Janghoon Ock

Assistant Professor

Department of Chemical and Biomolecular Engineering, University of Nebraska–Lincoln

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PROFESSIONAL EXPERIENCES

Assistant Professor Aug. 2025 – Present
Department of Chemical & Biomolecular Engineering, University of Nebraska–Lincoln
Courtesy Appointment, Department of Mechanical & Materials Engineering

BK Global Visiting Fellow *at Seoul National University, Seoul, Korea* Jun. – Aug. 2026

Research Intern at *Energy & Materials Division, Toyota Research Institute, Los Altos, CA* May. – Aug. 2024

Associate Researcher at *R&D Center, SK Innovation, Daejeon, Korea* Jan. 2018 – Jul. 2021

EDUCATION

Ph.D. **Carnegie Mellon University** Aug. 2025
Chemical Engineering (Advisor: Prof. Amir Barati Farimani)

M.S. **Seoul National University** Feb. 2018
Chemical and Biological Engineering (Advisor: Prof. Kyung Hyun Ahn)

B.S. **Seoul National University** Feb. 2016
Chemical and Biological Engineering

PUBLICATIONS

† co-first authorship; * corresponding authorship

Peer-reviewed Journal Articles

11. A. Chaudhari, J. Ock*, A. Barati Farimani*, "Modular Large Language Model Agents for Multi-Task Computational Materials Science", ***Communications Materials***, 2026. [Link]
10. Y. Yeh†, J. Ock†, A. Chandrasekhar, S. Maheshwari, A. Barati Farimani*, "Text. to Band Gap: Pre-trained Language Models as Encoder for Semiconductor Band Gap Prediction", ***Computational Materials Science***, 2026. [Link]
9. J. Ock†, R. S. Meda†, S. Badrinarayanan, N. Aluru, A. Chandrasekhar, A. Barati Farimani*, "Large Language Model Agent for Modular Task Execution in Drug Discovery", ***Journal of Chemical Information and Modeling***, 2026. [Link]
8. J. Ock, R. S. Meda, T. Vinchurkar, Y. Jadhav, A. Barati Farimani*, "Adsorb-Agent: Autonomous Identification of Stable Adsorption Configurations via Large Language Model Agent", ***Digital Discovery***, 2026. [Link]
7. T. Zeng, S. Badrinarayanan, J. Ock, C. Lai, A. Barati Farimani*, "LLM-guided Chemical Process Optimization with a Multi-Agent Approach", ***Machine Learning: Science and Technology****, 2025*. [Link]
6. J. Ock, S. Badrinarayanan, R. Magar, A. Antony, A. Barati Farimani*, "Multimodal Language and Graph Learning of Adsorption Configuration in Catalysis," ***Nature Machine Intelligence***, 2024. [Link]
5. J. Ock, P. Mollaei, A. Barati Farimani*, "GradNav: Accelerated Exploration of Potential Energy Surfaces with Gradient-Based Navigation," ***Journal of Computational Theory and Chemistry***, 2024. [Link]
4. Z. Cao, O. Barati Farimani, J. Ock, A. Barati Farimani*, "Machine Learning in Membrane Design: From Property Prediction to AI-Guided Optimization", ***Nano Letters***, 2024. [Link]
3. J. Ock, C. Guntuboina, A. Barati Farimani*, "Catalyst Energy Prediction with *CatBERTa*: Unveiling Feature Exploration Strategies through Large Language Models," ***ACS Catalysis***, 2023. [Link]
2. J. Ock, T. Tian, J. Kitchin, Z. Ulissi*, "Beyond Independent Error Assumptions in Large GNN Atomistic

Models," ***Journal of Chemical Physics***, 2023. (Featured Article) [Link]

1. J. Ock, J.S. Hong*, and K.H. Ahn, "Acceleration of Instability during the Capillary Thinning Process due to the Addition of Particles to a Poly(ethylene oxide) Solution," ***Journal of Non-Newtonian Fluid Mechanics***, 2018. [Link]

