Shengli (Bruce) Jiang

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Education

University of Wisconsin-Madison, Madison, WI — 2023
Ph.D. in Chemical Engineering (Advisor: Victor M. Zavala)
Thesis: *Data Representations and Transformations in Chemical Engineering*

University of California, San Diego, La Jolla, CA — 2018
B.S. in Chemical Engineering (Advisor: Zheng Chen)

Appointments

Incoming Assistant Professor — Starting August 2026
University of South Carolina, Columbia, SC
Department of Chemical Engineering
Principal Investigator, Computational Materials and Product Design (CMPD) Laboratory

Postdoctoral Associate — 2023–2026
Princeton University, Princeton, NJ
Department of Chemical and Biological Engineering (Advisor: Michael A. Webb)
Research: *Polymer design using machine learning and molecular dynamics simulations*

Lecturer — 2024–2025
Princeton University, Princeton, NJ
Department of Chemical and Biological Engineering
Course: *Machine learning in chemical science and engineering*

Research Intern — 2022
Dow Chemical, Freeport, TX
Chemometrics and Artificial Intelligence Group
Research: *Electricity price forecasting; large language models for quality note analysis*

Givens Associate — 2020
Argonne National Laboratory, Lemont, IL
Mathematics and Computer Science Division
Research: *Graph neural architecture search for molecular property prediction*

Undergraduate Researcher — 2016–2018
University of California, San Diego, La Jolla, CA
Department of NanoEngineering
Research: *Design of organic cathodes for lithium-ion batteries*

Publications

Journal Publications

[J21] **S. Jiang** and M. A. Webb. Generative active learning across polymer architectures and solvophobicities for targeted rheological behavior. *npj Computational Materials*, 2025. doi:10.1038/s41524-025-01900-2.

[J20] **S. Jiang** and M. A. Webb. Physics-guided neural networks for transferable property prediction in architecturally diverse copolymers. *Macromolecules*, 58(10):4971–4984, 2025. doi:10.1021/acs.macromol.5c00720.

[J19] S. Dhamankar*, **S. Jiang***, and M. A. Webb. Accelerating multicomponent phase-coexistence calculations with physics-informed neural networks. *Molecular Systems Design & Engineering*, 10(2):89–101, 2025. doi:10.1039/D4ME00168K. *Equal contribution.

[J18] L. D. González, J. L. Pulsipher, **S. Jiang**, A. Mukherjee, T. Soderstrom, and V. M. Zavala. A digital twin simulator of a pastillation process with applications to automatic control based on computer vision. *Computers & Chemical Engineering*, 201:109205, 2025. doi:10.1016/j.compchemeng.2025.109205.

[J17] J. E. González-Pérez, **S. Jiang**, O. Jiménez-González, V. M. Zavala, A. Romo-Hernández, J. Á. Guerrero-Beltrán, A. López-Malo, and N. Ramírez-Corona. Implementing Topological Data Analysis for Monitoring Mass Transfer during Vacuum-Assisted Osmotic Dehydration of Apples. *ACS Omega*, 2025. doi:10.1021/acsomega.5c00531.

[J16] C. Lucky, **S. Jiang**, C.-R. Shih, V. M. Zavala, and M. Schreier. Understanding the interplay between electrocatalytic C(sp3)–C(sp3) fragmentation and oxygenation reactions. *Nature Catalysis*, 7(1):1–11, 2024. doi:10.1038/s41929-024-01218-0.

[J15] **S. Jiang**, A. B. Dieng, and M. A. Webb. Property-guided generation of complex polymer topologies using variational autoencoders. *npj Computational Materials*, 10(1):139, 2024. doi:10.1038/s41524-024-01328-0.

[J14] **S. Jiang**, S. Qin, R. C. Van Lehn, P. Balaprakash, and V. M. Zavala. Uncertainty quantification for molecular property predictions with graph neural architecture search. *Digital Discovery*, 3(8):1534–1553, 2024. doi:10.1039/D4DD00088A.

