

# Sungsoo Ahn

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## Education

MS/Ph.D Integrated Course in Electrical Engineering Mar. 2015 – Mar. 2021  
*Korea Advanced Institute of Science and Technology (KAIST), Daejeon, South Korea*  
*Advisor: Jinwoo Shin*

BS in Electrical Engineering Mar. 2011 – Mar. 2015  
*Korea Advanced Institute of Science and Technology (KAIST), Daejeon, South Korea*

## Employment

Assistant Professor Jan. 2025 – Present  
*Korea Advanced Institute of Science and Technology (KAIST), Daejeon, South Korea*

Assistant Professor Dec. 2021 – Jan. 2025  
*Pohang University of Science and Technology (POSTECH), Pohang, South Korea*  
*Graduate School of AI and Department of Computer Science and Engineering*

Research Associate Mar. 2021 – Nov. 2021  
*Mohamed Bin Zayed University of Artificial Intelligence (MBZUAI),  
Abu Dhabi, United Arab Emirates*  
*Supervisors: Le Song and Eric Xing*

Research Intern Jun. 2018 – Aug. 2018  
*Amazon Cambridge Development Center, Cambridge, England*  
*Supervisor: Zhenwen Dai*

Visiting Student Mar. 2018 – May 2018  
*University of Cambridge, Cambridge, England*  
*Host: Adrian Weller*

Research Intern Jun. 2017 – Aug. 2017  
*Los Alamos National Laboratory, New Mexico, United States*  
*Host: Michael Chertkov*

Research Intern Jun. 2016 – Aug. 2016  
*Los Alamos National Laboratory, New Mexico, United States*  
*Host: Michael Chertkov*

## Publications

 \*Equal contribution. †Corresponding author.

### CONFERENCE

1. Minsu Kim, Jean-Pierre R. Falet, Oliver Ethan Richardson, Xiaoyin Chen, Moksh Jain, Sungjin Ahn, **Sungsoo Ahn**, and Yoshua Bengio, Latent Veracity Inference for Identifying Errors in Stepwise Reasoning, In *International Conference on Learning Representations (ICLR)*, 2026. [\[arXiv\]](#)
2. Hyunjin Seo\*, Taewon Kim\*, Sihyun Yu, and **Sungsoo Ahn**, Learning Flexible Forward Trajectories for Masked Molecular Diffusion, In *International Conference on Learning Representations (ICLR)*, 2026. [\[arXiv\]](#)
3. Seonghyun Park, Kiyong Seong, Soojung Yang, Rafael Gomez-Bombarelli, and **Sungsoo Ahn**, Learning Collective Variables from BioEmu with Time-Lagged Generation, In *International Conference on Learning Representations (ICLR)*, 2026. [\[arXiv\]](#)
4. Seonghwan Seo, Minsu Kim, Tony Shen, Martin Ester, Jinkyoo Park, **Sungsoo Ahn**, and Woo Youn Kim, Generative Flows on Synthetic Pathway for Drug Design, In *International Conference on Learning Representations (ICLR)*, 2025. [\[arXiv\]](#)
5. Nayoung Kim, Seongsu Kim, Minsu Kim, Jinkyoo Park, and **Sungsoo Ahn**, MOFFlow: Flow Matching for Structure Prediction of Metal-Organic Frameworks, In *International Conference on Learning Representations (ICLR)*, 2025. [\[arXiv\]](#)
6. Kiyong Seong, Seonghyun Park, Seonghwan Kim, Woo Youn Kim, and **Sungsoo Ahn**, Transition Path Sampling with Improved Off-Policy Training of Diffusion Path Samplers, In *International Conference on Learning Representations (ICLR)*, 2025. [\[arXiv\]](#)
7. Taewon Kim\*, Hyunjin Seo\*, **Sungsoo Ahn**, and Eunho Yang, ReBind: Enhancing Ground-state Molecular Conformation Prediction via Force-Based Graph Rewiring, In *International Conference on Learning Representations (ICLR)*, 2025. [\[arXiv\]](#)
8. Minsu Kim, Sanghyeok Choi, Taeyoung Yun, Emmanuel Bengio, Leo Feng, Jarrid Rector-Brooks, **Sungsoo Ahn**, Jinkyoo Park, Nikolay Malkin, and Yoshua Bengio, Adaptive Teachers for Amortized Samplers, In *International Conference on Learning Representations (ICLR)*, 2025. [\[arXiv\]](#)
9. Dongyoon Hahm, Woogyel Jin, June Suk Choi, **Sungsoo Ahn**, and Kimin Lee, Enhancing LLM Agent Safety via Causal Influence Prompting, In *Annual Meeting of the Association for Computational Linguistics (ACL) Findings*, 2025. [\[arXiv\]](#)
10. Yunhui Jang, Jaehyung Kim, and **Sungsoo Ahn**, Structural Reasoning Improves Molecular Understanding of LLM, In *Annual Meeting of the Association for Computational Linguistics (ACL)*, 2025. [\[arXiv\]](#)
11. Federico Berto, Chuanbo Hua, Junyoung Park, Laurin Luttmann, Yining Ma, Fanchen Bu, Jiarui Wang, Haoran Ye, Minsu Kim, Sanghyeok Choi, Nayeli Gast Zepeda, André Hottung, Jianan Zhou, Jieyi Bi, Yu Hu, Fei Liu, Hyeonah Kim, Jiwoo Son, Haeyeon Kim, Davide Angioni, Wouter Kool, Zhiguang Cao, Qingfu Zhang, Joungho Kim, Jie Zhang, Kijung Shin,

