Yongchul G. Chung

Professor

- College of Engineering
  - School of Chemical Engineering (BK21 FOUR)
  - Department of Chemical and Biomolecular Engineering
- (affiliated) Graduate School of Data Science
- (affiliated) University College
  - School of Transdisciplinary Engineering, AI Convergence Computational Science

Contact

address	2, Busandaehak-ro 63beon-gil, Busan 46241 Korea (South)
phone	+82 51-510-3757
email	drygchung@gmail.com
website	https://sites.google.com/view/mtap-lab

Current Research Interests

- AI for Materials and Chemical Discovery
- Digital Reticular Chemistry and Engineering
- Quantum

Representative Publications

- MOFClassifier: A Machine Learning Approach for Validating Computation-Ready Metal-Organic Frameworks, *Journal of the American Chemical Society*, **2025 (corresponding author)**
- CoRE MOF DB: a curated experimental metal-organic framework database with machine-learned properties for integrated material-process modeling, *Matter*, **2025 (corresponding author)**
  *** Highly Cited Paper (September/October 2025);** top 1% of academic field of **Materials Science**
- Progress toward the computational discovery of new metal-organic framework adsorbents for energy applications, *Nature Energy*, **2024 (co-1st author)**
  * **Highly Cited Paper (September/October 2025);** top 0.1% of academic field of **Engineering**
- Advanced, Updates, and Analytics for the Computation-Ready, Experimental Metal-Organic Framework Database: CoRE MOF 2019
  Journal of Chemical and Engineering Data, **2019 (corresponding author)**
  *** Highly Cited Paper (September/October 2025);** top 1% of academic field of **Chemistry**
- Surface Area Determination of Porous Materials Using the Brunauer-Emmett-Teller (BET) Method: Limitations and Improvements
  Journal of Physical Chemistry C, **2019 (corresponding author)**
  *** Highly Cited Paper (September/October 2025);** top 1% of academic field of **Chemistry**

Academic 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 – current	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 – current	Department Chair Artificial Intelligence (AI) Convergence Computational Science School of Transdisciplinary Engineering Pusan National University
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
Sept. 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 & 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	*Molecular Systems Design & Engineering* Emerging Investigator
	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

Summary of Research Performance (from 2020 – 2026)

Field-Weighted Citation Impact (FWCI): 2.08

Citations per Publication: 26.8

Publications (**bold** = group members, * = corresponding, $^{+}$ = co-first)

Google Scholar citation (as of 2026/06/15: 6,219)

Submitted/Under Review/Revision

. S. Lee, **T. Lee, A. Jo, J. Yu, I.S. Kim, **Y.G. Chung***, S. Ahn*
Local environmental modification of Ti-SiO2 via terminal alcohols grafting for liquid-phase cyclohexene epoxidation with H2O2

. 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 (6)

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)
https://doi.org/10.1002/ijch.70028
- Invited contribution to the special collection **"Reticular Chemistry and New Materials"** dedicated to Prof. Omar Yaghi's **2025 Nobel Prize in Chemistry**

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

Journal of Chemical Physics, 164, 114502 (2026)
https://doi.org/10.1063/5.0307954

70. **M. Hassan**, **C. Shin**, **T. 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)
https://doi.org/10.1016/j.cej.2026.175117

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, (2026)
https://doi.org/10.1002/aenm.202504672

68. **M. Hassan**, **S. Yoon**, **Y. Chen**, P. Kim, H. Yun, H.T. Kwon, Y.S. Bae, C.Y. Yoo, C.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)
https://doi.org/10.1016/j.cpc.2025.109944

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 System Design & Engineering, 11, 181 – 194 (2026)
https://doi.org/10.1039/D5ME00131E

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)
https://doi.org/10.1021/acs.iecr.5c03794

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 Isotherm
Langmuir, 41, 44, 29851 – 20858 (2025)
https://doi.org/10.1021/acs.langmuir.5c04369

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 using pressure/vacuum swing adsorption process
Separation and Purification Technology, 378, 3, 1347866 (2025)
https://doi.org/10.1016/j.seppur.2025.134786

