Yongchul G. Chung

Professor (tenured), School of Chemical Engineering (BKFOUR 21)

Affiliated: Department of Chemical & Biomolecular Engineering
Graduate School of Data Science; AI Convergence Computational Science Program
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Research Interests

- Computation
- Artificial Intelligence
- Materials
- Chemical Separation

Representative Publications

* Corresponding author; + co-first author.

1. G. Zhao, P. Zhao, **Y.G. Chung***
   MOFClassifier: A Machine Learning Approach for Validating Computation-Ready Metal-Organic Frameworks
   Journal of the American Chemical Society, 147(37), 33343–33349 (2025).

2. G. Zhao, L. M. Brabson, S. Chheda, J. Huang, H. Kim, K. Liu, K. Mochida, T.D. Pham, Prerna, G.G. Terrones, S. Yoon, L. Zoubritzky, F.-X. Coudert, M. Haranczyk, H.J. Kulik, S. M. Moosavi, D.S. Sholl, J.I. Siepmann, R.Q. Snurr, **Y.G. Chung***
   CoRE MOF DB: a curated experimental metal-organic framework database with machine-learned properties for integrated material-process screening
   Matter, 8, 102140 (2025).

3. P.Z. Moghadam+, **Y.G. Chung+**, R.Q. Snurr*
   Progress toward the computational discovery of new metal–organic framework adsorbents for energy applications
   Nature Energy, 9, 121–133 (2024).

4. **Y.G. Chung+***, E. Haldoupis+, B.J. Bucior+, M. Haranczyk, S. Lee, H. Zhang, K.D. Vogiatzis, M. Milisavljevic, S. Ling, J.S. Camp, B. Slater, J.I. Siepmann*, D.S. Sholl*, R.Q. Snurr*
   Advances, updates, and analytics for the computation-ready, experimental metal-organic framework database: CoRE MOF 2019
   Journal of Chemical & Engineering Data, 64 (12), 5985–5998 (2019).

5. P. Sinha+, A. Datar+, C. Jeong, X. Deng, **Y.G. Chung***, L.C. Lin*
   Surface area determination of porous materials using the Brunauer–Emmett–Teller (BET) method: limitations and improvements
   The Journal of Physical Chemistry C, 123 (33), 20195–20209 (2019).

Education and Postdoctoral Training

Jan. 2013 – Feb. 2016	Postdoctoral Fellow, Chemical & Biological Engineering, Northwestern University Advisor: Prof. Randall Q. Snurr
Jan. 2013	Ph.D. in Chemical Engineering, Case Western Reserve University Advisor: Prof. Daniel J. Lacks
May 2007	B.S. in Chemical Engineering, Texas Tech University

Professional Appointments

Mar. 2025 – Present	Professor School of Chemical Engineering (BKFOUR 21) Department of Chemical & Biomolecular Engineering (affiliated) Graduate School of Data Science (affiliated) Artificial Intelligence (AI) Convergence Computational Science (affiliated) Pusan National University
Mar. 2026 – Present	Department Chair Artificial Intelligence (AI) Convergence Computational Science School of Transdisciplinary Engineering Pusan National University
Aug. 2026 – Sep. 2026	Visiting Professor, Materials Science & Engineering, University of California, Berkeley Affiliate, Materials Science Division, Lawrence Berkeley National Laboratory (Host: Kristin Persson, MSE)
Mar. 2020 – Feb. 2025	Associate Professor School of Chemical & Biomolecular Engineering, Pusan National University
Mar. 2023 – Feb. 2025	Department Chair School of Chemical & Biomolecular Engineering, Pusan National University
Mar. 2023 – Feb. 2024	Graduate School Chair Graduate School of Chemical Engineering, Pusan National University
May 2022 – Jun. 2022	Guest Researcher (Host: Evgeny Pidko, Chemical Engineering) Department of Chemical Engineering, Delft University of Technology
Jan. 2022 – May 2022	Visiting Scientist (Host: Heather J. Kulik, Chemical Engineering) Department of Chemical Engineering, Massachusetts Institute of Technology
Sep. 2021 – Dec. 2021	Visiting Researcher Clean Energy Research Center, Korea Institute of Science and Technology
Mar. 2016 – Feb. 2020	Assistant Professor School of Chemical & Biomolecular Engineering, Pusan National University

Honors and Awards

2025	PNU School of Engineering Excellent Researcher Award (Spring)
2024	*I&EC Research* Excellence in Review Award
	PNU School of Engineering Excellent Researcher Award (Spring)
2023	*I&EC Research* 2023 Class of Influential Researchers – Asia and Pacific
	PNU School of Engineering Excellent Researcher Award (Spring)
2022	PNU School of Engineering Excellent Researcher Award (Fall)
	Service Award, Korean Society of Industrial and Engineering Chemistry
	PNU School of Engineering Excellent Researcher Award (Spring)

2020	Service Award, Korean Institute of Chemical Engineers
2017	Special Presentation Award, 2017 Joint Korea/Japan/Taiwan Chemical Engineering Conference
2016	New Investigator Award, Korean Institute of Chemical Engineers
	New Investigator Award, Korean Society of Industrial and Engineering Chemistry
2011	CWRU Graduate Studies Travel Grant
2010	Student Travel Grant, Society of Rheology
2006–2007	Vernon J. & Bendell Yeakly Memorial Scholarship
2005–2006	TTU Tradition Designated Scholarship
2004–2006	Don Carter Endowed Scholarship
2005–2006	Dean's List

Research Performance 2020–2026

Field-Weighted Citation Impact (FWCI): 2.32; **Citations per Publication:** 29.9

Publications

Google Scholar Citations: 6,604 (September 8, 2026)

Bold author names denote group members; * corresponding author; + co-first author.

Manuscripts under Review or Revision

. **Y.G. Chung*, T. Siah, M. Hassan, C. Shin, P. Zhao, H. Kim, Y. Chen
Beyond Crystal Rankings: Data-Driven Discovery of Metal-Organic Framework Adsorbents
(Invited contribution for Annual Review of Chemical and Biomolecular Engineering, Vol.18)

. D.W. Kim, **Y. Chen, N. Kim, C.G. Kim, **T. Lee**, **Y.G. Chung***, C.S. Hong*
Harnessing structural flexibility of porous aromatic frameworks for high methane storage capacity

. S. Jang, J.W. Leem, Y. Jung, J. Im, C. Park, **C. Shin, **Y.G. Chung**, B. Jeong, S. W. Hong*, J. Lee*
Binder-Free Pure Carbon Nanotube Aerogel Electrodes for Deformation Tolerant Flexible Supercapacitors

2026 (7)

73. S. Lee, **T. Lee**, A. Jo, J. Yu, I.S. Kim, **Y.G. Chung***, S. Ahn*
Local environmental modification of Ti-SiO_2 via terminal alcohol grafting for liquid-phase cyclohexene epoxidation with H_2O_2
Langmuir, in press