- Cathy Wu, **Sungsoo Ahn**, Guojie Song, Changhyun Kwon, Kevin Tierney, Lin Xie, and Jinkyoo Park, RL4CO: an Extensive Reinforcement Learning for Combinatorial Optimization Benchmark, In *Knowledge Discovery and Data Mining (KDD) Datasets and Benchmarks*, 2025. [\[arXiv\]](#)
12. Hyosoon Jang, Yunhui Jang, Sungjae Lee, Jungseul Ok, and **Sungsoo Ahn**, Self-Training Large Language Models with Confident Reasoning, In *Empirical Methods in Natural Language Processing (EMNLP)*, 2025. [\[arXiv\]](#)
  13. Hyomin Kim, Yunhui Jang, and **Sungsoo Ahn**, MT-Mol: Multi Agent System with Tool-based Reasoning for Molecular Optimization, In *Empirical Methods in Natural Language Processing (EMNLP)*, 2025. [\[arXiv\]](#)
  14. Yunhui Jang, Jaehyung Kim, and **Sungsoo Ahn**, Improving Chemical Understanding of LLMs via SMILES Parsing, In *Empirical Methods in Natural Language Processing (EMNLP)*, 2025. [\[arXiv\]](#)
  15. Dongyeop Woo, Minsu Kim, Minkyu Kim, Kiyoung Seong, and **Sungsoo Ahn**, Energy-based Generator Matching: A Neural Sampler for General State Space, In *Conference on Neural Information Processing Systems (NeurIPS)*, 2025. [\[arXiv\]](#)
  16. Minkyu Kim, Kiyoung Seong, Dongyeop Woo, **Sungsoo Ahn**, and Minsu Kim, On Scalable and Efficient Training of Diffusion Samplers, In *Conference on Neural Information Processing Systems (NeurIPS)*, 2025. [\[arXiv\]](#)
  17. Nayoung Kim, Seongsu Kim, and **Sungsoo Ahn**, Flexible MOF Generation with Torsion-Aware Flow Matching, In *Conference on Neural Information Processing Systems (NeurIPS)*, 2025. [\[arXiv\]](#)
  18. Seongsu Kim, Nayoung Kim, Dongwoo Kim, and **Sungsoo Ahn**, High-order Equivariant Flow Matching for Density Functional Theory Hamiltonian Prediction, In *Conference on Neural Information Processing Systems (NeurIPS)*, 2025. [\[arXiv\]](#)
  19. Hyosoon Jang, Minsu Kim, and **Sungsoo Ahn**, Learning Energy Decompositions for Partial Inference in GFlowNets, In *International Conference on Learning Representations (ICLR)*, 2024, [oral presentation \(86/7304 = 1.18% accept rate\)](#). [\[arXiv\]](#)
  20. Yunhui Jang, Seul Lee, and **Sungsoo Ahn**, A Simple and Scalable Representation for Graph Generation, In *International Conference on Learning Representations (ICLR)*, 2024. [\[arXiv\]](#)
  21. Yunhui Jang, Dongwoo Kim, and **Sungsoo Ahn**, Graph Generation with  $K^2$  Trees, In *International Conference on Learning Representations (ICLR)*, 2024. [\[arXiv\]](#)
  22. Minsu Kim, Taeyoung Yun, Emmanuel Bengio, Dinghuai Zhang, Yoshua Bengio, **Sungsoo Ahn**, and Jinkyoo Park, Local Search GFlowNets, In *International Conference on Learning Representations (ICLR)*, 2024, [spotlight presentation \(366/7304 = 5.0% accept rate\)](#). [\[arXiv\]](#)
  23. Hyomin Kim, Yunhui Jang, Jaeho Lee, and **Sungsoo Ahn**, Hybrid Neural Representation for Spherical Data, In *International Conference on Machine Learning (ICML)*, 2024. [\[arXiv\]](#)