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)
https://doi.org/10.1021/jacs.5c10126

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)
https://doi.org/10.1016/j.cej.2025.164419

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)
https://doi.org/10.1016/j.memsci.2025.124298

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)
https://doi.org/10.1016/j.matt.2025.102140

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)
https://doi.org/10.1016/j.cej.2025.160517

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)
https://doi.org/10.1002/adfm.202417288

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)
https://doi.org/10.1002/adfm.202412577

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)
https://doi.org/10.1021/acsami.4c11953

55. **S. Yoon⁺, M. Hassan⁺, Y.G. Chung***
Multiscale computational modeling and process economic optimization of all-silica zeolites for adsorptive separation of ternary ($H_2S/CO_2/CH_4$) gas mixture
Chemical Engineering Journal, 496, 154116, (2024)
https://doi.org/10.1016/j.cej.2024.154116

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, 5352–5367, (2024)
- Virtual Special Issue "Machine Learning and Statistical Mechanics: Shared Synergies for Next Generation of Chemical Theory and Computation"
https://doi.org/10.1021/acs.jctc.4c00434

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)
https://doi.org/10.1007/s11144-024-02656-4

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)
https://doi.org/10.1016/j.seppur.2024.127752

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)
https://doi.org/10.1002/adma.202401739

50. **G. Zhao⁺, H. Kim⁺, C.W. Yang, Y.G. Chung***
Leveraging Machine Learning to Predict the Atmospheric Lifetime and the Global Warming Potential (GWP) of SF_6 Replacement Gases
Journal of Physical Chemistry A, 128(12), 2399 – 2408, (2024)
- Virtual Special Issue "Machine Learning in Physical Chemistry Vol. 2"
https://doi.org/10.1021/acs.jpca.3c07339

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)
https://doi.org/10.1016/j.jechem.2024.02.032

48. P. Moghadam[+], **Y.G. Chung[+]**, R.Q. Snurr*
Progress toward the computational discovery of new MOF adsorbents for energy applications
Nature Energy, 9, 121 – 133 (2024)
https://doi.org/10.1038/s41560-023-01417-2

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)
https://doi.org/10.1007/s11814-024-00048-x

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)
https://doi.org/10.1021/acs.iecr.3c02211

45. S. Han[+], S. Lee[+], D. Kim, J. Seong, A. Sharma, J. Lim**, 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)
https://doi.org/10.1021/acs.chemmater.3c00694

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)
https://doi.org/10.1016/j.cej.2023.143644

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)
https://doi.org/10.21105/joss.05429

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)
https://doi.org/10.1016/j.matt.2023.03.009

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, 113856, (2023)
https://doi.org/10.1016/j.cattod.2022.07.024

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)
https://doi.org/10.1016/j.ijhydene.2022.09.199

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)
https://doi.org/10.1039/d2ta05420e

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)
https://doi.org/10.1021/acs.langmuir.2c01390

37. **S. Ga, Y.G. Chung***
Recent advances in software tools for adsorption science and engineering
Molecular Systems Design & Engineering, 6, 686 – 701 (2022)
- MSDE Emerging Investigator Series
https://doi.org/10.1039/D2ME00036A

36. **Y. Gu, A. Bai, S. Yoon, Y.G. Chung***, D.W. Park*
Defect-engineered MOF-801 for cycloaddition of CO2 with epoxides
Journal of Materials Chemistry A, 6 (5), 1585 - 1603, (2022)
https://doi.org/10.1039/D2TA00503D

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)
https://doi.org/10.1002/advs.202201559

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)
https://doi.org/10.1021/acsami.1c18440

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 SF6/N2 separation
Chemical Engineering Journal, 426, 131787 (2021)
https://doi.org/10.1016/j.cej.2021.131787

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)
- Porous Materials and Their Applications in Korea (invited contribution)
https://doi.org/10.1002/bkcs.12380

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)
https://doi.org/10.1002/advs.202004999

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)
https://doi.org/10.1002/advs.202004940

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)
https://doi.org/10.1021/acsanm.1c00740