Preprint

3. A. Chandrasekhar, J. Ock, A. Barati Farimani*, "Catalyst-Agent: Autonomous heterogeneous catalyst screening with an LLM agent", *arXiv:2603.01311*, 2026. [Link] (will be submitted in June 2026)
2. S. Badrinarayanan, Y. Su, J. Ock, A. Pham, S. Ahuja, A. Barati Farimani*, "Meta-Learning for Cross-Task Generalization in Protein Mutation Property Prediction", *arXiv:2510.20943*, 2025. [Link] (will be submitted in July 2026)
1. S. Maheshwari†, Z. Tang†, J. Ock, A. Kolluru, J. R. Kitchin, A. Barati Farimani*, "Beyond Force Metrics: Pre-training MLFFs for Stable MD Simulations", *arXiv:2506.14850*, 2025. [Link] (will be submitted in July 2026)

PATENTS

3. H.S. Kim, J. Ock, Y.J. Yim, B.C. Kang, "Electrode coating device," US20240162407A1 (filed)
2. I.H. Song, H.C. Kim, J. Ock, J.A. Lee, W.J. Jeong, "Method of producing ethylene-carboxylic acid copolymer," US12391776B2
1. H.S. Lee, S.J. Kim, J.H. Park, M.G. Kim, J. Ock, "Method of producing ethylene-carboxylic acid copolymer," US11685795B2

PRESENTATIONS

Conference Presentations

11. Adsorb-Agent: LLM-driven Autonomous Identification of Stable Adsorption Configurations, *AIChE 2025 Fall Annual Meeting*
10. LLM-Powered Agent for Identifying Stable Adsorption Configurations on Catalytic Surfaces, *AIChE 2025 Fall Annual Meeting*
9. Large Language Model and Multimodal Learning Framework for Catalyst Discovery, *AIChE 2024 Fall Annual Meeting*
8. Tying It All Together: Multimodal Learning in Catalyst and Inorganic Crystal Exploration, *AIChE 2024 Fall Annual Meeting*
7. Multimodal Language and Graph Learning of Adsorption Energy Prediction, *AIChE 2024 Fall Annual Meeting*
6. Catberta: Catalyst Energy Prediction and Feature Analysis through Language Models, *AIChE 2024 Fall Annual Meeting*
5. CarBERTa and Graph-assisted Pretraining for Open Catalyst Challenge, *AI for Science Workshop, Open Catalyst Challenge Lightening Talk, NeurIPS 2023. (Invited)*
4. Machine Learning Potential for Preferred Adsorption Site Prediction, *KIChE-US Chapter Open Forum, AIChE 2022 Fall Annual Meeting. (Invited)*
3. Machine Learning Potential for site enumeration prediction, *AIChE 2022 Fall Annual Meeting*
2. Correlations in adsorption energy uncertainties in Open Catalyst dataset, *PCCS 2022*
1. Experimental study on aggregates breakage under extensional flow, *KIChE 2017* Spring Annual Meeting

Invited Seminar Talks and Workshops

3. Reimagining Catalyst Discovery with Large Language Models, *Dankook University*, Nov 2025 (virtual)

2. Bridging Text, Graph, and Action: AI-assisted Catalyst Discovery, Bridging Text, Graph, and Action: AI-assisted Catalyst Discovery

   Department of Mechanical and Materials Engineering, University of Nebraska-Lincoln, Oct 2025

   Department of Chemical and Biomolecular Engineering, University of Nebraska-Lincoln, Feb 2025

   SK Innovation, KRICT, KAIST ECE Dr. Jaemin Yoo's group, Mar 2025

1. Catalyst Property Prediction with CatBERTa: Unveiling Feature Exploration Strategies through Large Language Models, *Crunch Seminar, Brown University*, Oct 2023. (virtual) [Link]

Others

2. Language Model and Multimodal Enhancement for Adsorption Energy Modeling, *Kitchin Group Seminar*, *Carnegie Mellon University*, Feb 2024
1. Instabilities in Capillary Thinning of Complex Fluids, *EEPL Group Seminar, Dankook University*, Oct 2023