24. Seongsu Kim and **Sungsoo Ahn**, Gaussian Plane-Wave Neural Operator for Electron Density Estimation, In *International Conference on Machine Learning (ICML)*, 2024. [\[arXiv\]](#)
25. Nayeong Kim, Juwon Kang, **Sungsoo Ahn**, Jungseul Ok, and Suha Kwak, Improving Robustness to Multiple Spurious Correlations by Multi-Objective Optimization, In *International Conference on Machine Learning (ICML)*, 2024.
26. Hyeonah Kim, Minsu Kim, **Sungsoo Ahn**, and Jinkyoo Park, Enhancing Sample Efficiency in Black-box Combinatorial Optimization via Symmetric Replay Training, In *International Conference on Machine Learning (ICML)*, 2024. [\[arXiv\]](#)
27. Fanchen Bu, Hyeonsoo Jo, Soo Yong Lee, **Sungsoo Ahn**, and Kijung Shin, Tackling Complex Conditions in Unsupervised Combinatorial Optimization, In *International Conference on Machine Learning (ICML)*, 2024. [\[arXiv\]](#)
28. Youngsik Yoon, Gangbok Lee, **Sungsoo Ahn**, and Jungseul Ok, Breadth-First Exploration in Adaptive Grid-based Reinforcement Learning, In *International Conference on Machine Learning (ICML)*, 2024.
29. Jaeseung Heo, Seungbeom Lee, **Sungsoo Ahn**, and Dongwoo Kim, EPIC: Graph Augmentation with Edit Path Interpolation via Learnable Cost, In *International Joint Conference on Artificial Intelligence (IJCAI)*, 2024. [\[arXiv\]](#)
30. Hyosoon Jang, Yunhui Jang, Minsu Kim, Jinkyoo Park, and **Sungsoo Ahn**, Pessimistic Backward Policy for GFlowNets, In *Conference on Neural Information Processing Systems (NeurIPS)*, 2024. [\[arXiv\]](#)
31. Junsu Kim, Younggyo Seo, **Sungsoo Ahn**, Kyunghwan Son, and Jinwoo Shin, Imitating Graph-Based Planning with Goal-Conditioned Policies, In *International Conference on Learning Representations (ICLR)*, 2023. [\[arXiv\]](#)
32. Sungbin Shin, Yohan Jo, **Sungsoo Ahn**, and Namhoon Lee, A Closer Look at the Intervention Procedure of Concept Bottleneck Models, In *International Conference on Machine Learning (ICML)*, 2023. [\[arXiv\]](#)
33. Hyuna Cho, Minjae Jeong, Sooyeon Jeon, **Sungsoo Ahn**, and Won Hwa Kim, Multi-resolution Spectral Coherence for Graph Generation with Score-based Diffusion, In *Conference on Neural Information Processing Systems (NeurIPS)*, 2023.
34. Hyosoon Jang, Seonghyun Park, Sangwoo Mo, and **Sungsoo Ahn**, Diffusion Probabilistic Models for Structured Node Classification, In *Conference on Neural Information Processing Systems (NeurIPS)*, 2023. [\[arXiv\]](#)
35. Minsu Kim, Federico Berto, **Sungsoo Ahn**, and Jinkyoo Park, Bootstrapped Training of Score-Conditioned Generator for Offline Design of Biological Sequences, In *Conference on Neural Information Processing Systems (NeurIPS)*, 2023. [\[arXiv\]](#)
36. Jaehyung Kim, Dongyeop Kang, **Sungsoo Ahn**, and Jinwoo Shin, What Makes Better Augmentation Strategies? Augment Difficult but Not Too Different, In *International Conference on Learning Representations (ICLR)*, 2022.

