

Sukwon Yun

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RESEARCH INTEREST

AI for Science

Building AI systems that collaborate, learn from experiments, and close the loop in scientific discovery

- Methods: AI Co-Scientists, Multi-Agent Systems, Mixture-of-Experts, Multimodal Learning
- Domains: Single-Cell Biology, Protein Design

EDUCATION

University of North Carolina at Chapel Hill, Chapel Hill, NC, USA

Aug 2024 – Dec 2025

- M.S. in Computer Science (Advisor: [Prof. Tianlong Chen](#))

KAIST, Daejeon, South Korea

Aug 2021 – Aug 2023

- M.S. in Industrial and Systems Engineering (Advisor: [Prof. Chanyoung Park](#))

Hanyang University, Seoul, South Korea

Mar 2015 – Aug 2021

- B.S. in Industrial Engineering, *Summa Cum Laude* (incl. 2-year military service)

POSITIONS & RESEARCH EXPERIENCE

Xaira Therapeutics, South San Francisco, CA, USA

- AI Scientist

Sep 2026 – Present

- Manager: [Prof. Bo Wang](#)
- Test-time scaling and Post-training for De Novo Antibody Design

- AI Resident

Jun 2026 – Sep 2026

- Mentors: [Prof. Bo Wang](#), [Dr. Mehran Karimzadeh](#), [Dr. Yongju Lee](#)
- Project: Autoresearch for Virtual Cell

University of Washington, Seattle, WA, USA

May 2026 – Sep 2026

- Researcher

- Advisor: [Prof. Su-In Lee](#)
- Project: AI Co-Scientists with Bayesian Optimization (*MLCB 2026 Spotlight*)

Genentech, South San Francisco, CA, USA

May 2025 – Aug 2025

- Research Intern

- Mentors: [Prof. Aviv Regev](#), [Dr. Russell Littman](#)
- Project: Mixture-of-Experts for Vision Transformers (*NeurIPS 2025 AI for Science*)

Tokyo Institute of Technology (Tokyo Tech), Tokyo, Japan

Oct 2022 – Feb 2023

- Visiting Researcher

- Host: [Prof. Tsuyoshi Murata](#)
- Project: Graph Diffusion for Missing Feature Problem (*KDD 2025*)

SELECTED

PUBLICATIONS

(FULL LIST IN THE END)
*: Equal contribution

Graph-of-Agents: A Graph-Based Framework for Multi-Agent LLM Collaboration

Sukwon Yun, *et al.*, Tianlong Chen

International Conference on Learning Representations (**ICLR 2026**)

When to Trust Your AI Co-Scientist? Learning Prior Reliability in Closed-Loop Bayesian Optimization

Sukwon Yun, *et al.*, Su-In Lee

Machine Learning in Computational Biology (**MLCB 2026 Spotlight**)

Flex-MoE: Modeling Arbitrary Modality Combination via the Flexible Mixture-of-Experts

Sukwon Yun, *et al.*, Tianlong Chen

Conference on Neural Information Processing Systems (**NeurIPS 2024 Spotlight**)

Single-cell RNA-seq data imputation using Feature Propagation

Sukwon Yun*, *et al.*, Chanyoung Park

International Conference on Machine Learning (**ICML 2023 Workshop on Comp. Bio. Best Paper Award**)

AWARDS & SCHOLARSHIPS

NeurIPS Top Reviewer

2025

- The Thirty-Ninth Annual Conference on Neural Information Processing Systems, San Diego, CA, USA

Best Paper Award

2025

- AAAI Workshop on Large Language Models and Generative AI for Health, Philadelphia, PA, USA

Best Paper Award

2024

- KDD Workshop on Federated Learning for Data Mining and Graph Analytics, Barcelona, Spain