72. **Y.G. Chung***, M.S. Lah
Hunting Structural Demons in Digital Reticular Chemistry: Lessons from Metal-Organic Frameworks
Israel Journal of Chemistry, 66 (4), e70028 (2026)

71. **H. Kim+, T. Lee+, S. Hong,** K.-H. Kim**, Y.G. Chung***
Data-driven Prediction of Ionic Conductivity in Solid-State Electrolytes with Machine Learning and Large Language Models
The Journal of Chemical Physics, 164, 114502 (2026)

70. **M. Hassan**, **C. Shin**, **T. Lee,** S. Lee, S. Chowdhury, H.T. Kwon, S.G. Kang*, S. Ahn*, **Y.G. Chung***
Direct Air Capture with Solid Sorbents: Adsorbent Design, Process Engineering, and CO_2 Conversion
Chemical Engineering Journal**,** 534, 175117 (2026)

69. Y. Wang, **Y.G. Chung,** W. Wu, W. Li*, S. Li*
Bridging the gap between materials and engineering: large-scale screening of metal-organic frameworks for adsorption cooling from device level
Advanced Energy Materials, 16 (5), e04672 (2026)

68. **M. Hassan**, **S. Yoon**, **Y. Chen**, P. Kim, H. Yun, H.T. Kwon, Y.S. Bae, C.Y. Yoo, D.Y. Koh, C.S. Hong, K.B. Lee, **Y.G. Chung***
AIM: A User-friendly GUI Workflow Program for Isotherm Fitting, Mixture Prediction, Isosteric Heat of Adsorption Estimation, and Breakthrough Simulation
Computer Physics Communications, 319, 109944 (2026)

67. **C. Shin**, **S. Yoon**, **Y.G. Chung***
Multiscale, Techno-economic Evaluation of Isoreticular Series of CALF-20 for Biogas Upgrading using a Pressure/Vacuum Swing Adsorption (PVSA) Process
Molecular Systems Design & Engineering, 11, 181–194 (2026)

2025 (10)

66. **S. Yoon**+, J. Tu+, L.-C. Lin*, **Y.G. Chung***
Integrating Macrostate Probability Distributions with Swing Adsorption Modeling for Binary/Ternary Gas Separation
Industrial & Engineering Chemistry Research, 64, 52, 25017–25033 (2025)

65. **Y. Chen**, **G. Zhao**, L.-C. Lin**, Y.G. Chung***
A Master Isotherm Model Approach to Quantify Defects in UiO-66 from Nitrogen Adsorption Isotherms
Langmuir, 41, 44, 29851–29858 (2025)

64. **S. Yoon**, J. Jung, **G. Zhao**, **Y. Lee**, K.B. Lee*, **Y.G. Chung***
Techno-economic analysis of Cu(I)-loaded porous carbons for CO separation via pressure/vacuum swing adsorption process
Separation and Purification Technology, 378, 134786 (2025)

63. **G. Zhao**, **P. Zhao**, **Y.G. Chung***
MOFClassifier: A Machine Learning Approach for Validating Computation-Ready Metal-Organic Frameworks
Journal of the American Chemical Society **(Communication)**, 147 (37), 33343–33349 (2025)

62. Z. Liu, D. Shen, **Y.G. Chung**, W. Li, S. Li*
Accelerated Discovery of High-Performance MOFs for Water Adsorption Chillers through Molecular Simulation and Machine Learning
Chemical Engineering Journal, 517, 164419 (2025)

61. M.J. Jang, **Y. Chen**, J. Choi, H. Seo, **Y.G. Chung**, D-Y. Koh*
Enhancing Interchain Interactions in Spirobifluorene-Based Microporous Polyimides for High-Performance Organic Solvent Nanofiltration
Journal of Membrane Science, 733, 124298 (2025)

60. **G. Zhao**, L. M. Brabson, S. Chheda, J. Huang, **H. Kim**, K. Liu, K. Mochida, T.D. Pham, Prerna, G.G. Terrones, **S. Yoon**, L. Zoubritzky, F.-X. Coudert, M. Haranczyk, H.J. Kulik, S. M. Moosavi, D.S. Sholl, J.I. Siepmann, R.Q. Snurr, **Y.G. Chung***
CoRE MOF DB: a curated experimental metal-organic framework database with machine-learned properties for integrated material-process screening
Matter, 8, 102140 (2025)

59. **S. Yoon**+, H. Mun+, **S. Ga**+, J. Park, I. Lee*, **Y.G. Chung***
Modeling, screening, and techno-economic evaluation of metal-organic frameworks for boil-off gas capture during intercontinental transportation of LNG
Chemical Engineering Journal, 507, 160517 (2025)

58. H.R. Park, G. Jang, J.S. Byun, Y. Park, W.I. Kim, S.J. Lee, **Y.G. Chung**, Y.M. Jung*, H.S. Park*
Hierarchically Structured Conductive Lanthanide Metal Organic Framework Nanorods for Ultrastable Flexible Magnesium Ion Capacitors
Advanced Functional Materials, 35 (11), 2417288 (2025)

57. J.S. Byun, W.I. Kim, S.H. Baek, F. Hao, **H. Kim**, **Y.G. Chung**, L.-X. Li, R. Zhang, H.S. Park*
Polyoxometalate Initiated In situ Conformal Coating of Multifunctional Hybrid Artificial Layers for High Performance Zinc Metal Anodes
Advanced Functional Materials, 35 (10), 2412577 (2025)

2024 (10)

56. **Y. Chen**, **G. Zhao**, **S. Yoon**, P. Habibi, C.S. Hong, S. Li, O.A. Moultos, P. Dey, T.J.H. Vlugt, **Y.G. Chung***
Computational Exploration of Adsorption-based Hydrogen Storage in Mg-alkoxide Functionalized Covalent-Organic Frameworks (COFs): Force-field and Machine Learning Models
ACS Applied Materials & Interfaces, 16, 45, 61995–62009 (2024)

55. **S. Yoon+, M. Hassan+, Y.G. Chung***
Multi-scale computational screening of all-silica zeolites for adsorptive separation of ternary ($H_2S/CO_2/CH_4$) mixtures
Chemical Engineering Journal, 496, 154116 (2024)

54. **G. Zhao, Y.G. Chung***
PACMAN: A Robust Partial Atomic Charge Predicter for Nanoporous Materials based on Crystal Graph Convolution Networks
Journal of Chemical Theory and Computation, 20, 12, 5368–5380 (2024)

53. **Y. Gu+, S. Yoon+,** R. Babu, **Y.G. Chung,** D.W. Park*
Linker-defect assisted catalytic fixation of CO_2 in a dual-linker metal-organic framework
Reaction Kinetics, Mechanisms and Catalysis, 137, 2197–2213 (2024)

52. Z. Cai, W. Li*, **Y.G. Chung**, S. Li, T. Liang, T. Wu
Transfer learning-assisted computational screening of metal-organic frameworks and covalent-organic frameworks for the separation of Xe/Kr noble gas
Separation and Purification Technology, 348, 127752 (2024)