37. **Sungsoo Ahn**, Binghong Chen, Tianzhe Wang, and Le Song, Spanning Tree-based Graph Generation for Molecules, In *International Conference on Learning Representations (ICLR)*, 2022, [spotlight presentation \(174/3422 = 5.2% accept rate\)](#).
38. Kyunghwan Son, Junsu Kim, **Sungsoo Ahn**, Roben Delos Reyes, Yung Yi, and Jinwoo Shin, Disentangling Sources of Risk for Distributional Multi-Agent Reinforcement Learning, In *International Conference on Machine Learning (ICML)*, 2022.
39. Nayeong Kim, Sehyun Hwang, **Sungsoo Ahn**, Jaesik Park, and Suha Kwak, Learning Debiased Classifier with Biased Committee, In *Conference on Neural Information Processing Systems (NeurIPS)*, 2022. [\[arXiv\]](#)
40. Jaeho Lee, Sejun Park, Sangwoo Mo, **Sungsoo Ahn**, and Jinwoo Shin, Layer-adaptive sparsity for the Magnitude-based Pruning, In *International Conference on Learning Representations (ICLR)*, 2021. [\[arXiv\]](#)
41. Junsu Kim, **Sungsoo Ahn**, Hankook Lee, and Jinwoo Shin, Self-Improved Retrosynthetic Planning, In *International Conference on Machine Learning (ICML)*, 2021. [\[arXiv\]](#)
42. Hankook Lee, **Sungsoo Ahn**, Seung-Woo Seo, You Young Song, Eunho Yang, Sung Ju Hwang, and Jinwoo Shin, RetCL: A Selection-based Approach for Retrosynthesis via Contrastive Learning, In *International Joint Conference on Artificial Intelligence (IJCAI)*, 2021. [\[arXiv\]](#)
43. Sihyun Yu, **Sungsoo Ahn**, Le Song, and Jinwoo Shin, RoMA: Robust Model Adaptation for Offline Model-based Optimization, In *Conference on Neural Information Processing Systems (NeurIPS)*, 2021. [\[arXiv\]](#)
44. **Sungsoo Ahn**, Younggyo Seo, and Jinwoo Shin, Learning What to Defer for Maximum Independent Sets, In *International Conference on Machine Learning (ICML)*, 2020. [\[arXiv\]](#)
45. Junhyun Nam, Hyuntak Cha, **Sungsoo Ahn**, Jaeho Lee, and Jinwoo Shin, Learning from Failure: Training Debiased Classifier from Biased Classifier, In *Conference on Neural Information Processing Systems (NeurIPS)*, 2020. [\[arXiv\]](#)
46. **Sungsoo Ahn**, Junsu Kim, Hankook Lee, and Jinwoo Shin, Guiding Deep Molecular Optimization with Genetic Exploration, In *Conference on Neural Information Processing Systems (NeurIPS)*, 2020. [\[arXiv\]](#)
47. **Sungsoo Ahn**, Shell Hu, Andreas Damianou, Neil Lawrence, and Zhenwen Dai, Variational Information Distillation for Knowledge Transfer, In *IEEE Conference on Computer Vision and Pattern Recognition (CVPR)*, 2019. [\[arXiv\]](#)
48. **Sungsoo Ahn**, Michael Chertkov, Adrian Weller, and Jinwoo Shin, Bucket-Renormalization for Approximate Inference, In *International Conference on Machine Learning (ICML)*, 2018. [\[arXiv\]](#)
49. **Sungsoo Ahn**, Michael Chertkov, Jinwoo Shin, and Adrian Weller, Gauged Mini-Bucket Elimination for Approximate Inference, In *International Conference on Artificial Intelligence and Statistics (AISTATS)*, 2018. [\[arXiv\]](#)

