. W. Myung, B. Hirshberg & M. Parrinello, Prediction of a supersolid phase in high-pressure deuterium. Phys. Rev. Lett. (in review) arXiv:2103.13974 (2021).
2. M. Ha, D. Y. Kim, M. Umer, V. Gladkikh, C. W. Myung*, Kwang S. Kim*(*co-corresponding author), High-performance electrochemical catalysis tuning of metal single-atoms by embedding in NxCy moiety of N-doped graphene. Energy Environ. Sci. DOI:10.1039/d1ee00154j (2021).
3. C. W. Myung* & K. S. Kim*, Anharmonicity-Driven Rashba Cohelical Excitons Break Quantum Efficiency Limitation. Adv. Mater. 2005400 (2020).
4. C. W. Myung, S. Javaid, K. S. Kim & G. Lee, Rashba-Dresselhaus effect in inorganic/organic lead iodide perovskite interfaces. ACS Energy Lett. 3, 1294-1300 (2018).
5. C. W. Myung, J. Yun, G. Lee & K. S. Kim, A new perspective on the role of A-site cations in perovskite solar cells. Adv. Energy Mater. 8, 1702898 (2018).
6. J. Kim, Kwang S. Kim*, & C. W. Myung*(*co-corresponding author) Superb band alignment, defect tolerance, and carrier injection property of SnO_2 electron transport layer for perovskite solar cells. npj Computational Mater. 6, 100 (2020).
7. S. Sultan, M. Ha, D. Y. Kim, J. N. Tiwari*, C. W. Myung*, A. Meena, T. J. Shin, K. H. Chae, & K. S. Kim* (*co-corresponding), Superb water splitting activity of the electrocatalyst $Fe_3Co(PO_4)_4$ designed with computation-aid. Nat. Commun. 10, 5195 (2019).
8. A. Hajibabaei, C. W. Myung, & K. S. Kim, Towards Universal Sparse Gaussian Process Potentials: Application to Lithium Diffusivity in Superionic Conducting Solid Electrolytes. Phys. Rev. B 103, 214102 (2021).
9. N. Clark, D. J. Kelly, M. Zhou, Y. Zhou, C. W. Myung, D. G. Hopkinson, C. Schran, A. Michaelides, R. Gorbachev, S. J. Haigh, Tracking single atoms in a liquid environment. Nature, accepted (2021) .

Machine learning design of energy materials: challenges and opportunities

Chang Woo Myung

Department of Chemistry, Chungnam National University, Korea

The biggest challenge the theoretical chemistry community is facing today is an exponential wall in the Schrödinger equation [1]. Without any approximations, the exact solution of the Schrödinger equation scales exponentially so that any calculation attempts over ~100 electrons become formidable tasks. Although, the scalability of materials simulation has increased significantly over the last decades because of the success of various wavefunction methods in chemistry and density functional theory in physics, a realistic large scale quantum mechanical simulation is still a challenge. Here, I will briefly introduce practical applications of first-principles (or ab initio from the beginning) calculations of novel energy materials, which are crucial for mitigating climate change, such as lead halide perovskites (LHP) solar cells[2], water splitting electrocatalysts[3], LHP light emitting diodes[4] and Li-battery materials[5]. Also, I will discuss current application of machine learning (ML) methods in chemistry, such as ML molecular dynamics[6], ML-assisted sampling[7] and ML materials design[8].

[1] Walter Kohn, "Electronic Structure of Matter – Wave Functions and Density Functional" Nobel Lecture (1999)
[2] C. W. Myung et al. Adv. Energy Mater. 8, 1702898 (2018).
[3] J. N. Tiwari et al. Nat. Energy 3, 773 (2018); S. Sultan et al. Nat. Commun. 10, 5195 (2019).
[4] C. W. Myung & K. S. Kim Adv. Mater. 33, 2005400 (2020).
[5] A. Hajibabaei, C. W. Myung & K. S. Kim Phys. Rev. B 103, 214102 (2021).
[6] C. W. Myung, B. Hirshberg & M. Parrinello arXiv:2103.13974 (2021).
[7] C. W. Myung, D. J. Wales & A. Michaelides in preparation (2021).
[8] M. Ha et al. Energy Environ. Sci., 14, 3455 (2021); V. Gladkikh et al. J. Phys. Chem. C 124, 890 (2020)