51. D.W. Kim+, **Y. Chen+**, H. Kim, N. Kim, Y.H. Lee, H. Oh, **Y.G. Chung***, C.S. Hong*
High Hydrogen Storage in Trigonal Prismatic Monomer-based Highly Porous Aromatic Frameworks
Advanced Materials, 36, 2401739 (2024)

50. **G. Zhao+, H. Kim+, C.W. Yang, Y.G. Chung***
Leveraging Machine Learning to Predict the Atmospheric Lifetime and the Global Warming Potential of SF_6 Replacement Gases
The Journal of Physical Chemistry A, 128 (12), 2399–2408 (2024)

49. T. Kang, P. Nakhanivej, K.J. Wang, **Y. Chen, Y.G. Chung**, H.S. Park*
Anion storing, oxygen vacancy incorporated perovskite oxide composites for high-performance aqueous dual ion hybrid supercapacitors
Journal of Energy Chemistry, 94, 646–655 (2024)

48. P.Z. Moghadam+, **Y.G. Chung+**, R.Q. Snurr*
Progress toward the computational discovery of new metal–organic framework adsorbents for energy applications
Nature Energy, 9, 121–133 (2024)

47. **Y. Gu[+], S. Yoon[+]**, R. Babu, S.J. Cho**, Y.G. Chung[*]**, D.W. Park[*]
Synthesis and characterization of bimetallic ZnCo-ZIF-71 with defect for an efficient catalytic CO_2 conversion
Korean Journal of Chemical Engineering, 41, 749–761 (2024)

2023 (6)

46. **G. Zhao, Y. Chen, Y.G. Chung[*]**
"High-Throughput, Multiscale Computational Screening of Metal-Organic Frameworks for Xe/Kr Separation with Machine-Learned Parameters"
Industrial & Engineering Chemistry Research, 62 (37), 15176–15189 (2023)

45. S. Han[+], S. Lee[+], D. Kim, J. Seong, A. Sharma, J. Lim**,** S. Jeong**, G. Zhao, Y. Chen**, S.B. Baek, **Y.G. Chung[*]**, M.S. Lah[*]
Construction of Chimeric Metal-Organic Frameworks with Symmetry-Mismatched Building Blocks
Chemistry of Materials, 35(15), 5903–5913 (2023)

44. S.H. Baek, J.S. Byun, H.J. Kim, S.J. Lee, J.M. Park, P. Xiong, **Y.G. Chung[*]**, H.S. Park[*]
Polyoxometalate–polymer hybrid artificial layers for ultrastable and reversible Zn metal anodes
Chemical Engineering Journal, 468, 143644 (2023)

43. G.G. Terrones, **Y. Chen**, A. Datar, L.C. Lin, H.J. Kulik, **Y.G. Chung[*]**
SESAMI APP: An Accessible Interface for Surface Area Calculation of Materials from Adsorption Isotherms
Journal of Open Source Software, 8 (86), 5429 (2023)

42. A. Nandy, S. Yue, C. Oh, C. Duan, G.G. Terrones, **Y.G. Chung**, H.J. Kulik[*]
A database of ultrastable MOFs reassembled from stable fragments with machine learning models
Matter, 6 (5), 1585–1603 (2023)

41. G.H. Lee, E. Jang, T. Lee, Y. Jeong, H. Kim, **S. Lee**, **Y.G. Chung**, K.S. Ha, H. Baik, H.G. Jang, S.J. Cho[*], J.K. Choi[*]
Effective delamination of a layered two-dimensional MCM-22 zeolite: Quantitative insights into the role of the delaminated structure on acid catalytic reactions
Catalysis Today, 411–412, 113856 (2023)

2022 (7)

40. Y. Liu, D. Shen, Z. Tu, L. Xing, **Y.G. Chung**, S. Li[*]
Room-temperature hydrogen storage performance of metal-organic framework/graphene oxide composites by molecular simulations
International Journal of Hydrogen Energy, 47 (97), 41055–41068 (2022)

39. S. Lee[+], I. Kevlishvili[+], H.J. Kulik, H.T. Kim, **Y.G. Chung[*]**, D.Y. Koh[*]
Highly Efficient Bromine Capture and Storage using N-containing Porous Organic Cages
Journal of Materials Chemistry A, 10 (46), 24802–24812 (2022)

38. A. Datar[+], **S. Yoon[+]**, L.C. Lin[*], **Y.G. Chung[*]**
Brunauer–Emmett–Teller Areas from Nitrogen and Argon Isotherms Are Similar
Langmuir, 38 (38), 11631–11640 (2022)

37. **S. Ga, Y.G. Chung[*]**
Recent advances in software tools for adsorption science and engineering
Molecular Systems Design & Engineering, 7 (7), 686–701 (2022)

36. **Y. Gu, A. Bai, S. Yoon,** Y. Choe**, Y.G. Chung[*]**, D.W. Park[*]
Defect-engineered MOF-801 for cycloaddition of CO_2 with epoxides
Journal of Materials Chemistry A, 10 (18), 10051–10061 (2022)

35. S.Y. Kim[+], **S. Han[+], S. Lee,** J.H. Kang, **S. Yoon**, W. Park, M.W. Shin, J. Kim, **Y.G. Chung[*],** Y. S. Bae[*]
Discovery of High-Performing Metal-Organic Frameworks for On-Board Methane Storage and Delivery via LNG–ANG Coupling: High-Throughput Screening, Machine Learning, and Experimental Validation
Advanced Science 9 (21), 2201559 (2022)

34. D. Kurniawan[+], **A. Bai[+]**, O. Setiawan, K.K. Ostrikov, **Y.G. Chung[*]**, W.H. Chiang[*]
Microplasma Band Structure Engineering in Graphene Quantum Dots for Sensitive and Wide-Range pH Sensing
ACS Applied Materials & Interfaces 14 (1), 1670–1683 (2022)

2021 (7)

33. **J. Cha[+], S. Ga[+],** S. Lee, **S. Nam,** Y.S. Bae[*], **Y.G. Chung[*]**
Integrated material and process evaluation of metal-organic frameworks database for energy-efficient SF_6/N_2 separation
Chemical Engineering Journal, 426, 131787 (2021)

32. **S. Yoon, Y.G. Chung[*]**
Limitation of model-based estimations of the hydrogen adsorption capacities in nanoporous materials: a molecular simulation study
Bulletin of the Korean Chemical Society 42 (11), 1539–1548 (2021)

31. H. Seo, **S. Yoon,** B. Oh, **Y.G. Chung,** D.Y. Koh[*]
Shape-Selective Ultramicroporous Carbon Membranes for Sub-0.1 nm Organic Liquid Separation
Advanced Science 8 (17), 2004999 (2021)

30. M. Kang[+], **S. Yoon[+], S. Ga[+],** D.W. Kang, S. Han, J.H. Choe, H. Kim, D.W. Kim, **Y.G. Chung[*],** C.S. Hong[*]
High-Throughput Discovery of $Ni(IN)_2$ for Ethane/Ethylene Separation
Advanced Science 8 (11), 2004940 (2021)