50. **Sungsoo Ahn**, Michael Chertkov, and Jinwoo Shin, Gauging Variational Inference, In *Conference on Neural Information Processing Systems (NeurIPS)*, 2017. [\[arXiv\]](#)
51. **Sungsoo Ahn**, Michael Chertkov, and Jinwoo Shin, Synthesis of MCMC and Belief Propagation, In *Conference on Neural Information Processing Systems (NeurIPS)*, 2016, **oral presentation (46/2500 = 1.8% accept rate); first NeurIPS oral from a South Korean institution.** [\[arXiv\]](#)
52. **Sungsoo Ahn**, Sejun Park, Michael Chertkov, and Jinwoo Shin, Minimum Weight Perfect Matching via Blossom Belief Propagation, In *Conference on Neural Information Processing Systems (NeurIPS)*, 2015, **spotlight presentation (82/1838 = 4.5% accept rate).** [\[arXiv\]](#)

## JOURNAL

1. Nayoung Kim, Minsu Kim, **Sungsoo Ahn**, and Jinkyoo Park, Decoupled Sequence and Structure Generation for Realistic Antibody Design, In *Transactions of Machine Learning Research (TMLR)*, 2024. [\[arXiv\]](#)
2. Seonghyun Park\*, Narae Ryu\*, Gahee Kim, Dongyeop Woo, Se-Young Yun<sup>†</sup>, and **Sungsoo Ahn<sup>†</sup>**, Non-backtracking Graph Neural Networks, In *Transactions of Machine Learning Research (TMLR)*, 2024. [\[arXiv\]](#)
3. Seojin Kim, Jaehyun Nam, Junsu Kim, Hankook Lee, **Sungsoo Ahn**, and Jinwoo Shin, Holistic Molecular Representation Learning via Multi-view Fragmentation, In *Transactions of Machine Learning Research (TMLR)*, 2024.
4. **Sungsoo Ahn**, Michael Chertkov, Adrian Weller, and Jinwoo Shin, Bucket-Renormalization for Approximate Inference, In *Journal of Statistical Mechanics: Theory and Experiment*, 2019(12), 124015, 2019. [\[arXiv\]](#)
5. **Sungsoo Ahn**, Michael Chertkov, and Jinwoo Shin, Gauging Variational Inference, In *Journal of Statistical Mechanics: Theory and Experiment*, 2019(12), 124022, 2019. [\[arXiv\]](#)
6. **Sungsoo Ahn**, Michael Chertkov, Andrew E. Gelfand, Sejun Park, and Jinwoo Shin, Maximum Weight Matching using Odd-sized Cycles: Max-Product Belief Propagation and Half-Integrality, In *IEEE Transactions on Information Theory*, 64(3), 1471–1480, 2018.

## PREPRINT

1. Yinhua Piao, Hyomin Kim, Seonghwan Kim, Yunhak Oh, Junhyeok Jeon, Sang-Yeon Hwang, Jaechang Lim, Woo Youn Kim, Chanyoung Park, and **Sungsoo Ahn**, Learning Adaptive Perturbation-Conditioned Contexts for Robust Transcriptional Response Prediction, *arXiv*, 2026. [\[arXiv\]](#)
2. Seongsu Kim, Chanhui Lee, Yoonho Kim, Seongjun Yun, Honghui Kim, Nayoung Kim, Changyoung Park, Sehui Han, Sungbin Lim\*, and **Sungsoo Ahn\***, Machine Learning Hamiltonians are Accurate Energy-Force Predictors, *arXiv*, 2026. [\[arXiv\]](#)
3. Hyosoon Jang, Hyunjin Seo, Yunhui Jang, Seonghyun Park, and **Sungsoo Ahn**, Boltz is a Strong Baseline for Atom-level Representation Learning, *arXiv*, 2026. [\[arXiv\]](#)