Session II 13:10 ~ 13:40
Speaker general information
Name: Chenjie XU (https://orcid.org/0000-0002-8278-3912) Email: Chenjie.xu@cityu.edu.hk Personal Website: www.xulab4nanomedicine.net
Education
• 2009.05, PhD in Chemistry, Brown University • 2004.10, MPhil in Chemistry, Hong Kong University of Science and Technology • 2002.07, BSc in Chemistry, Nanjing University
Experience
• 2020.01 ~ present Associate Professor, Department of Biomedical Engineering, City University of Hong Kong, Hong Kong SAR • 2019.01 ~ Present Adjunct Principal Investigator, National Dental Centre, Singapore • 2018.01 ~ 2019.12 Cluster leader of Environmental Chemistry and Materials Centre (ECMC), Nanyang Environment & Water Research Institute (NEWRI), Nanyang Technological University, Singapore • 2021.08 ~ 2019.12 Assistant Professor, School of Chemical & Biomedical Engineering, Nanyang Technological University, Singapore • 2009.06 ~ 2012.06 Research Associate, Department of Medicine, Brigham & Women's Hospital, Harvard Medical School • 2004.08 ~ 2005.06 Visiting Scholar, Department of Medicine, Stanford University
Representative publications
1. RZ. Seeni, DCS Lio, C Wiraja, MFB Yusoff, WTY Koh, Y Liu, BT Goh*, C Xu*. Targeted Delivery of Anaesthetic Agents to Bone Tissues using Conductive Microneedles Enhanced Iontophoresis for Painless Dental Anaesthesia. Advanced Functional Materials, 2021, 2105686. 2. M Cui, M Zheng, C Wiraja, SWT Chew, A Mishra, V Mayandi, R Lakshminarayanan*, C Xu*. Ocular delivery of predatory bacteria with cryo-microneedles against eye infection. Advanced Science, 2021, 2102327. DOI:10.1002/advs.202102327 3. C Wiraja, Y Mori, T Ichimura, J Hwang, C Xu*, JV Bonventre*. Tubuloids using Spherical Nucleic Acid-based mRNA Nanoflares. Nano Letters, 2021, 21, 13, 5850 4. H Chang, SWT Chew, M Zheng, DCS Lio, C Wiraja, Y Mei, A Than, S Peng, D Wang, K Pu, P Chen, H Liu, C Xu*. Cryomicroneedles for Transdermal Cell Delivery. Nature Biomedical Engineering, 2021, doi:10.1038/s41551-021-00720-1 5. DCS Lio, RN Chia, MSY Kwek, C Wiraja, LE Madden, H Chang, SMA Khadir, X Wang*, DL Becker*, C Xu*. Temporal Pressure Enhanced Topical Drug Delivery through Micropore Formation. Science Advances. 2020. 6 (22), eaaz6919 6. C Wiraja, Y Zhu, DCS Lio, DC Yeo, M Xie, W Fang, Q Li, M Zheng, MV Steensel, L Wang, C Fan*, C Xu* Framework Nucleic Acids as Programmable Carrier for Transdermal Drug Delivery. Nature Communication, 2019, 10, 1147 7. A Than, C Liu, H Chang, P.K Duong, X Wang*, C Xu*, P Chen*. Self-implantable double-layered micro-drug-reservoirs for efficient and controlled ocular drug delivery, Nature Communication. 2018, 9, 4433 8. DC Yeo, C Wiraja, AS Paller*, CA Mirkin*, C Xu*. Abnormal Scar Identification with Spherical Nucleic Acids Technology, Nature Biomedical Engineering, 2018, 2, 227 9. H Chang, M Zheng, X Yu, A Than, RZ Seeni, R Kang, J Tian, DP Khanh, L Liu, P Chen*, C Xu*. A swellable microneedle patch to rapidly extract skin interstitial fluid for timely metabolic analysis. Advanced Materials. 2017, 29 (37), 1702243 10. Gao Y, Chan CU, Gu Q, Lin X, Zhang W, Yeo DCL, Alsema AM, Arora M, Chong MSK, Shi P, Ohl CD*, Xu CJ*, Controlled nanoparticle release from stable magnetic microbubble oscillations, NPG Asia Materials, 2016, 8, e260