[J13] F. Long*, **S. Jiang***, E. Bar-Ziv, and V. M. Zavala. Robust plastic waste classification using wavelet transform multi-resolution analysis and convolutional neural networks. *Computers & Chemical Engineering*, 181:108516, 2024. doi:10.1016/j.compchemeng.2023.108516. *Equal contribution.

[J12] **S. Jiang**, N. Bao, A. D. Smith, S. Byndoor, R. C. Van Lehn, M. Mavrikakis, N. L. Abbott, and V. M. Zavala. Scalable extraction of information from spatiotemporal patterns of chemoresponsive liquid crystals using topological descriptors. *The Journal of Physical Chemistry C*, 127(32):16081–16098, 2023. doi:10.1021/acs.jpcc.3c03076.

[J11] S. Qin, **S. Jiang**, J. Li, P. Balaprakash, R. C. Van Lehn, and V. M. Zavala. Capturing molecular interactions in graph neural networks: a case study in multi-component phase equilibrium. *Digital Discovery*, 2(1):138–151, 2023. doi:10.1039/D2DD00045H.

[J10] F. Long*, **S. Jiang***, A. G. Adekunle, V. M. Zavala, and E. Bar-Ziv. Online characterization of mixed plastic waste using machine learning and mid-infrared spectroscopy. *ACS Sustainable Chemistry & Engineering*, 10(48):16064–16069, 2022. doi:10.1021/acssuschemeng.2c06052. *Equal contribution.

[J9] N. Bao*, **S. Jiang***, A. Smith, J. J. Schauer, M. Mavrikakis, R. C. Van Lehn, V. M. Zavala, and N. L. Abbott. Sensing gas mixtures by analyzing the spatiotemporal optical responses of liquid crystals using 3D convolutional neural networks. *ACS Sensors*, 7(9):2545–2555, 2022. doi:10.1021/acssensors.2c00362. *Equal contribution.

[J8] **S. Jiang**, Z. Xu, M. Kamran, S. Zinchik, S. Paheding, A. G. McDonald, E. Bar-Ziv, and V. M. Zavala. Using ATR-FTIR spectra and convolutional neural networks for characterizing mixed plastic waste. *Computers & Chemical Engineering*, 155:107547, 2021. doi:10.1016/j.compchemeng.2021.107547.

[J7] S. Zinchik, **S. Jiang**, S. Friis, F. Long, L. Høgstedt, V. M. Zavala, and E. Bar-Ziv. Accurate characterization of mixed plastic waste using machine learning and fast infrared spectroscopy. *ACS Sustainable Chemistry & Engineering*, 9(42):14143–14151, 2021. doi:10.1021/acssuschemeng.1c04281.

[J6] **S. Jiang** and V. M. Zavala. Convolutional neural nets in chemical engineering: Foundations, computations, and applications. *AIChE Journal*, 67(9):e17282, 2021. doi:10.1002/aic.17282.

[J5] **S. Jiang**, J. Noh, C. Park, A. D. Smith, N. L. Abbott, and V. M. Zavala. Using machine learning and liquid crystal droplets to identify and quantify endotoxins from different bacterial species. *Analyst*, 146(4):1224–1233, 2021. doi:10.1039/D0AN02220A.

[J4] A. K. Chew, **S. Jiang**, W. Zhang, V. M. Zavala, and R. C. Van Lehn. Fast predictions of liquid-phase acid-catalyzed reaction rates using molecular dynamics simulations and convolutional neural networks. *Chemical Science*, 11(46):12464–12476, 2020. doi:10.1039/D0SC03261A.

[J3] F. Ji, L. Wang, J. Yang, X. Wu, M. Li, **S. Jiang**, S. Lin, and Z. Chen. Highly compact, free-standing porous electrodes from polymer-derived nanoporous carbons for efficient electrochemical capacitive deionization. *Journal of Materials Chemistry A*, 7(4):1768–1778, 2019. doi:10.1039/C8TA10268F.