4. Dongyeop Woo, Marta Skreta, Seonghyun Park, Kirill Neklyudov<sup>†</sup>, and **Sungsoo Ahn**<sup>†</sup>, Riemannian MeanFlow, *arXiv*, 2026. [\[arXiv\]](#)
5. Hyomin Kim, Sang-Yeon Hwang, Jaechang Lim, Yinhua Piao, Yunhak Oh, Woo Youn Kim, Chanyoung Park, **Sungsoo Ahn**, and Junhyeok Jeon, Progressive Multi-Agent Reasoning for Biological Perturbation Prediction, *arXiv*, 2026. [\[arXiv\]](#)
6. Nayoung Kim, Honghui Kim, Sihyun Yu, Minkyu Kim, Seongsu Kim, and **Sungsoo Ahn**, AtomMOF: All-Atom Flow Matching for MOF-Adsorbate Structure Prediction, *arXiv*, 2026. [\[arXiv\]](#)
7. Minkyu Kim, Nayoung Kim, Honghui Kim, and **Sungsoo Ahn**, CatFlow: Co-generation of Slab-Adsorbate Systems via Flow Matching, *arXiv*, 2026. [\[arXiv\]](#)
8. Yunhui Jang, Seonghyun Park, Jaehyung Kim, and **Sungsoo Ahn**, INDIBATOR: Diverse and Fact-Grounded Individuality for Multi-Agent Debate in Molecular Discovery, *arXiv*, 2026. [\[arXiv\]](#)
9. Taewon Kim, Jihwan Shin, Hyomin Kim, Youngmok Jung, Jonhoon Lee, Won-Chul Lee, Insu Han<sup>†</sup>, and **Sungsoo Ahn**<sup>†</sup>, DNACHUNKER: Learnable Tokenization for DNA Language Models, *arXiv*, 2026. [\[arXiv\]](#)
10. Hyosoon Jang, Yunhui Jang, Jaehyung Kim, and **Sungsoo Ahn**, Can LLMs Generate Diverse Molecules? Towards Alignment with Structural Diversity, *arXiv*, 2024. [\[arXiv\]](#)
11. Dongyeop Woo and **Sungsoo Ahn**, Iterated Energy-based Flow Matching for Sampling from Boltzmann Densities, *arXiv*, 2024. [\[arXiv\]](#)

## Services

1. Local Chair, Probabilistic Machine Learning Conference (ProbML) 2026
2. Workshop Organizer, International Conference on Machine Learning (ICML), AI4Science 2026
3. Area Chair, International Conference on Machine Learning (ICML) 2022 – 2026
4. Area Chair, International Conference on Learning Representations (ICLR) 2024 – 2026
5. Area Chair, Conference on Neural Information Processing Systems (NeurIPS) 2022 – 2025
6. Area Chair, Intl. Conference on Artificial Intelligence and Statistics (AISTATS) 2022 – 2024
7. Area Chair, Association for the Advancement of Artificial Intelligence (AAAI) 2024
8. Action Editor, Transactions of Machine Learning Research (TMLR) 2024 – 2026
9. Workflow Chair, International Conference on Machine Learning (ICML) 2022
10. Board of Directors, Korean Society of AI Frontier (KSAIF) 2025 –
11. Reviewer, NeurIPS 2018 – 2021
12. Reviewer, ICML 2019 – 2021