29. P.C. Yeh[+], **S. Yoon[+],** D. Kurniawan, **Y.G. Chung[*],** W.H. Chiang[*]
Unraveling the fluorescence quenching of colloidal graphene quantum dots for selective metal ion detection
ACS Applied Nano Materials 4 (6), 5636–5642 (2021)

28. **H. Kwon,** K.C. Oh, Y. Choi, **Y.G. Chung,** J. Kim[*]
Development and application of machine learning-based prediction model for distillation column
International Journal of Intelligent Systems 36 (5), 1970–1997 (2021)

27. D.H. Song, J.H. Kang, H.S. Park, **Y.G. Chung,** H. Song[*]
Simultaneous Removal of NO and SO_2 using Microbubble and Reducing Agent
Clean Technology 27 (4), 341–349 (2021)

2020 (3)

26. A. Datar, **Y.G. Chung[*],** L.C. Lin[*]
Beyond the BET analysis: The surface area prediction of nanoporous materials using a machine learning method
The Journal of Physical Chemistry Letters 11 (14), 5412–5417 (2020)

25. **H. Kwon,** K.C. Oh, **Y.G. Chung,** H. Cho, J. Kim[*]
Development of machine learning model for predicting distillation column temperature
Applied Chemistry for Engineering 31 (5), 520–525 (2020)

24. **S. Kang, Y.G. Chung,** J.H. Kang, H. Song[*]
CO_2 absorption characteristics of amino group functionalized imidazolium-based amino acid ionic liquids
Journal of Molecular Liquids 297, 111825 (2020)

2019 (7)

23. C.V. Nguyen[+], **S. Lee[+], Y.G. Chung[*],** W.H. Chiang[*], K.C.W. Wu[*]
Synergistic effect of metal-organic framework-derived boron and nitrogen heteroatom-doped three-dimensional porous carbons for precious-metal-free catalytic reduction of nitroarenes
Applied Catalysis B: Environmental 257, 117888 (2019)

22. **Y.G. Chung[+*],** E. Haldoupis[+], B.J. Bucior[+], M. Haranczyk, **S. Lee,** H. Zhang, K.D. Vogiatzis, M. Milisavljevic, S. Ling, J.S. Camp, B. Slater, J.I. Siepmann[*], D.S. Sholl[*], R.Q. Snurr[*]
Advances, updates, and analytics for the computation-ready, experimental metal-organic framework database: CoRE MOF 2019
Journal of Chemical & Engineering Data 64 (12), 5985–5998 (2019)

21. A. Sturluson, M.T. Huynh, A.R. Kaija, C. Laird, **S. Yoon,** F. Hou, Z. Feng, C.E. Wilmer[*], Y.J. Colón[*], **Y.G. Chung[*],** D.W. Siderius[*], C.M. Simon[*]
The role of molecular modelling and simulation in the discovery and deployment of metal-organic frameworks for gas storage and separation
Molecular Simulation, 45 (14–15), 1082–1121 (2019)

20. S.I. Kim[+], **S. Lee[+], Y.G. Chung[*],** Y.S. Bae[*]
The Origin of p-Xylene Selectivity in a DABCO Pillar-Layered Metal-Organic Framework: A Combined Experimental and Computational Investigation
ACS Applied Materials & Interfaces 11 (34), 31227–31236 (2019)

19. P. Sinha[+], A. Datar[+], **C. Jeong,** X. Deng, **Y.G. Chung[*],** L.C. Lin[*]
Surface area determination of porous materials using the Brunauer–Emmett–Teller (BET) method: limitations and improvements
The Journal of Physical Chemistry C 123 (33), 20195–20209 (2019)

18. K.T. Leper[i+], **Y.G. Chung[+],** F. You[*], R.Q. Snurr[*]
Development of a General Evaluation Metric for Rapid Screening of Adsorbent Materials for Postcombustion CO_2 Capture
ACS Sustainable Chemistry & Engineering 7 (13), 11529–11539 (2019)

17. J.H. Lee, S. Jeoung, **Y.G. Chung[*],** H.R. Moon[*]
Elucidation of flexible metal-organic frameworks: Research progresses and recent developments
Coordination Chemistry Reviews 389, 161–188 (2019)

2018 (2)

16. G.G. Choi, J.F. Kurisingal, **Y.G. Chung[*]**, D.W. Park[*]
Two dimensional Zn-stilbenedicarboxylic acid (SDC) metal-organic frameworks for cyclic carbonate synthesis from CO_2 and epoxides
Korean Journal of Chemical Engineering 35, 1373–1379 (2018)

15. G.S. Jeong, A.C. Kathalikkattil, R. Babu, **Y.G. Chung,** D.W. Park[*]
Cycloaddition of CO_2 with epoxides by using an amino-acid-based Cu (II)–tryptophan MOF catalyst
Chinese Journal of Catalysis 39 (1), 63–70 (2018)

2017 (5)

14. S. Li, **Y.G. Chung**, C.M. Simon, R.Q. Snurr[*]
High-Throughput Computational Screening of Multivariate Metal-Organic Frameworks (MTV-MOFs) for CO_2 Capture
The Journal of Physical Chemistry Letters 8 (24), 6135–6141 (2017)

13. **Y. G. Chung[+],** P. Bai[+], M. Haranczyk, K. T. Leperi, P. Li, H. Zhang, T.C. Wang, T. Duerinck, F. You, J. T. Hupp, O. K. Farha, J. I. Siepmann, R.Q. Snurr[*]
Computational screening of nanoporous materials for hexane and heptane isomer separation
Chemistry of Materials 29 (15), 6315–6328 (2017)

12. W. Li, Z. Rao, **Y.G. Chung,** S. Li*
    The Role of Partial Atomic Charge Assignment Methods on the Computational Screening of Metal-Organic Frameworks for CO_2 Capture under Humid Conditions
    ChemistrySelect 2 (29), 9458–9465 (2017)

11. D. Nazarian, J.S. Camp, **Y.G. Chung,** R.Q. Snurr, D.S. Sholl*
    Large-scale refinement of metal-organic framework structures using density functional theory
    Chemistry of Materials 29 (6), 2521–2528 (2017)

10. K.M. Bhin, J. Tharun, K.R. Roshan, D.W. Kim, **Y.G. Chung,** D.W. Park*
    Catalytic performance of zeolitic imidazolate framework ZIF-95 for the solventless synthesis of cyclic carbonates from CO_2 and epoxides
    Journal of CO_2 Utilization 17, 112–118 (2017)

2016 (2)

9. **Y.G. Chung+,** D.A. Gómez-Gualdrón+, P. Li, K.T. Leperi, P. Deria, H. Zhang, N.A. Vermeulen, J.F. Stoddart, F. You, J.T. Hupp, O.K. Farha, R.Q. Snurr*
    In silico discovery of metal-organic frameworks for precombustion CO_2 capture using a genetic algorithm
    Science Advances, 2 (10), e1600909 (2016)