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)
https://doi.org/10.1002/int.22368

27. D.H. Song, J.H. Kang, H.S. Park, **Y.G. Chung,** H. Song*
Simultaneous Removal of NO and SO2 using Microbubble and Reducing Agent
Clean Technology 27 (4), 341-349 (2021)
https://doi.org/10.7464/ksct.2021.27.4.341

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
Journal of Physical Chemistry Letters 11 (14), 5412-5417 (2020)
https://doi.org/10.1021/acs.jpclett.0c01518

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)
https://doi.org/10.14478/ace.2020.1057

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)
https://doi.org/10.1016/j.molliq.2019.111825

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)
https://doi.org/10.1016/j.apcatb.2019.117888

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)
- Selected as a front Cover
https://doi.org/10.1021/acs.jced.9b00835

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)
https://doi.org/10.1080/08927022.2019.1648809

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)
https://doi.org/10.1021/acsami.9b11343

19. R. 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
Journal of Physical Chemistry C 123 (33), 20195-20209 (2019)
https://doi.org/10.1021/acs.jpcc.9b02116

18. K.T. Leper[+], **Y.G. Chung[+],** F. You*, R.Q. Snurr*
Development of a General Evaluation Metric for Rapid Screening of Adsorbent Materials for Post-combustion CO2 Capture
ACS Sustainable Chemistry & Engineering 7 (13), 11529-11539 (2019)
https://doi.org/10.1021/acssuschemeng.9b01418

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)
https://doi.org/10.1016/j.ccr.2019.03.008

2018 (2)

16. G.G. Choi, J.F. Kurisingal, **Y.G. Chung***, D.W. Park*
Two-dimensional Zn-stilbene-dicarboxylic acid (SDC) metal-organic frameworks for cyclic carbonate synthesis from CO2 and epoxides
Korean Journal of Chemical Engineering 35, 1373-1379 (2018)
https://doi.org/10.1007/s11814-018-0023-y

15. G.S. Jeong, A.C. Kathalikkattil, R. Babu, **Y.G. Chung,** D.W. Park*
Cycloaddition of CO2 with epoxides by using an amino-acid-based Cu (II)–tryptophan MOF catalyst
Chinese Journal of Catalysis 39 (1), 63-70 (2018)
https://doi.org/10.1016/S1872-2067(17)62916-4

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 CO2 Capture
Journal of Physical Chemistry Letters 8 (24), 6135-6141 (2017)
https://doi.org/10.1021/acs.jpclett.7b02700

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)
https://doi.org/10.1021/acs.chemmater.6b04226

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 CO2 Capture under Humid Conditions
ChemistrySelect 2 (29), 9458-9465 (2017)
https://doi.org/10.1002/slct.201701934

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)
https://doi.org/10.1021/acs.chemmater.6b04226

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 CO2 and epoxides
Journal of CO2 Utilization 17, 112-118 (2017)
https://doi.org/10.1016/j.jcou.2016.12.001

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 CO2 capture using a genetic algorithm
Science Advances, 2 (10), e1600909 (2016)
https://doi.org/10.1126/sciadv.1600909

8. Song Li, **Y.G. Chung,** R.Q. Snurr*
High-Throughput Screening of Metal-Organic Frameworks for CO2 Capture in the Presence of Water
Langmuir 32 (40), 10368-10376 (2016)
https://doi.org/10.1021/acs.langmuir.6b02803

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)
https://doi.org/10.1039/C5SC01784J

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)
https://doi.org/10.1039/C4EE03515A

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)
https://doi.org/10.1021/cm502594j

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)
https://doi.org/10.1002/polb.23166

3. **Y.G. Chung**, D.J. Lacks*
Atomic mobility in a polymer glass after shear and thermal cycles
Journal of Physical Chemistry B 116 (48), 14201-14205 (2012)
https://doi.org/10.1021/jp309772f

2. **Y.G. Chung**, D.J. Lacks*
How deformation enhances mobility in a polymer glass
Macromolecules 45 (10), 4416-4421 (2012)
https://doi.org/10.1021/ma300431x