Nucleic acid-based functional nanoparticles for biosensing

Chenjie XU

Department of Biomedical Engineering, City University of Hong Kong, Kowloon Tong, Hong Kong SAR, China

Timely monitoring and assessment of human health plays a crucial role in maintaining the well-being of our advancing society. Besides medical tools and devices, suitable probe agents are crucial to assist such monitoring, either in passive or active ways (i.e. sensor) through inducible signals.

Out of the different category of activatable sensors, a category which has gathered significant attention over recent years is the nucleic acid (NA)-based sensors. Comprised largely of nucleic acids warrants bio-degradation and clearance from the body, with minimal risks of toxicity as compared to chemically-synthesized sensors. With its highly defined base-pairing assembly, its recognition (i.e. specificity) is largely predictable and tuneable through simple sequence alteration. This allows precise programmability of the sensing performance. Moreover, NA-based sensors are versatile as well, with targeting ability to both nucleic acids and proteins (e.g. aptamer), besides innate compatibility to serve both therapeutic-diagnostic (theranostic) purposes with antisense oligonucleotides or interfering RNAs.

In this talk, Dr. Xu will highlight his development of activatable optical sensors, based on nucleic acids. Focusing on the wound healing and skin regeneration, sensing mechanism and bio-applications of these nucleic acid sensors in ex vivo assays, intracellular and in vivo settings will be discussed.

Session II 13:40 ~ 14:10
Speaker general information
Name: Jaheon Kim E-mail: jaheon@ssu.ac.kr Personal Website: http://www.ssu-inorg.org/index.htm
Education
• 1991. 08 ~ 1996. 08, Ph.D., Inorganic Chemistry, POSTECH, Korea • 1987. 03 ~ 1989. 08, M.S., Chemistry, Seoul National University, Korea • 1983. 03 ~ 1987. 02, B.S., Chemistry, Seoul National University, Korea
Experience
• 2015. 03 ~ Professor at Dept. of Chem., SSU • 2009. 03 ~ 2015. 02, Associate professor at Dept. of Chem., SSU • 2005. 04 ~ 2009. 02, Assistant professor at Dept. of Chem., SSU • 2003, 03 ~ 2005. 03, Full-time lecturer at Dept. of Chem., Soongsil University(SSU) • 1999. 03 ~ 2003. 02, Research Fellow, University of Michigan, Ann Arbor, USA • 1998. 06 ~ 1999. 10, Researcher, Center for Smart Supramolecules, POSTECH • 1996. 11 ~ 1998. 06, Researcher, Daelim R&D Institute, Daejeon, Korea
Representative publications
1. H. J. Park, J. Oh, J. Kim, <u>J. Kim</u>, Two-step gas adsorption induced by the transmetallation in a two-dimensional metal-organic framework. *Chem. Commun.* 2020, *56*, 9727. 2. Y. Choi, K. Noh, J. Lee, <u>J. Kim</u>, Porosity Properties of the Conformers of Sodalite-like Zeolitic Imidazolate Frameworks. *J. Am. Chem. Soc.* 2018, *140*, 14586. 3. N. Ko, J. Hong, S. Sung, K. E. Cordova, H. J. Park, J. K. Yang, <u>J. Kim</u>, Significant enhancement of water vapour uptake at low pressure by amine-functionalization of UiO-67, *Dalton Trans.* 2015, *44*, 2047. 4. S. B. Choi, H. Furukawa, H. J. Nam, D.-Y. Jung, Y. H. Jhon, A. Walton, D. Book, M. O'Keeffe, O. M. Yaghi, <u>J. Kim</u>, Reversible Interpenetration in a Metal-Organic Framework Triggered by Ligand Removal and Addition. *Angew. Chem. Int. Ed.* 2012, *51*, 8791. 5. H. Furukawa, N. Ko, Y. B. Go, N. Aratani, S. B. Choi, E. Choi, A. Ö. Yazaydin, R. Q. Snurr, M. O'Keeffe, <u>J. Kim</u>, O. M. Yaghi, Ultrahigh Porosity in Metal-Organic Frameworks. *Science* 2010, *329*, 424.