8. Song Li, **Y.G. Chung,** R.Q. Snurr*
    High-Throughput Screening of Metal-Organic Frameworks for CO_2 Capture in the Presence of Water
    Langmuir 32 (40), 10368–10376 (2016)

2015 (2)

7. P. Deria, **Y.G. Chung**, R.Q. Snurr, J.T. Hupp*, O.K. Farha*
    Water stabilization of Zr_6-based metal-organic frameworks via solvent-assisted ligand incorporation
    Chemical Science 6 (9), 5172–5176 (2015)

6. C. M. Simon, J. Kim, D.A. Gomez-Gualdron, J.S. Camp, **Y.G. Chung**, R.L. Martin, R. Mercado, M.W. Deem, D. Gunter, M. Haranczyk, D.S. Sholl, R.Q. Snurr*, B. Smit*
    The materials genome in action: identifying the performance limits for methane storage
    Energy & Environmental Science, 8 (4), 1190–1199 (2015)

2014 (1)

5. **Y.G. Chung**, J. Camp, M. Haranczyk, B.J. Sikora, W. Bury, V. Krungleviciute, T. Yildirim, O.K. Farha, D.S. Sholl*, R.Q. Snurr*
    Computation-ready, experimental metal-organic frameworks: A tool to enable high-throughput screening of nanoporous crystals
    Chemistry of Materials 26 (21), 6185–6192 (2014)

2012 (4)

4. **Y.G. Chung**, D.J. Lacks*
    Atomic mobility in strained glassy polymers: The role of fold catastrophes on the potential energy surface
    Journal of Polymer Science Part B: Polymer Physics 50 (24), 1733–1739 (2012)

3. **Y.G. Chung**, D.J. Lacks*
    Atomic mobility in a polymer glass after shear and thermal cycles
    The Journal of Physical Chemistry B 116 (48), 14201–14205 (2012)

2. **Y.G. Chung**, D.J. Lacks*
    How deformation enhances mobility in a polymer glass
    Macromolecules 45 (10), 4416–4421 (2012)

1. **Y.G. Chung**, D.J. Lacks*
   Sheared polymer glass and the question of mechanical rejuvenation
   The Journal of Chemical Physics 136 (12), 124907 (2012)

Patents and Registered Software

- **Granted Korean patent.** KR 10-2707528; application no. 10-2022-0085362.
- **Pending Korean patent applications.** 10-2022-0059393 and 10-2023-0061292.
- **Registered software.** 2 registrations.

Presentations

Department & Research Groups (invited)

Feb. 2026	AI and Computational Chemistry Division, Korea Institute of Energy Research, Daejeon Korea
Jan. 2026	Department of Chemical & Biomolecular Engineering, Yonsei University, Seoul Korea
Jul. 2025	Department of Energy Engineering, Daegu Gyeongbuk Institute of Science and Technology (DGIST), Daegu Korea
Apr. 2025	Department of Chemistry, Pohang University of Science and Technology, Pohang Korea
Feb. 2025	Department of Chemical Engineering, National Taiwan University of Science and Technology, Taipei Taiwan
Feb. 2025	Department of Chemical Engineering, National Taiwan University, Taipei Taiwan
Feb. 2025	The Sargent Centre for Process Systems Engineering, Imperial College London, London UK
Feb. 2025	Cambridge Crystallographic Data Centre, Cambridge UK
Feb. 2025	Department of Chemical Engineering, University College London, London UK
Oct. 2024	Department of Chemical Engineering, Texas Tech University, Lubbock TX USA
Apr. 2024	Department of Chemistry, Sungkyunkwan University, Suwon, Korea
May 2023	School of Chemical Engineering, Sungkyunkwan University, Suwon, Korea
Nov. 2022	Department of Chemistry, Hanyang University, Seoul, Korea
Jul. 2022	Process & Energy, Delft University of Technology, Delft, the Netherlands
Jul. 2022	Computational Chemistry Group Meeting, Universiteit van Amsterdam, Amsterdam, The Netherlands
Apr. 2022	Earth & Environmental Engineering, Lenfest Center for Sustainable Energy, Columbia University, New York, NY, USA
Apr. 2022	Department of Chemical Engineering, MIT, Cambridge, MA USA
Mar. 2022	Materials Colloquium, Department of Chemical Engineering, University of Massachusetts - Amherst, Amherst, MA USA
Feb. 2022	Department of Chemical & Biomolecular Engineering, Case Western Reserve University, Cleveland, OH USA
May 2021	Department of Chemical Engineering, Konkuk University, Seoul, Korea (zoom)
Apr. 2021	Department of Chemistry, Korea University, Seoul, Korea (zoom)
Mar. 2021	Department of Chemical and Biomolecular Engineering, Yonsei University, Seoul, Korea (zoom)
Jul. 2019	Environmental Engineering, Kyunghee University, Suwon, Korea
Mar. 2018	Department of Chemical Engineering, University of Ulsan, Ulsan, Korea
May 2017	Department of Chemistry, UNIST, Ulsan, Korea
Mar. 2017	Department of Chemistry, Pohang University of Science and Technology, Pohang Korea
Jan. 2016	Department of Chemical and Biomolecular Engineering, Case Western Reserve University, Cleveland, OH USA
Mar. 2015	Department of Chemical Engineering, University of Illinois - Chicago, Chicago, IL USA

International Conferences & Workshops (invited)