1. **Y.G. Chung**, D.J. Lacks*
Sheared polymer glass and the question of mechanical rejuvenation
Journal of Chemical Physics 136 (12) (2012)
https://doi.org/10.1063/1.3698473

Domestic Patents & Licenses

- (1) KR patent registered
  - KR 10-2707528 (app number: 10-2022-0085362)
- (2) KR patents pending
  - 10-2022-0059393
  - 10-2023-0061292
- (2) software program licenses registered

Presentations

Department & Research Groups (invited)

1. AI and Computational Chemistry Division, Korea Institute of Energy Research, Daejeon Korea, February 2026
2. Department of Chemical & Biomolecular Engineering, Yonsei University, Seoul Korea, January 2026
3. Department of Energy Engineering, Daegu Gyeongbuk Institute of Science and Technology (DGIST), Daegu Korea, July 2025
4. Department of Chemistry, Pohang University of Science and Technology, Pohang Korea, April 2025
5. Department of Chemical Engineering, National Taiwan University of Science and Technology, Taipei Taiwan, February 2025
6. Department of Chemical Engineering, National Taiwan University, Taipei Taiwan, February 2025
7. The Sargent Centre for Process Systems Engineering, Imperial College London, London UK, February 2025
8. Cambridge Crystallographic Data Centre, Cambridge UK, February 2025
9. Department of Chemical Engineering, University College London, London UK, February 2025
10. Department of Chemical Engineering, Texas Tech University, Lubbock TX USA Oct 2024
11. Department of Chemistry, Sungkyunkwan University, Suwon, Korea, April 2024
12. School of Chemical Engineering, Sungkyunkwan University, Suwon, Korea, May 2023
13. Department of Chemistry, Hanyang University, Seoul, Korea, November 2022
14. Process & Energy, Delft University of Technology, Delft, the Netherlands, July 2022
15. Computational Chemistry Group Meeting, Universiteit van Amsterdam, Amsterdam, The Netherlands, July 2022
16. Earth & Environmental Engineering, Lenfest Center for Sustainable Energy, Columbia University, New York, NY, April 2022
17. Department of Chemical Engineering, MIT, Cambridge, MA USA April 2022
18. Materials Colloquium, Department of Chemical Engineering, University of Massachusetts - Amherst, Amherst, MA USA March 2022
19. Department of Chemical & Biomolecular Engineering, Case Western Reserve University, Cleveland, OH USA February 2022
20. Department of Chemical Engineering, Konkuk University, Seoul, Korea, May 2021 (zoom)
21. Department of Chemistry, Korea University, Seoul, Korea, April 2021 (zoom)
22. Department of Chemical and Biomolecular Engineering, Yonsei University, Seoul, Korea, March 2021 (zoom)
23. Environmental Engineering, Kyunghee University, Suwon, Korea, July 2019
24. Department of Chemical Engineering, University of Ulsan, Ulsan, Korea March 2018
25. Department of Chemistry, UNIST, Ulsan, Korea May 2017

26. Department of Chemistry, Pohang University of Science and Technology, Pohang Korea, March 2017
27. Department of Chemical and Biomolecular Engineering, Case Western Reserve University, Cleveland, OH USA January 2016
28. Department of Chemical Engineering, University of Illinois - Chicago, Chicago IL USA March 2015