Design, synthesis, and gas adsorption applications of zeolitic imidazolate frameworks

Jaheon Kim

Department of Chemistry, Soongsil University, Republic of Korea

Zeolitic imidazolate frameworks (ZIFs), which are composed of tetrahedral divalent metal ions (mostly Zn^{2+}, Co^{2+}, and Cd^{2+}) and bridging imidazolate ligand, giving rise to 4-coordinate metal-organic extended structures analogous to zeolites. Since ZIFs have good water and thermal stability, and interesting porosity as well, they are useful for gas adsorption applications. However, their building blocks are simple and limited compared with metal-organic frameworks (MOFs) in terms of available metal ions and organic linkers, it is challenging to discover new structures or topologies of ZIFs. One proven strategy is to incorporate mixed-imidazolates into frameworks so that the functional groups substituted on imidazole rings affect the coordination geometry of metal centers and in turn, generate the connectivity diversity of building blocks. In contrast, we may use other metal ions in synthesis than the common ones such as Zn^{2+}, which can also induce mere distortion of the coordination geometry around metal centers. In this presentation, we will show our ongoing exploration for synthesizing new ZIFs by using mixed-ligand methods via post-treatments of as-synthesized ZIFs, and linking copper ions with sole imidazolates.

First, we demonstrate functionalized ZIFs can be obtained through post-synthetic modification of as-synthesized ZIFs that are prepared from Zn^{2+} ion and unfunctionalized imidazole (ImH). For example, the reactions with ZIF-**afi** crystals with 2-nitromimidazole (nImH), 2-methylimidazole (mImH), or benzimidazole (BImH) give functionalized ZIFs with **gme**, **sod** (ZIF-8), and **sod** (ZIF-7) topology, respectively. In contrast, ZIF-**aco** crystals transform to **gme**, **sod** (ZIF-8), or **cag** type ZIFs with the same imidazoles as those used for the ZIF-**afi** modification. All these structural transformations take place via crystal-to-crystal conversion. The ratios of Im/mIm in the produced **sod**-ZIFs (or termed ZIF-8x with compositions of $Zn(Im)_{2-x}(mIm)_x$) can be adjusted simply by changing the amounts of added mImH in the reactions with ZIF-**aco** crystals. Indeed, the gas adsorption properties of the resulting ZIF-8x are dependent on the Im/mIm ratios. Second, we present the synthesis, crystal structures, and porosities of three new Cu-ZIFs: Cu-ZIF-**sql** ($Cu(fIm)_2$, fIm = 2-formylimidazolate), Cu-ZIF-**gis** ($Cu(nIm)_2$, nIm = 2-nitroimidazolate), and Cu-ZIF-**rho** ($Cu(nIm)_2$). Cu-ZIF-**sql** is a non-porous square grid structure, Cu-ZIF-**gis** adsorbs only small gases such as H_2 and records a high isosteric heat of H_2 adsorption, and Cu-ZIF-**rho** has large pores that can store various gases such as H_2, CO_2, N_2, or CH_4. The Cu-ZIFs are stable in both acidic and basic aqueous solutions, and most importantly, the coordination geometry of Cu^{2+} is not tetrahedral but severely flattened tetrahedral.