Dec. 2026	2026 Annual Meeting of TwIChE, Feng Chia University, Taichung, Taiwan (scheduled)
Nov. 2026	Special Session of Prof. Randall Snurr's 60th Birthday II, AIChE Annual Meeting 2026, Minneapolis, MN, USA (scheduled)
Nov. 2026	Nanomaterials for CO_2 conversion and H_2 generation, AIChE Annual Meeting 2026, Minneapolis, MN, USA (scheduled)
Oct. 2026	Pioneering Next-Generation Porous Materials and Scientific Progress Through Artificial Intelligence Innovations, Korean Chemical Society (KCS), Suwon, Korea (scheduled)
Jun. 2026	Chemistry with AI for Carbon Neutrality 2026 (C-AICN 2026), Higashi Hiroshima, Japan
May 2026	Canadian Societies for Chemistry and Chemical Engineering 2026 Conferences and Exhibition (x2026), Toronto, Canada
Nov. 2025	2025 Annual Meeting of TwIChE, Taiwan-Japan-Korea (TJK) Symposium, National Cheng Kung University, Tainan, Taiwan
Oct. 2024	AI for Materials Chemistry, Korean Chemical Society, Daegu, Korea
Sep. 2024	"Machine Learning", Thermodynamics 2024, Delft, the Netherlands
Sep. 2024	iRASPA/RASPA Workshop 2024, Delft, the Netherlands
Apr. 2024	Symposium on Computational Chemistry & Artificial Intelligence for Advanced Catalyst and Materials Design, KIChE, Jeju Island, Korea
Oct. 2023	PSK-LG Chemical Special Session, Korea Polymer Society, Jeju Island, Korea
Oct. 2021	KIChE Fall Meeting and International Symposium on Separation Technology for Carbon Neutrality, Busan, Korea
Sep. 2021	Clean Technology Fall Meeting, Yeosu, Korea
Dec. 2019	Division of Thermodynamics KIChE Winter Workshop, Yonsei University, Seoul, Korea
Dec. 2018	The 2nd Conference on Advanced Separation Science and Engineering (CASSE), Hanoi, Vietnam
Apr. 2018	Korean Institute of Chemical Engineers (KIChE) Symposium on Applications of Molecular Modeling in New and Renewable Energy Fields, Changwon, Korea
Mar. 2018	American Chemical Society (ACS) Sustainable Chemistry & Engineering Lectureship Awards: Symposium in honor of Fengqi You, New Orleans, USA
Nov. 2017	Korea-Japan-Taiwan (KJT) Chemical Engineering Conference, Busan, Korea
Nov. 2017	BIOVIA User Group Meeting, Seoul, Korea
Nov. 2017	The 4th International Symposium on Hybrid Materials and Processing, Busan, Korea
Aug. 2017	US-Korea Conference (UKC), Washington D.C., USA
May 2017	Korea Carbon Society Spring Meeting, Changwon, Korea
Feb. 2017	Vietnam-Korea Chemical Engineering Joint Symposium, Nha-trang, Vietnam
Dec. 2016	MOF and Beyond Workshop, Daejeon, Korea
Oct. 2014	Nanoporous Materials Genome All-Hands Meeting, St. Paul, Minnesota USA
Jul. 2014	Northwestern/UOP Molecular Modeling Workshop, Evanston Illinois, USA
Nov. 2013	Nanoporous Materials Genome Center, University of Minnesota – Twin Cities, Minneapolis, MN USA
Oct. 2013	Nanoporous Materials Genome All-Hands Meeting, Berkeley, CA USA
Jun. 2012	6th Simulators Meeting, Carnegie Mellon University, Pittsburgh, PA USA
May 2012	ACS 10th National Graduate Research Polymer Conference, Cleveland OH USA
Oct. 2011	AIChE Annual Meeting, Minneapolis MN USA
Oct. 2011	83rd Annual Meeting of the Society of Rheology, Cleveland OH USA
Oct. 2010	82nd Annual Meeting of the Society of Rheology, Santa Fe, NM USA
Jun. 2010	4th Simulators Meeting, Carnegie Mellon University, Pittsburgh, PA USA
May 2010	Midwest Thermodynamics and Statistical Mechanics Conference, University of Notre Dame, South Bend IN USA

Research Funding

Approximately US$2.31 million allocated to my research group from national agencies and industry. Industrial support includes KEPCO, KHNP, and LG Chem, with additional in-kind GPU support from NVIDIA.

Active

- **National Research Foundation of Korea (sole PI)** **2024–2029**
  Development of physics-informed machine learning interatomic potential towards integrated material-process investigation for Xe-selective MOF
  Total funding: $800k
- **National Research Foundation of Korea (co-PI)** **2025–2026**
  Materials and Systems Modeling for Light and Ultrastable low-density Porous Materials for Hydrogen Storage
  Total funding: $700k (PI: C.S. Hong, Korea University); $160k to Y.G. Chung

Completed

- **National Research Foundation of Korea (co-PI)** **2021–2024**
  Materials and Systems Modeling for Light and Ultrastable low-density Porous Materials for Hydrogen Storage
  Total funding: $800k (PI: C.S. Hong, Korea University); $200k to Y.G. Chung
- **National Research Foundation of Korea (co-PI)** **2021–2024**
  Development of modeling and experimentation for the adsorptive separation processes for CO capture
  Total funding: $600k (PI: Ki Bong Lee, Korea University); $200k to Y.G. Chung
- **Korea Electric Power Corporation (co-PI)** **2021–2024**
  Computational Exploration of SF_6 Replacement Gases
  Total funding: $600k ($250k to Y.G. Chung)
- **Korea Hydro & Nuclear Power (co-PI)** **2021–2023**
  Production of High-purity Hydrogen via Sorption-Enhanced System
  Total funding: $250k ($120k to Y.G. Chung)
- **Korea Evaluation Institute of Industrial Technology (co-PI)** **2020–2021**
  Green Ammonia for Hydrogen Storage
  Group allocation: approximately $20k
- **Korea Institute of Industrial Technology (sole PI)** **2020**
  Computational Screening of High-Performance Zeolites for Pre-treatment of Natural Gas
  Group allocation: approximately $20k
- **National Research Foundation of Korea (sole PI)** **2020–2024**
  Modeling and Experimentation for Nanoporous Materials Characterization and the BET Theory
  Total funding: $350k
- **Korea Institute of Industrial Technology (sole PI)** **2020–2021**
  DFT Investigation of Olefin Synthesis
  Total funding: $80k
- **LG Chem (sole PI)** **2018**
  Using Molecular Simulation for Gas Purification Adsorbent Discovery
  Total funding: $10k
- **National Research Foundation of Korea (sole PI)** **2016–2019**
  Materials Genome Approach to Discovery of Novel Adsorbent Materials for CO_2/SO_2 Separation and Purification
  Total funding: $100k

Supercomputing Allocation

- **Korea Supercomputing Center** **2016–2026**
  Periodic CPU and GPU allocations through Korea Supercomputing Center Proposals
- **ASCR Leadership Computing Challenge (ALCC) Allocation (U.S. DOE)** **2018**
  58 million process hours (PI: J. Ilja Siepmann; co-PI: Y.G. Chung)
- **ASCR Leadership Computing Challenge (ALCC) Allocation (U.S. DOE)** **2017**
  146 million process hours (PI: J. Ilja Siepmann; co-PI: Y.G. Chung)

Equipment Grants

- **NVIDIA Academic Grant Program** **Sep. 2026**
  GPU-Accelerated MLIP-Ising Simulation of UiO-66 Defect Ensemble
  In-kind award: four NVIDIA RTX PRO 6000 Server Edition GPUs.