International Conferences & Workshops

29. AICHE Annual Meeting 2026, November 2026
30. Chemistry with AI for Carbon Neutrality 2026 (C-AICN 2026), Higashi Hiroshima Japan, June 2026
31. x2026, Toronto Canada, May 2026
32. 2025 Annual Meeting of TwIChE, Taiwan-Japan-Korea (TJK) Symposium, November 2025
33. AI for Materials Chemistry, Korean Chemical Society, Daegu, Korea, October 2024
34. "Machine Learning", Thermodynamics 2024, Delft, the Netherlands, September 2024
35. iRASPA/RASPA Workshop 2024, Delft, the Netherlands, September 2024
36. Symposium on Computational Chemistry & Artificial Intelligence for Advanced Catalyst and Materials Design, KIChE, Jeju Island, Korea April 2024
37. PSK-LG Chemical Special Session, Korea Polymer Society, Jeju Island, Korea, October 2023
38. KIChE Fall Meeting and International Symposium on Separation Technology for Carbon Neutrality, October 2021
39. Clean Technology Fall Meeting, September 2021
40. Division of Thermodynamics KIChE Winter Workshop, Yonsei University, Seoul, Korea, December 2019
41. The 2nd Conference on Advanced Separation Science and Engineering (CASSE), Hanoi, Vietnam, December 2018
42. Korean Institute of Chemical Engineers (KIChE) Symposium on Applications of Molecular Modeling in New and Renewable Energy Fields, Changwon, Korea, April 2018
43. American Chemical Society (ACS) Sustainable Chemistry & Engineering Lectureship Awards: Symposium in honor of Fengqi You, New Orleans, USA, March 2018
44. Korea-Japan-Taiwan (KJT) Chemical Engineering Conference, Busan, Korea, November 2017
45. BIOVIA User Group Meeting, Seoul, Korea, November 2017
46. The 4th International Symposium on Hybrid Materials and Processing, Busan, Korea, November 2017
47. US-Korea Conference (UKC), Washington D.C., USA, August 2017
48. Korea Carbon Society Spring Meeting, Changwon, Korea, May 2017
49. Vietnam-Korea Chemical Engineering Joint Symposium, Nha-trang, Vietnam, February 2017
50. MOF and Beyond Workshop, Daejeon, Korea, December 2016
51. Nanoporous Materials Genome All-Hands Meeting, St. Paul, Minnesota USA October 2014
52. Northwestern/UOP Molecular Modeling Workshop, Evanston Illinois, USA July 2014
53. Nanoporous Materials Genome Center, University of Minnesota – Twin Cities, Minneapolis, MN USA November 2013
54. Nanoporous Materials Genome All-Hands Meeting, Berkeley, CA USA, October 2013
55. 6th Simulators Meeting, Carnegie Mellon University, Pittsburgh, PA USA, June 2012
56. ACS 10th National Graduate Research Polymer Conference, Cleveland OH USA, May 2012
57. AICHE Annual Meeting, Minneapolis MN USA, Oct. 2011
58. 83rd Annual Meeting of the Society of Rheology, Cleveland OH USA, Oct. 2011
59. 82nd Annual Meeting of the Society of Rheology, Santa Fe, NM USA, Oct. 2010
60. 4th Simulators Meeting, Carnegie Mellon University, Pittsburgh, PA USA, June 2010

61. Midwest Thermodynamics and Statistical Mechanics Conference, University of Notre Dame, South Bend IN USA, May 2010

Funded Research (total: $2.61 M equivalent)

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*

Korea Electric Power Corporation (co-PI) 2021 – 2024

- *Computational Exploration of SF6 Replacement Gases*

Korea Hydro & Nuclear Power (co-PI) 2021 – 2023

- *Production of High-purity Hydrogen via Sorption-Enhanced System*

Korea Evaluation Institute of Industrial Technology (co-PI) 2020 – 2021

- *Green Ammonia for Hydrogen Storage*

Korea Institute of Industrial Technology (sole PI) 2020

- *Computational Screening of High-Performance Zeolites for Pre-treatment of Natural Gas*

National Research Foundation of Korea (sole PI) 2020 – 2024

- *Modeling and Experimentation for Nanoporous Materials Characterization and the BET Theory*

Korea Institute of Industrial Technology (sole PI) 2020 – 2021

- *DFT Investigation of Olefin Synthesis*

LG Chemical (sole PI) 2018

- *Using Molecular Simulation for Gas Purification Adsorbent Discovery*

National Research Foundation of Korea (sole PI) 2016 – 2019

- *Materials Genome Approach to Discovery Novel Adsorbent Materials for CO_2/SO_2 Separation and Purification*