Session II 14:10 ~ 14:40
Speaker general information
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Education
• 2016 Ph.D. In Nanofusion Technology (Nanomaterials), Pusan National University with Prof. Yoon-Hwae Hwang and Prof. Hyung Kook Kim • 2011 M.S. In Nanofusion Technology (Nanomaterials), Pusan National University with Prof. Yoon-Hwae Hwang and Prof. Hyung Kook Kim • 2009 B.S. In Nanoscience and Nanotechnology, Pusan National University
Experience
• 2019 ~ present Assistant Professor of Mechanical Engineering, The University of Hong Kong • 2017 ~ 2019 Postdoctoral Scholar of Chemistry, University of California, Berkeley with Prof. Jeffrey R. Long • 2016 ~ 2017 Postdoctoral Fellow, Pusan National University with Prof. Kyujung Kim • 2016 ~ 2016 Lecturer of Nanoenergy Engineering, Pusan National University • 2013 ~ 2016 Researcher of Alternative Military Service as Technical Research Personnel
Representative publications
1. J. Jeong, S. Jeon, X. Ma, Y. W. Kwon, D.-M. Shin*, S. W. Hong*, "Sustainable and flexible microbrush-faced triboelectric generator for portable/wearable applications", Advanced Materials, in press (IF=30.849). 2. D.-M. Shin, J. E. Bachman, M. K. Taylor, J. Kamcev, J. G. Park, M. E. Ziebel, E. Velasquez, N. N. Jarenwattananon, G. K. Sethi, Y. Cui, J. R. Long,"A single-ion conducting borate network polymer as a viable quasi-solid electrolyte for lithium metal batteries", Advanced Materials (2020) 32, 1905771 (IF=30.849). 3. J. Kamcev, M. K. Taylor, D.-M. Shin, N. N. Jarenwattananon, K. A. Colwell, J. R. Long, "Functionalized porous aromatic frameworks as high-performance adsorbents for the rapid removal of boric acid from water", Advanced Materials (2019) 31, 1808027 (IF=30.849). 4. Y. Yan, W.-G. Kim, X. Ma, T. Tegafaw, T. M. Nguyen, J.-M. Lee, E.-J. Choi, H. Ahn, S.-H. Ha, K. Kim, J.-M. Kim, H. K. Kim, J.-W. Oh*, D.-M. Shin*, Y.-H. Hwang*, "Nanogenerators facilitated piezoelectric and flexoelectric characterizations for bioinspired energy harvesting materials", Nano Energy (2021) 81, 105607 (IF=17.881). 5. Y. Zhang, S.-C. Fu, K. C. Chan, D.-M. Shin, C. Y. H. Chao, "Boosting power output of flutter- driven triboelectric nanogenerator by flexible flagpole", Nano Energy (2021) 88, 106284 (IF=17.881). 6. D.-M. Shin†, H. J. Han†, W.-G. Kim, E. Kim, C. Kim, S. W. Hong, H. K. Kim, J.-W. Oh, Y.-H. Hwang, "Bioinspired piezoelectric nanogenerators based on vertically aligned phage nanopillars", Energy & Environmental Science (2015) 8, 3198-3203 (IF=38.532). † These authors contributed equally to this work.

Energy scavenging from the mechanical resource, and energy storage to high performing battery

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In the era of the internet of things, the billions of connected devices will require not only high battery cost but also an enormous scale of maintenance expenses, so that we need an alternative for powering the devices beyond plugging all of the intelligent devices into the grid. The power supply for future technology requires independent, sustainable, continuous operation, and maintenance-free. The possible solution for easily powering those devices includes harvesting the tiny energy when available, from environmentally friendly sources like the sun, thermal, and mechanical energy. Our recent research interest has been dedicated to the developing the main components of self-powered nanoelectronics, which includes the energy harvesting and storage devices. In this talk, I will address a simple strategy for energy harvesting from mechanical energy based on the smart piezoelectric nanomaterials, such as ZnO nanorods/graphene/ZnO nanorods heterostructure and aligned M13 bacteriophage, as well as triboelectric nanomaterials. Further I will present the future energy storage technology based on a single-ion conducting electrolyte to improve the power density, safety concerns as well as high capacity retention at rapid discharging.