GRANT PROPOSALS

Submitted

5. DOE Genesis Mission, "From Observables to Connectivity: Learning and Designing Self-assembly of Disordered System via Graph-Based Machine Learning", Budget: $748,912, PI: Janghoon Ock, Co-PI: Ravi Saraf, In Soo Kim
4. DOE Genesis Mission, "From Patterns to Function: AI-Driven Reverse Ecology for Predicting Microbial Interactions and Community Function", Budget: $749,917, PI: Hyun-Seob Song, Co-PI: Janghoon Ock
3. NSF CHE-DRP, "ML-Assisted Molecular Design of Decoupled Conductivity-Viscosity in Complex Electrolytes", Budget: $594,177, PI: Vitaly Alexandrov, Co-PI: Janghoon Ock
2. NSF EPSCoR, "WISE-AI: Wastewater Innovation for Sustainable Treatment of Emerging Contaminants Guided by AI", Budget $2,078,655, PI: Isabel Escobar & Nirupam Aich, Co-PI: Janghoon Ock
1. NSF EPSCoR, "Coordinated Research Infrastructure and Training for Critical Mineral Recovery through Ligand Networks and AI-Driven Approaches", Budget: $1,500,000, PI: Kavita Sharma & Barry Cheung, Key personnel: Janghoon Ock

TEACHING AND MENTORING

Teaching	CHME212: Introduction to Chemical Engineering Computation	Spring 2026
	CHME482/882: Polymers (Guest Lecture: Accelerating Materials Innovation with ML)	Nov. 2026
	06663A: Analysis and Modeling of Transport Phenomena (T.A.)	Spring 2022 & 2023
	06705A: Advanced Chemical Engineering Thermodynamics (T.A.)	Fall 2022

Mentoring

University of Nebraska–Lincoln

Ph.D. Obed Issakah (Spring 2026–Present)

Undergrad. Tran Nhat Khang Nguyen (Spring 2026–Present), Noah Hazen (Spring 2026–Present), Anh Nguyen (Summer 2026–Present)

Carnegie Mellon University

Jonghoon Park (ChemE M.S., Fall 2023), Gauri Dalwankar (ChemE M.S., Fall 2023), Tirtha Vinchurkar (ChemE M.S., Fall 2023–Fall 2024), Ying-Ting Yeh (ChemE M.S., Fall 2023–Spring 2025), Genmao Zhuang (MSE M.S., Fall 2024), Srivathsan Badrinarayanan (ChemE M.S., Summer 2024), Shagun Maheshwari (MSE B.S., Fall 2024–Spring 2025), Cheng Kai Lai (ChemE M.S., Spring 2025), Tong Zheng (ChemE M.S., Spring

2025), Tom Li (ChemE M.S., Spring 2025–Fall 2025), Zhengxian Tang (MSE M.S., Fall 2024–Spring 2026), Jennifer Gonzales-Pasion (ChemE M.S., Fall 2025–Present)

AWARDS AND HONORS

2025	Ken Meyer Award (research excellence award), Carnegie Mellon University
2024 – 2025	H. Robert Sharbaugh Presidential Fellowship, Carnegie Mellon University
2024, 2022	Hanwha Travel Award (AIChE 2024, 2022 Annual Meeting), Hanwha Solution
2023	Bradford and Diane Smith Graduate Fellowship, Carnegie Mellon University
2016 – 2017	Brain Korea 21 Plus, BK21 Plus Groups
2016	Merit-based Scholarship (2nd semester, full tuition), Seoul National University
2013	Samsung Mentoring Scholarship, Samsung Welfare Foundation
2009 – 2014	National Science and Technology Scholarship (full tuition), Ministry of Science, Korea

ACADEMIC SERVICE

Reviewer	Nature Machine Intelligence, npj Computational Materials, Journal of Chemical Information and Modeling, Cell Reports Physical Science, Digital Discovery
Memberships	American Institute of Chemical Engineering (AIChE)
	Korean Institute of Chemical Engineering (KIChE)
UNL Internal	The Prairie AI Initiative Committee (2025–Present)