[J2] F. Ji, Y. Shi, M. Li, **S. Jiang**, G. Chen, F. Liu, and Z. Chen. Scalable synthesis of uniform nanosized microporous carbon particles from rigid polymers for rapid ion and molecule adsorption. *ACS Applied Materials & Interfaces*, 10(30):25429–25437, 2018. doi:10.1021/acsami.8b07353.

[J1] Y. Shi, H. Tang, **S. Jiang**, L. V. Kayser, M. Li, F. Liu, F. Ji, D. J. Lipomi, S. P. Ong, and Z. Chen. Understanding the electrochemical properties of naphthalene diimide: implication for stable and high-rate lithium-ion battery

electrodes. *Chemistry of Materials*, 30(10):3508–3517, 2018. doi:10.1021/acs.chemmater.8b01304.

Conference Publications

[C2] Y. Peng, Z. Wang, I. Castillo, L. Gunnell, and **S. Jiang**. A new modeling framework for real-time extreme electricity price forecasting. In *12th IFAC International Symposium on Advanced Control of Chemical Processes*. IFAC, 2024. doi:10.1016/j.ifacol.2024.08.451.

[C1] **S. Jiang** and P. Balaprakash. Graph neural network architecture search for molecular property prediction. In *2020 IEEE International Conference on Big Data*, pages 1346–1353. IEEE, 2020. doi:10.1109/BigData50022.2020.9378060.

Book Chapters, Technical Reports, and Others

[B1] **S. Jiang**, S. Qin, J. L. Pulsipher, and V. M. Zavala. Convolutional neural networks: Basic concepts and applications in manufacturing. In *Artificial Intelligence in Manufacturing*, pages 63–102. Elsevier, 2024. doi:10.1016/B978-0-323-99134-6.00007-4.

Presentations

Invited Talks

[T4] Polymer physics meets machine learning: A synergistic approach to complex polymer design. *MIT PSE Seminar*, Cambridge, MA, 2025.

[T3] Physics-informed machine learning for complex polymer design. *Yungu Young Scholars Forum 2025*, Hangzhou, China, 2025.

[T2] Scalable extraction of information from spatio-temporal responses of liquid crystals using topology. *PPG Graduate Student Symposium*, Madison, WI, 2023.

[T1] Real-time characterization of mixed plastic waste using machine learning and infrared spectroscopy. *FOCAPO-CPC*, San Antonio, TX, 2023.

Conference Talks

[K14] Physics-guided, data-driven design of polymer chemistry and architecture for tuning rheological properties. *MRS Fall Meeting & Exhibit*, Boston, MA, 2025.

[K13] Accelerating multicomponent phase-coexistence calculations with physics-informed neural networks. *AIChE Annual Meeting*, Boston, MA, 2025.

[K12] Data-driven design of polymer chemistry and architecture for tuning rheological properties. *AIChE Annual Meeting*, Boston, MA, 2025.

[K11] Data-centric modeling, design, and optimization of soft materials. *AIChE Annual Meeting*, Boston, MA, 2025.

[K10] Property-guided generation of complex polymer topologies using variational autoencoders. *AIChE Annual Meeting*, San Diego, CA, 2024.

[K9] Physics-guided machine learning for transferable prediction of polymer properties. *AIChE Annual Meeting*, San Diego, CA, 2024.

[K8] Polymer physics meets machine learning: A symbiosis to unravel polymer complexity in design. *ACS Annual Meeting*, Denver, CO, 2024.

[K7] Property-guided generation of topologically complex polymers using variational autoencoders. *ACS Annual Meeting*, Denver, CO, 2024.

[K6] Molecular property uncertainty quantification using automatic graph neural architecture search. *AIChE Annual Meeting*, Phoenix, AZ, 2022.

[K5] Characterization of chemoresponsive liquid crystals using topological descriptors and machine learning. *AIChE Annual Meeting*, Phoenix, AZ, 2022.

[K4] Rapid and real-time mixed-plastic waste analysis using infrared spectroscopy and machine learning. *AIChE Annual Meeting*, Boston, MA, 2021.