Best Paper Award

2023

- ICML Workshop on Computational Biology, Honolulu, Hawai'i, USA

	Korea National Scholarship ▪ Awarded by the Ministry of Science and ICT, South Korea	2021 – 2023
	Poster Competition Excellence Award ▪ Awarded at Industrial/Social Problem Solving Session held by Department of ISysE, KAIST	2022
	SIGIR Student Travel Award ▪ ACM International Conference on Information and Knowledge Management, Georgia, USA	2022
	Merit Based Scholarship ▪ Awarded by the Department of Industrial Engineering, Hanyang University	2021
	Hanyang Academic Achievement Award ▪ Awarded within the top 3% among the College of Engineering, Hanyang University	2021
	Certificate of Recognition ▪ Awarded when serving military service as an auxiliary police by Seoul Metropolitan Police	2018
TEACHING EXPERIENCE	University of North Carolina at Chapel Hill ▪ COMP283: Discrete Structures	Fall, 2025
	KAIST ▪ IE343: Statistical Machine Learning	Spring, 2022
PROFESSIONAL SERVICES	Event Organizations ▪ Session Chair, Knowledge Representation 3, Birmingham, UK, CIKM (2023)	
	Program Committee ▪ AAAI (2025, 2026)	
	Conference Reviews ▪ NeurIPS (2023 -), ICLR (2024 -), ICML (2024 -), CVPR (2025), ICCV (2025), ECCV (2024), MICCAI (2025), ACL (2025), COLM (2025), KDD (2025), CPAL (2024 -)	
	Workshop Reviews ▪ ICBINB-BIO @ NeurIPS (2026), GenAI4Health @ AAAI (2025), ML4LMS @ ICML (2024)	
FULL PUBLICATIONS *: Equal contribution #: Co-correspondence	CONFERENCES [C24] When to Trust Your AI Co-Scientist? Learning Prior Reliability in Closed-Loop Bayesian Optimization Sukwon Yun , Xiaojian Chen, Su-In Lee Machine Learning in Computational Biology (MLCB 2026 Spotlight)	
	[C23] SPATIA: Multimodal Generation and Prediction of Spatial Cell Phenotypes Zhenglun Kong, Mufan Qiu, John Boesen, Xiang Lin, Sukwon Yun , Tianlong Chen, Manolis Kellis, Marinka Zitnik International Conference on Machine Learning (ICML 2026)	
	[C22] Symbolic Mixture-of-Experts: Adaptive Skill-based Routing for Heterogeneous Reasoning Justin Chih-Yao Chen*, Sukwon Yun *, Elias Stengel-Eskin*, Tianlong Chen, Mohit Bansal International Conference on Machine Learning (ICML 2026)	
	[C21] Graph-of-Agents: A Graph-Based Framework for Multi-Agent LLM Collaboration Sukwon Yun , Jie Peng, Pingzhi Li, Wendong Fan, Jie Chen, James Zou, Guohao Li, Tianlong Chen International Conference on Learning Representations (ICLR 2026)	
	[C20] BetaConform: Efficient MAP Estimation of LLM Ensemble Judgment Performance with Prior Transfer Huaizhi Qu, Inyoung Choi, Zhen Tan, Song Wang, Sukwon Yun , Qi Long, Faizan Siddiqui, Kwonjoon Lee, Tianlong Chen Conference on Neural Information Processing Systems (NeurIPS 2025)	
	[C19] Training Robust Graph Neural Networks by Modeling Noise Dependencies Yeonjun In, Kanghoon Yoon, Sukwon Yun , Kibum Kim, Sungchul Kim, Chanyoung Park Conference on Neural Information Processing Systems (NeurIPS 2025)	
	[C18] Oldie but Goodie: Re-illuminating Label Propagation on Graphs with Partially Observed Features Sukwon Yun , Xin Liu, Yunhak Oh, Junseok Lee, Tianlong Chen, Tsuyoshi Murata, Chanyoung Park ACM SIGKDD Conference on Knowledge Discovery and Data Mining (KDD 2025)	