Supercomputing Allocation

Korea Supercomputing Center 2016 – 2026

- Periodic CPU and GPU allocations through Korea Supercomputing Center Proposals

ASCR Leadership Computing Challenge (ALCC) Allocation (US. DOE) 2018

- 58 million process hours
- J. Ilja Siepmann PI, Yongchul G. Chung co-PI

ASCR Leadership Computing Challenge (ALCC) Allocation (U.S. DOE) 2017

- 146 million process hours
- J. Ilja Siepmann PI, Yongchul G. Chung co-PI

Professional Society Affiliations

American Institute of Chemical Engineers (2013 – current)

- Computational Molecular Science and Engineering Forum (CoMSEF)

American Chemical Society (2015 – current)

- Chemical Information Division
- Computers in Chemistry Division
- Physical Chemistry Division
- CATL Division

International Adsorption Society (2018 – current)

- Education committee

Korean Institute of Chemical Engineers (2016 – current)

- Thermodynamics and Molecular Simulation Division
- Separation Technology Division

Korean Society of Industrial Chemistry (2016 – current)

- AI and Computational Science Division (2026 – current)

Korean Chemical Society (2016 – current)

- Materials Chemistry Division

Professional and Faculty Services & Activities

Editorial Activities

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

Conference and Workshop Organizer

•	Organizer	International Adsorption Society (IAS) Asia-Pacific Webinar Series Online	2023
•	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 "Synthesis and Application of Inorganic Materials I: Synthesis"	Nov. 2026
•	Chair	2025 AICHE Annual Meeting "MOFs, COFs, and Porous Materials" Cambridge, 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 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 – current

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
• Swiss National Science Foundation	2023 – 2025
• Samsung Future Technology Center	2017
• Korea Supercomputing Center	2018 – 2021

Journal Review

- **Journal reviewer for >400 articles**, invited by more than **80** journals such as:
- **ACS (23)**
  - *Accounts of Chemical Research, ACS Applied Energy Materials, ACS Applied Materials & Interfaces, ACS Applied Nano Materials, ACS Materials Letters, ACS Sustainable Chemistry & Engineering, Chem & Bio Engineering, Chemical Reviews, ACS Central Science, ACS Omega, ACS Sensors, Chemistry of Materials, Crystal Growth & Design, Environmental Science & Technology, Energy & Fuel, Industrial & Engineering Chemistry Research, Inorganic Chemistry, Langmuir, Journal of the American Chemical Society (JACS), JACS Au, The Journal of Physical Chemistry C, The Journal of Physical Chemistry Letters, Journal of Chemical Information and Modeling*
- **Elsevier (14)**
  - *Applied Catalysis B: Environmental, Chemical Engineering Journal, Chemical Engineering Science, Computational Materials Science*, *Coordination Chemistry Reviews*, Composites Part B, *eScience*, *Fuel*, *Journal of Cleaner Production*, *Journal of Environmental Chemical Engineering, Inorganic Chemistry Communications, Computers & Chemical Engineering, Separation and Purification Technology, International Journal of Hydrogen Energy*
- **RSC (12)**
  - *Chemical Communications, Energy & Environmental Materials, Digital Discovery, Journal of Materials Chemistry A/B/C, Physical Chemistry Chemical Physics, RSC Advances, Industrial Chemistry & Materials, Sustainable Energy & Fuels, Materials Advances, Molecular Systems Design & Engineering, Nanoscale*
- **Society Journals (8)**
  - *Adsorption, AICHE Journal, Bulletin of the Korean Chemical Society, The Canadian Journal of*

Chemical Engineering, Journal of the Taiwan Institute of Chemical Engineers, Korean Journal of Chemical Engineering, Microporous and Mesoporous Materials

- **Wiley (9)**
  - *Advanced Materials, Advanced Functional Materials, Angewantde Chemie, Advanced Science, Chemical Engineering & Technology, ChemistrySelect, ChemSusChem, EcoEnergy, International Journal of Quantum Chemistry*
- **Nature Portfolio (5)**
  - *Nature Energy, Nature Communications, Nature Computational Science, npj computational materials, Scientific Reports*
- **Springer Nature (3)**
  - *Discover Nano, Science China Chemistry, Nano-Micro Letters*
- **ScienceDirect (2)**
  - *Separation and Purification Technology, Computational and Theoretical Chemistry*
- **APS (2)**
  - *Physical Review Letters, Physics Review X Energy*
- **Taylor & Francis (2)**
  - *Separation Science and Technology*, *Molecular Simulation*
- **AAAS (1)**
  - *Science Advances*
- **AIP (1)**
  - *Journal of Chemical Physics*