[K3] Characterizing complex solvent environments in acid-catalyzed reactions using molecular dynamics simulations and 3D convolutional neural nets. *AIChE Annual Meeting*, Virtual, 2020.

[K2] Color as a source of information in liquid crystal sensors. *AIChE Annual Meeting*, Virtual, 2020.

[K1] Endotoxin sensors using liquid crystals and machine learning. *AIChE Annual Meeting*, Orlando, FL, 2019.

Honors and Awards

Givens Associate Fellowship, Argonne National Laboratory 2020

Poster Award, Computing in Engineering Forum, University of Wisconsin-Madison 2020

Travel Award, Machine Learning in Science and Engineering (MLSE), Georgia Institute of Technology 2019

Provost Honors, University of California, San Diego 2014–2018

Research Grants

NSF BIO-AI: Designing plant rhizobacteria communities for sustainable agriculture ($944,832), *PI: Jonathan M. Conway; Co-PI: Michael A. Webb.* Contributed to proposal writing (AI components).

Mentoring Experience

Princeton University, Princeton, NJ

Andrew Chen (PhD Student, 2025)
Marios Giannakou (Visiting Scholar, 2025)
Michelle Gao (Laboratory Learning Program Intern, 2024)
Sophia Colmenares (Senior Thesis, 2023–2024)

University of Wisconsin-Madison, Madison, WI

Yoonsung Jeong (Informatics Skunkworks Researcher, 2021–2023)
Tatchapol Jettanachai (Informatics Skunkworks Researcher, 2021–2022)
Mushtaq Mohamud Ali (URS Scholar, 2021–2022)
Jaehun Kim (URS Scholar, 2021–2022)
Shraddha Byndoor (URS Scholar, 2021–2022)
Sydney Knepfel (Undergraduate Researcher, 2021–2022)
Khoa Bui (Undergraduate Researcher, 2021–2022)
Aditya Sharma (Undergraduate Researcher, 2020–2021)

Teaching Experience

Princeton University, Princeton, NJ

Machine Learning in Chemical Science and Engineering (Lecturer) Fall 2024

University of Wisconsin-Madison, Madison, WI

Statistics for Chemical Engineers (Teaching Assistant) Spring 2021
Introduction to Chemical Process Modeling (Teaching Assistant) Spring 2020

University of California, San Diego, La Jolla, CA

Physical Chemistry (Undergraduate Teaching Assistant) Spring 2015

Professional Services

Peer Review

Journals: *Chemical Reviews; Chemical Science; npj Computational Materials; Environmental Science & Technology; Expert Systems With Applications; Waste Management; Digital Discovery; Journal of Chemical Information and Modeling; Molecular Systems Design & Engineering; Communications Chemistry; Chemical Engineering Science; Computers & Chemical Engineering; Engineering Applications of Artificial Intelligence; Industrial & Engineering Chemistry Research; Computational Materials Science; RSC Advances; ACS Omega; Journal of Computational Physics; Engineering Reports; Chinese Journal of Chemical Engineering.*

Conferences: *American Control Conference; IEEE Conference on Decision and Control.*

Committee Service

Department DECI Committee Member, Princeton University 2023–2025
Department DEI Committee Member, University of Wisconsin-Madison 2022–2023

Professional Affiliations

American Chemical Society (Computers in Chemistry Division)

American Institute of Chemical Engineers

Materials Research Society

Software Products

[S4] **AutoGNNUQ (Main Developer)**

- Uncertainty quantification for molecular property predictions with graph neural architecture search [link].

[S3] **TopoGNN (Main Developer)**

- Property-guided generation of complex polymer topologies using variational autoencoders [link].

[S2] **GCGNN (Main Developer)**

- Physics-guided neural networks for transferable prediction of polymer properties [link].

[S1] **DeepHyper (Contributor)**

- Scalable neural architecture and hyperparameter search for deep neural networks [link].

Last updated: April 3, 2026