13. Reviewer, ICLR 2019 – 2024
14. Reviewer, AISTATS 2019 – 2021

## Talks

1. Foundation Models for Material Discovery Jul. 2025  
*Korea Institute of Material Science (KIMS), Changwon, South Korea*
2. Generative Models for Molecular Discovery Jul. 2025  
*Seoul National University, Seoul, South Korea*
3. A Generative Model for Metal Organic Frameworks Jul. 2025  
*KAIST-MILA Annual Workshop, Montreal, Canada*
4. Machine Learning for Transition Path Sampling Jul. 2025  
*Korean In silico bio Design and Discovery Society (KIDDS), Daejeon, South Korea*
5. Generative Models for Molecular Discovery May. 2025  
*LG AI Research, Seoul, South Korea*
6. Optimization Methods for Material Science Dec. 2024  
*POSCO Holdings, Seoul, South Korea*
7. Structure- and Energy-Based Machine Learning for Molecules Dec. 2024  
*KAIST-MILA Prefrontal AI Workshop, Montreal, Canada*
8. Amortizing Intractable Inference for Molecular Discovery Nov. 2024  
*Physics Informed Machine Learning Workshop, New Mexico, United States*
9. Opportunities and Challenges in Deep Graph Generative Models Nov. 2023  
*AI Korea, Seoul, South Korea*
10. Machine Learning for Drug Discovery Oct. 2023  
*Korea Advanced Institute of Science and Technology (KAIST), Daejeon, South Korea*
11. Graph Structured Prediction and Graph Generation with Deep Learning Jun. 2023  
*Korea Advanced Institute of Science and Technology (KAIST), Daejeon, South Korea*
12. Deep Neural Networks for Graph Optimization Nov. 2022  
*University of Arizona, Arizona, United States*
13. Geometric Deep Learning for Drug Discovery Aug. 2022  
*Korean Artificial Intelligence Association (KAIA), Jeju, South Korea*
14. Machine Learning for Drug Discovery Jun. 2022  
*Centre for Frontier AI Research, Singapore*
15. Elimination Techniques in Probabilistic Graphical Models Jun. 2021  
*Skolkovo Institute of Science and Technology (Skoltech), Moscow, Russia*
16. Guiding Deep Molecular Optimization with Genetic Exploration Dec. 2020  
*Samsung Advanced Institute of Technology (SAIT), Suwon, South Korea*

17. Scaling Deep Reinforcement Learning to Large Combinatorial Problems Feb. 2020  
*Pohang University of Science and Technology (POSTECH), Pohang, South Korea*
18. Bucket Renormalization for Approximate Inference Jul. 2018  
*University of Oxford, Oxford, England*
19. Mini-Bucket Renormalization Feb. 2018  
*Physics Informed Machine Learning Workshop, Santa Fe, New Mexico, United States*
20. Gauge Transformation of Graphical Models Jul. 2017  
*Los Alamos National Laboratory (LANL), New Mexico, United States*
21. Optimizing Gauge Transformation for Inference in Graphical Models Feb. 2017  
*Banff Workshop, Alberta, Canada*
22. Synthesis of MCMC and Belief Propagation Jul. 2016  
*Los Alamos National Laboratory (LANL), New Mexico, United States*
23. Minimum Weight Perfect Matching via Blossom Belief Propagation Nov. 2015  
*Korea Advanced Institute of Science and Technology (KAIST), Daejeon, South Korea*

## Courses

1. Proteins and AI (CoE499) Spring 2026  
*Korea Advanced Institute of Science and Technology (KAIST)*
2. Machine learning for molecules (AI899) Fall 2025  
*Korea Advanced Institute of Science and Technology (KAIST)*
3. Geometric deep learning (AI810) Spring 2025  
*Korea Advanced Institute of Science and Technology (KAIST)*
4. Introduction to artificial intelligence (CSED105) Fall 2024  
*Pohang University of Science and Technology (POSTECH)*
5. Machine learning for graphs (CSED/AIGS703I) Spring 2024  
*Pohang University of Science and Technology (POSTECH)*
6. Introduction to artificial intelligence (CSED105) Fall 2023  
*Pohang University of Science and Technology (POSTECH)*
7. Probabilistic graphical models (CSED/AIGS524) Spring 2023  
*Pohang University of Science and Technology (POSTECH)*
8. Introduction to machine learning (CSED490B) Fall 2022  
*Pohang University of Science and Technology (POSTECH)*
9. Probabilistic graphical models (CSED/AIGS524) Spring 2022  
*Pohang University of Science and Technology (POSTECH)*

## **Awards and Grants**

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|-------------------------------------|-------------|
| 1. KAIST Outstanding Teaching Award | Spring 2026 |
| 2. NVIDIA Academic Grant Program    | 2026        |
| 3. NVIDIA Academic Grant Program    | 2025        |
| 4. KAIST Q-Day Award                | Winter 2025 |