Professional Society Affiliations

American Institute of Chemical Engineers (2013 – Present)
- Computational Molecular Science and Engineering Forum (CoMSEF)

American Chemical Society (2015 – Present)
- Chemical Information Division
- Computers in Chemistry Division
- Physical Chemistry Division
- CATL Division

International Adsorption Society (2018 – Present)
- Education Committee

Korean Institute of Chemical Engineers (2016 – Present)
- Thermodynamics and Molecular Simulation Division
- Separation Technology Division

Korean Society of Industrial and Engineering Chemistry (2016 – Present)
- AI and Computational Science Division

Korean Chemical Society (2016 – Present)
- Materials Chemistry Division

Professional and Faculty Services & Activities

Editorial Activities

- Associate Editor, *The Canadian Journal of Chemical Engineering* 2026 – Present
- Editorial Advisory Board, *Langmuir* (ACS Publication) 2024 – Present
- Editorial Board Member, *Main Group Chemistry* (IOP Publication) 2022–2025
- Editor, *News & Information for Chemical Engineers* 2020–2021

Conference and Workshop Organizer

- Organizing Committee Member, PBAST10
  10th Pacific Basin Conference on Adsorption Science and Technology
  Yonsei University, Seoul, Korea May–Jun. 2027
- Organizer, International Adsorption Society (IAS) Asia-Pacific Webinar Series
  Online 2023, 2024, 2026
- Co-organizer, KIChE Fall Symposium
  "Computational Chemistry"
  Daejeon, Korea (South) Oct. 2023
- Co-organizer, MOF and Beyond Workshop
  Daejeon, Korea (South) Dec. 2017
- Co-organizer, KJT Chemical Engineering Conference
  Busan, Korea (South) Nov. 2017

Sessions Chaired or Co-chaired at Major International Conferences

- Co-Chair, 2026 AIChE Annual Meeting Nov. 2026 (scheduled)
  "Synthesis and Application of Inorganic Materials I: Synthesis"
  Minneapolis, MN, USA
- Co-organizer, 2026 KSIEC Annual Meeting Oct. 2026 (scheduled)
  "AI-Driven Computational Industrial Chemistry for Advanced Materials Development"
  Busan, Korea
- Chair, 2025 AIChE Annual Meeting
  "MOFs, COFs, and Porous Materials"
  Boston, MA, USA Nov. 2025
- Chair, Thermodynamics 2024
  "Porous/confined media"
  Delft, the Netherlands Sep. 2024
- Chair, 2023 Ji-San-Hak Busan
  "Future Technology Session"
  Busan, Korea Oct. 2023
- Co-chair, 2022 Asian Crystallographic Association Conference
  "Database Development and Machine Learning for Crystal Structures"
  Jeju Korea Oct. 2022
- Co-chair, 2017 AIChE Annual Meeting
  "Accelerated Discovery and Development of Inorganic Materials"
  "MOFs, COFs, and Porous Polymer Materials I: Synthesis"
  "MOFs, COFs, and Porous Polymer Materials II: Applications"
  Minneapolis, MN USA Nov. 2017

Professional Societies

KIChE (Korean Institute of Chemical Engineers)

- Member, International Relations Committee 2025–2026

- Secretary, Thermodynamics and Molecular Simulation Division 2020–2024
- Secretary, Separation Technology Division 2016–2019
- Member, Research and Development Committee 2022–2023
- Member, International Relations Committee 2019–2022
- Member, 50th Board of the KIChE 2019

KSIEC (Korean Society of Industrial and Engineering Chemistry)

- Secretary, AI and Computational Science Division 2026–2027

International Adsorption Society (IAS)

- Member, PhD Thesis Award Committee 2024
- Member, International Adsorption Society (IAS) Education Committee 2021 – Present

University & Department

Department

- Department Chair, Chemical & Biomolecular Engineering Mar. 2023 – Feb. 2025
- Division Chair, Graduate School of Chemical Engineering Mar. 2023 – Feb. 2024
- Principal Investigator, University Innovation on Undergraduate Teaching 2019–2022
- Member, Faculty Search Committee 2017–2021

College of Engineering

- Member, Faculty Compensation Committee 2018, 2019, 2026
- Member, Education Reform Committee Mar. 2022 – Feb. 2024
- Liaison, Semiconductor Convergence Major 2023

University College

- Department Chair, AI Convergence Computational Science Mar. 2026 – Present
- Member, Faculty Search Committee 2025
- Chair, Faculty Search Committee 2026

University

- Chair, AIX-Computational Science Curriculum TF May 2025 – Aug. 2025

Proposal Reviewer

- National Research Foundation of Korea 2021–2026
- Korea Institute of Energy Technology Evaluation and Planning 2017, 2021, 2025
- Korea Technology Credit Bureau Co. LTD 2024
- ACS Petroleum Research Fund 2021, 2023, 2025, 2026
- Swiss National Science Foundation 2023–2025
- Samsung Future Technology Center 2017
- Korea Supercomputing Center 2018–2021

Journal Reviewing

Reviewed more than 400 manuscripts for more than **80** journals, including:

ACS

Accounts of Chemical Research; ACS Applied Energy Materials; ACS Applied Materials & Interfaces; ACS Applied Nano Materials; ACS Central Science; ACS Materials Letters; ACS Nano; ACS Omega; ACS Sensors; ACS Sustainable Chemistry & Engineering; Chem & Bio Engineering; Chemical Reviews; Chemistry of Materials; Crystal Growth & Design; Energy & Fuels; Environmental Science & Technology; Industrial & Engineering Chemistry Research; Inorganic Chemistry; JACS Au; Journal of Chemical Information and Modeling; Journal of the American Chemical Society (JACS); Langmuir; The Journal of Physical Chemistry C; The Journal of Physical Chemistry Letters.

Elsevier

Applied Catalysis B: Environmental; Chemical Engineering Journal; Chemical Engineering Science; Composites Part B; Computational and Theoretical Chemistry; Computational Materials Science; Computers & Chemical Engineering; Coordination Chemistry Reviews; eScience; Fuel; Inorganic Chemistry Communications; International Journal of Hydrogen Energy; Journal of Cleaner Production; Journal of Environmental Chemical Engineering; Separation and Purification Technology.

RSC

Chemical Communications; Chemical Science; Digital Discovery; Industrial Chemistry & Materials; Journal of Materials Chemistry A; Journal of Materials Chemistry B; Journal of Materials Chemistry C; Materials Advances; Molecular Systems Design & Engineering; Nanoscale; Physical Chemistry Chemical Physics; RSC Advances; Sustainable Energy & Fuels.

Society Journals

Adsorption; AIChE Journal; Bulletin of the Korean Chemical Society; Journal of the Taiwan Institute of Chemical Engineers; Korean Journal of Chemical Engineering; Microporous and Mesoporous Materials; The Canadian Journal of Chemical Engineering.

Wiley

Advanced Functional Materials; Advanced Materials; Advanced Science; Angewandte Chemie; Chemical Engineering & Technology; ChemistrySelect; ChemSusChem; EcoEnergy; Energy & Environmental Materials; International Journal of Quantum Chemistry.

Nature Portfolio

Nature Communications; Nature Computational Science; Nature Energy; npj Computational Materials; Scientific Reports.

Springer Nature

Discover Nano; Nano-Micro Letters; Science China Chemistry.

APS

Physical Review Letters; PRX Energy.

Taylor & Francis

Molecular Simulation; Separation Science and Technology.

AAAS

Science Advances.

AIP

Journal of Chemical Physics.