- [C17] Spatial Coordinates as a Cell Language: A Multi-Sentence Framework for Imaging Mass Cytometry Analysis
Chi-Jane Chen*, Yuhang Chen*, **Sukwon Yun***, Natalie Stanley, Tianlong Chen
Annual Meeting of the Association for Computational Linguistics (**ACL 2025 Findings**)
- [C16] GRNFormer: A Biologically-Guided Framework for Integrating Gene Regulatory Networks into RNA Foundation Models
Mufan Qiu, Xinyu Hu, Fengwei Zhan, **Sukwon Yun**, Jie Peng, Ruichen Zhang, Bhavya Kailkhura, Jiekun Yang, Tianlong Chen
Annual Meeting of the Association for Computational Linguistics (**ACL 2025 Findings**)
- [C15] Agents Under Siege: Breaking Pragmatic Multi-Agent LLM Systems with Optimized Prompt Attacks
Rana Shahroz, Zhen Tan, **Sukwon Yun**, Charles Fleming, Tianlong Chen
Annual Meeting of the Association for Computational Linguistics (**ACL 2025 Oral**)
- [C14] I²MoE: Interpretable Multimodal Interaction-aware Mixture-of-Experts
Jiayi Xin, **Sukwon Yun**, Jie Peng, Inyoung Choi, Jenna L. Ballard, Tianlong Chen, Qi Long
International Conference on Machine Learning (**ICML 2025**)
- [C13] Modalities Contribute Unequally: Enhancing Medical Multi-modal Learning through Adaptive Modality Token Re-balancing
Jie Peng, Jenna L. Ballard, Mohan Zhang, **Sukwon Yun**, Jiayi Xin, Qi Long, Yanyong Zhang, Tianlong Chen
International Conference on Machine Learning (**ICML 2025**)
- [C12] Sparse MoE as a New Treatment: Addressing Forgetting, Fitting, Learning Issues in Multi-Modal Multi-Task Learning
Jie Peng, **Sukwon Yun**, Kaixiong Zhou, Ruida Zhou, Thomas Hartvigsen, Yanyong Zhang, Zhangyang Wang, Tianlong Chen
Conference on Parsimony and Learning (**CPAL 2025**)
- [C11] Cut the Crap: An Economical Communication Pipeline for LLM-based Multi-Agent Systems
Guibin Zhang, Yanwei Yue, Zhixun Li, **Sukwon Yun**, Guancheng Wan, Kun Wang, Dawei Cheng, Jeffrey Xu Yu, Tianlong Chen
International Conference on Learning Representations (**ICLR 2025**)
- [C10] PortLLM: Personalizing Evolving Large Language Models with Training-Free and Portable Model Patches
Rana Muhammad Shahroz Khan, Pingzhi Li*, **Sukwon Yun***, Zhenyu Wang, Shahriar Nirjon, Chau-Wai Wong, Tianlong Chen
International Conference on Learning Representations (**ICLR 2025**)
- [C9] Subgraph Federated Learning for Local Generalization
Sungwon Kim, Yoonho Lee, Yunhak Oh, Namkyeong Lee, **Sukwon Yun**, Junseok Lee, Sein Kim, Carl Yang, Chanyoung Park
International Conference on Learning Representations (**ICLR 2025 Oral**)
- [C8] Flex-MoE: Modeling Arbitrary Modality Combination via the Flexible Mixture-of-Experts
Sukwon Yun, Inyoung Choi, Jie Peng, Yangfan Wu, Jingxuan Bao, Qiyiwen Zhang, Jiayi Xin, Qi Long[#], Tianlong Chen[#]
Conference on Neural Information Processing Systems (**NeurIPS 2024 Spotlight**)
- [C7] DALK: Dynamic Co-Augmentation of LLMs and KG to answer Alzheimer’s Disease Questions with Scientific Literature
Dawei Li, Shu Yang, Zhen Tan, Jae Young Baik, **Sukwon Yun**, Joseph Lee, Aaron Chacko, Bojian Hou, Duy Duong-Tran, Ying Ding, Huan Liu, Li Shen, Tianlong Chen
Conference on Empirical Methods in Natural Language Processing (**EMNLP 2024 Findings**)
- [C6] Mew: Multiplexed Immunofluorescence Image Analysis through an Efficient Multiplex Network
Sukwon Yun, Jie Peng, Alexandro Trevino, Chanyoung Park, Tianlong Chen
European Conference on Computer Vision (**ECCV 2024**)