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 – current
  - Member, Faculty Search Committee 2025
  - Chair, Faculty Search Committee 2026
- University
  - Chair, AIX-Computational Science Curriculum TF May 2025 – Aug. 2025

Research Mentoring

Graduate Students

Current

1. 2025 – current Changdon Shin
2. 2025 – current Pengyu Zhao

3. 2025 – current Siah Thong
4. 2024 – current Taekgi Lee
   - 2024 Samsung AI Challenge, 3rd place ($2,500 prize)
5. 2022 – current Hassan Muhammad
   - 2024 Best Poster Award, Separation Technology Division, KICHE
   - 2023 Best Poster Award, BKFOUR21 Workshop PNU ChBE
6. 2020 – current 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

7. 2019 – current 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

8. 2024 – current 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)

9. 2020 – current Guobin Zhao *Ph.D. Postdoctoral Fellow, NUS*
   - 2024 Best Poster Award, Busan-Gyeongnam Region, KICHE
   - 2024 Best Poster Award, Busan-Ulsan-Gyeongnam Region, KSIEC

10. 2019 – 2022 Seungyun Han
11. 2019 – 2021 Jaehoon Cha

12. 2019 – 2022 Dong-Hoon Song *M.S., (affiliated student co-advised with Hojun Song)*

13. 2019 – 2021 Hyuck Won Kwon *M.S., (affiliated student co-advised with Junghwan Kim)*
14. 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
15. 2018 – 2020 Sehee Kang *M.S. (affiliated student co-advised with Hojun Song)*
16. 2018 – 2020 Hyun Mo Je *M.S. (affiliated student co-advised with Jungkyu Roh)*
17. 2017 – 2019 Soo Myung Nam *M.S. Engineer, Hankuk Paper*

Postdoctoral Researchers

1. 2022 – 2023 Dr. Changwon Yang *Senior Scientist, Korean Quantum Computing Inc.*
2. 2021 – 2022 Dr. Yunjang Gu *Research Scientist, Nam Hae Chemicals Ltd.*
3. 2020 – 2022 Dr. Seongbin Ga *Faculty, Chemical Engineering, University of Ulsan*
   - 2021 NRF Sejong Fellowship
4. 2020 – 2022 Dr. Anjali Bai *Postdoc., National University of Singapore*

Undergraduate Students

1. 2025 – current Hyunji Kim

2.	2025	Nahyeon Lee	
3.	2025	Dahee Kang	
4.	2025	Sungeun Hong	
5.	2024 – 2025	Jaehoon Lee	
		- 2024 Samsung AI Challenge, 3rd place ($2,500 prize)	
6.	2024	Chaeyoung Park	
7.	2024	Younseo Yang	
8.	2023	Haewon Kim	continued as an MS student
9.	2023	Yeji Lee	KCC
10.	2021	Nayoung Kim	
11.	2021	Chaewon Park	
12.	2020	Hyeji Kim	
13.	2019	Byungkwan Sung	Kolon Industries
14.	2018 – 2020	Seungyun Han	continued as a MS student
15.	2018 – 2019	Juyong Kim	Samsung Display
16.	2018 – 2019	Sunghyun Yoon	continued as a MS/PhD student
17.	2017 – 2018	Nayoung Seo	SK pucore
18.	2016 – 2017	Jinwook Hwang	Samsung Engineering
19.	2016 – 2017	Hyeji Lee	Hanwha Energy
20.	2016 – 2019	Seulchan Lee	continued as BS/MS student
21.	2018	Geonjong Kim	SK Hynix
22.	2018 – 2019	Chungsik Jeong	

Teaching Activities

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