Research Mentoring

Graduate Students

Current

2025 – Present **Changdon Shin**

2025 – Present **Pengyu Zhao**

2025 – Present **Siah Thong**

2024 – Present **Taekgi Lee**

- 2024 Samsung AI Challenge, 3rd place ($2,500 prize)

2022 – Present **Hassan Muhammad**

- 2024 Best Poster Award, Separation Technology Division, KIChE
- 2023 Best Poster Award, BKFOUR21 Workshop PNU ChBE

2020 – Present **Yu Chen**

- 2024 Best Poster Award, Busan-Gyeongnam Region, KIChE
- 2023 Best Oral Presentation Award, Busan-Gyeongnam Region, KIChE
- 2023 Best Oral Presentation Award, BKFOUR21 Workshop PNU ChBE

Past

2019–2026 **Sunghyun Yoon**; *Ph.D.; Postdoctoral Researcher, PNU*
- 2024 Best Poster Award, Busan-Ulsan-Gyeongnam Region, KSIEC
- 2024 Excellent Oral Presentation Award, The Korean Society of Clean Technology
- 2023 PNU Research Award, PNU
- 2023 Best Poster Award, Separation Technology Division KIChE
- 2022 Winner Oral Presentation BKFOUR21 Workshop PNU ChBE

2024–2026 **Haewon Kim**; *M.S.; Engineer, SK hynix*
- 2024 Best Poster Award, Busan-Gyeongnam Region, KIChE
- 1st Medical AI Competition, Grand Prize Winner ($4,000 prize)

2020–2025 **Guobin Zhao**; *Ph.D.; Postdoctoral Fellow, NUS*
- 2024 Best Poster Award, Busan-Gyeongnam Region, KIChE
- 2024 Best Poster Award, Busan-Ulsan-Gyeongnam Region, KSIEC

2019–2022 **Seungyun Han**

2019–2021 **Jaehoon Cha**

2019–2022 **Dong-Hoon Song**; *M.S. (affiliated student co-advised with Hojun Song)*

2019–2021 **Hyuck Won Kwon**; *M.S. (affiliated student co-advised with Junghwan Kim)*

2016–2019 **Seulchan Lee**; *B.S./M.S. Engineer, SK Innovation*
- 2019 Best Poster Award, KCS
- 2019 Best Poster Award, KSIEC
- 2018 Best Poster Award, Separation Technology Division, KIChE

2018–2020 **Sehee Kang**; *M.S. (affiliated student co-advised with Hojun Song)*

2018–2020 **Hyun Mo Je**; *M.S. (affiliated student co-advised with Jungkyu Roh)*

2017–2019 **Soo Myung Nam**; *M.S. Engineer, Hankuk Paper*

Postdoctoral Researchers

2022–2023 **Dr. Changwon Yang**; *Senior Scientist, Korean Quantum Computing Inc.*

2021–2022 **Dr. Yunjang Gu**; *Research Scientist, Nam Hae Chemicals Ltd.*

2020–2022 **Dr. Seongbin Ga**; *Faculty, Chemical Engineering, University of Ulsan*
- 2021 NRF Sejong Fellowship

2020–2022 **Dr. Anjali Bai**; *Postdoc., National University of Singapore*

Undergraduate Students

2025–2026 **Hyunji Kim**

2025 **Nahyeon Lee**

2025 **Dahee Kang**

2025 **Sungeun Hong***; Ph.D. program, NUS, Singapore*

2024–2025 **Jaehoon Lee**
- 2024 Samsung AI Challenge, 3rd place ($2,500 prize)

2024 **Chaeyoung Park**

2024 **Younseo Yang**

2023 **Haewon Kim**; continued as an M.S. student

2023 **Yeji Lee**; KCC

2021 **Nayoung Kim**

2021 **Chaewon Park**

2020 **Hyeji Kim**

2019 **Byungkwan Sung**; Kolon Industries

2018–2020 **Seungyun Han**; continued as an M.S. student

2018–2019 **Juyong Kim**; Samsung Display

2018–2019 **Sunghyun Yoon**; continued as an M.S./Ph.D. student

2017–2018 **Nayoung Seo**; SK pucore

2016–2017 **Jinwook Hwang**; Samsung Engineering

2016–2017 **Hyeji Lee**; Hanwha Energy

2016–2019 **Seulchan Lee**; continued as a B.S./M.S. student

2018 **Geonjong Kim**; SK hynix

2018–2019 **Chungsik Jeong**

Teaching Activities

UG = undergraduate; G = graduate. Courses are grouped by year and semester; enrollment is per offering.

Year & Semester	Level	Course Name	Enrollment
2026 Spring	UG	Artificial Intelligence for Materials and Chemicals	13
2026 Spring	G	Molecular Thermodynamics and Statistical Mechanics	4
2025 Fall	UG	Technical Writing for Chemical Engineers	24
2025 Fall	UG	Current Events in Chemical & Biomolecular Engineering	27
2025 Spring	G	Applied Molecular Modeling	7
2025 Spring	UG	Introduction to Computational Nanoscience and Engineering	14
2024 Fall	UG	Current Events in Chemical & Biomolecular Engineering	44
2024 Spring	UG	Artificial Intelligence for Materials and Chemicals	6
2023 Fall	UG	Separation Process	30
2023 Spring	UG	Chemical Engineering Semiconductor	13
2022 Fall	UG	Introduction to Chemical Engineering Data Science	40
2022 Fall	UG	Separation Process	53
2021 Spring	UG	Engineering Mathematics	61
2021 Spring	UG	Introduction to Engineering Computing	61
2020 Fall	G	Numerical & Statistical Analysis	7
2020 Fall	UG	Numerical Analysis	21
2020 Spring	G	Advanced Chemical Engineering Thermodynamics	4
2020 Spring	UG	Engineering Mathematics	71
2019 Fall	G	Advanced Numerical Analysis	8
2019 Fall	UG	Numerical Analysis	23
2019 Spring	G	Fundamentals of Molecular Modeling	13
2019 Spring	UG	Creative Research	26
2019 Spring	UG	Engineering Mathematics	47
2018 Fall	UG	Separation Process	55
2018 Fall	UG	Numerical Analysis	33
2018 Spring	UG	Creative Research	24
2018 Spring	UG	Advanced Chemical Engineering Thermodynamics	2
2018 Spring	UG	Engineering Mathematics	62
2017 Fall	G	Advanced Catalyst Engineering	6
2017 Fall	UG	Catalyst Engineering	32
2017 Fall	UG	Separation Process	38
2017 Spring	UG	Creative Research	28
2017 Spring	G	Advanced Chemical Engineering Thermodynamics	10
2017 Spring	UG	Heat and Mass Transfer	52
2017 Spring	UG	Engineering Mathematics	72
2016 Fall	G	Advanced Numerical Methods	5
2016 Fall	UG	Separation Process	53
2016 Fall	UG	Introduction to Engineering	58
2016 Spring	G	Advanced Chemical Engineering Thermodynamics	8
2016 Spring	UG	Chemical Engineering Thermodynamics	73
2016 Spring	UG	Engineering Mathematics	66