- [C5] DEGNN: Dual Experts Graph Neural Network Handling Both Edge and Node Feature Noise
Tai Hasegawa, **Sukwon Yun**, Xin Liu, Yin Jun Phua, Tsuyoshi Murata
Pacific-Asia Conference on Knowledge Discovery and Data Mining (**PAKDD 2024**)
- [C4] MUSE: Music Recommender System with Shuffle Play Recommendation Enhancement
Yunhak Oh*, **Sukwon Yun***, Dongmin Hyun, Sein Kim, Chanyoung Park
ACM International Conference on Information and Knowledge Management (**CIKM 2023**)
- [C3] S-Mixup: Structural Mixup for Graph Neural Networks
Junghurn Kim*, **Sukwon Yun***, Chanyoung Park
ACM International Conference on Information and Knowledge Management (**CIKM 2023 Short**)
- [C2] MELT: Mutual Enhancement of Long-Tailed User and Item for Sequential Recommendation
Kibum Kim, Dongmin Hyun, **Sukwon Yun**, Chanyoung Park
ACM SIGIR Conference on Research and Development in Information Retrieval (**SIGIR 2023**)
- [C1] LTE4G: Long-Tail Experts for Graph Neural Networks
Sukwon Yun, Kibum Kim, Kanghoon Yoon, Chanyoung Park
ACM International Conference on Information and Knowledge Management (**CIKM 2022**)

JOURNALS

- [J2] Single-cell multiregion epigenomic rewiring in Alzheimer’s disease progression and cognitive resilience
Zunpeng Liu*, Shanshan Zhang*, Benjamin T. James, Kyriaki Galani, Riley J. Mangan, Stuart Benjamin Fass, Chuqian Liang, Manoj M Wagle, Carles A. Boix, Yosuke Tanigawa, **Sukwon Yun**, Yena Sung, Xushen Xiong, Na Sun, Lei Hou, Martin Wohlwend, Mufan Qiu, Xikun Han, Lei Xiong, Efthalia Preka, Lei Huang, William F. Li, Li-Lun Ho, Amy Grayson, Julio Mantero, Alexey Kozlenkov, Hansruedi Mathys, Tianlong Chen, Stella Dracheva, David A. Bennett, Li-Huei Tsai, Manolis Kellis
Cell 2025
- [J1] Single-cell RNA sequencing data imputation using bi-level feature propagation
Junseok Lee*, **Sukwon Yun***, Yeongmin Kim, Tianlong Chen, Manolis Kellis, Chanyoung Park
Briefings in Bioinformatics 2024

WORKSHOPS

- [W7] Sparse Mixture-of-Experts for Multi-Channel Imaging: Are All Channel Interactions Required?
Sukwon Yun, Heming Yao, Burkhard Hoeckendorf, David Richmond, Aviv Regev[#], Russell Littman[#]
NeurIPS 2025 AI for Science
- [W6] Graph-of-Agents: A Graph-Based Framework for Multi-Agent LLM Collaboration
Sukwon Yun, Jie Peng, Pingzhi Li, Wendong Fan, Jie Chen, James Zou, Guohao Li, Tianlong Chen
ICML 2025 MAS
- [W5] One Leaf Knows Autumn: A Piece of Data-Model Facilitates Efficient Cancer Prognosis with Histological and Genomic Modalities
Jie Peng, Jingxia Jiang, Yueliang Ying, **Sukwon Yun**, Qi Long, Yanyong Zhang, Tianlong Chen
AAAI GenAI4Health 2025
- [W4] Generate, Then Retrieve: Addressing Missing Modalities in Multimodal Learning via Generative AI and MoE
Sukwon Yun*, Jiayi Xin*, Inyoung Choi, Jie Peng, Qi Long, Tianlong Chen
AAAI GenAI4Health 2025 Best Paper Award
- [W3] Subgraph Federated Learning for Local Generalization
Sungwon Kim, Yoonho Lee, Yunhak Oh, Namkyeong Lee, **Sukwon Yun**, Junseok Lee, Sein Kim, Carl Yang, Chanyoung Park
KDD 2024 FedKDD Best Paper Award
- [W2] Noise Robust Graph Learning under Feature-Dependent Graph-Noise
Yeonjun In, Kanghoon Yoon, **Sukwon Yun**, Kibum Kim, Sungchul Kim, Chanyoung Park
WWW 2024 DCAI Oral
- [W1] Single-cell RNA-seq data imputation using Feature Propagation
Sukwon Yun*, Junseok Lee*, Chanyoung Park
ICML 2023 WCB Best Paper Award