Shengli (Bruce) Jiang

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EDUCATION

University of Wisconsin-Madison 2018–Present
Ph.D. Candidate in Chemical Engineering (Minor in Computer Science)
Advisor: Victor M. Zavala
Research Area: Geometric Deep Learning, Topological Data Analysis, Sustainability

University of California, San Diego 2014–2018
B.S. in Chemical Engineering (Magna Cum Laude)
Advisor: Zheng Chen
Research Area: Lithium-ion Battery Cathode Material Design

WORK EXPERIENCE

Dow Inc. 2022
Chemoinformatics, Statistics and AI Group
Supervisors: Zhenyu Wang and Ivan Castillo
- Extreme Electricity Price Prediction Using Autoencoders and Long Short-term Memory
- Text Root Cause Analysis Using Natural Language Processing and Graph Neural Networks

Argonne National Laboratory 2020
Mathematics and Computer Science Division
Supervisor: Prasanna Balaprakash
- Molecular Property Prediction Using Neural Architecture Search and Graph Neural Networks

MENTORING EXPERIENCE

- **Yoonsung Jeong** (Informatics Skunkworks Student) 2022–Present
- **Tatchapol Jettanachai** (Informatics Skunkworks Student) 2021–2022
- **Mushtaq Mohamud Ali** (URS Scholar) 2021–2022
- **Jaehun Kim** (URS Scholar) 2021–2022
- **Shraddha Byndoor** (URS Scholar) 2021–2022
- **Sydney Knepfel** (Undergraduate Student) 2021–2022
- **Khoa Bui** (Undergraduate Student, now at Amcor) 2021–2022
- **Aditya Sharma** (Undergraduate Student, now at P&G) 2020–2021

TEACHING EXPERIENCE

- **CBE 562** (Statistics for Chemical Engineers, Teaching Assistant) Spring 2021
- **CBE 255** (Introduction to Chemical Process Modeling, Teaching Assistant) Spring 2020
- **CHEM 6B** (Physical Chemistry, Undergraduate Tutor) Fall 2017

PEER REVIEW

- **Journals**: ACS Omega; Communications Chemistry; Computers & Chemical Engineering; Engineering Reports; Environmental Science & Technology
- **Conferences**: American Control Conference

PUBLICATIONS

In Preparation

[I1] **S. Jiang**, S. Qin, P. Balaprakash, R. C. Van Lehn, and V. M. Zavala. Uncertainty Quantification and Neural Architecture Search Using Graph Neural Networks for Molecular Property Prediction. *In Preparation*, 2022.

[I2] **S. Jiang**, J. L. Pulsipher, T. A. Soderstrom, and V. M. Zavala. Spatial-Temporal Control of a Pastillation Process using Convolutional Neural Network Sensors. *In Preparation*, 2022.

[I3] **S. Jiang**, A. D. Smith, J. J. Schauer, B. de Foy, and V. M. Zavala. Air Pollutant Concentration Analysis Using Preconditioned Dynamic Mode Decomposition. *In Preparation*, 2022.

[I4] **S. Jiang**, K. Carey, L. Denlinger, N. Jarjour, M. Schiebler, R. Sorkness, A. Hahn, S. B. Fain, and V. M. Zavala. Hybrid Deep Learning Model For Asthma Progression Prediction Using CT Scans And Clinical Data. *In Preparation*, 2022.

Under Review

[U1] **S. Jiang**, Z. Wang, and I. Castillo. Extreme Electricity Price Forecasting Using Autoencoders and Long Short-Term Memory. *Under Review*, 2022.

[U2] **S. Jiang**, N. Bao, A. D. Smith, J. J. Schauer, M. Mavrikakis, R. C. Van Lehn, N. L. Abbott and V. M. Zavala. Scalable Extraction of Information from Spatio-Temporal Patterns of Chemoresponsive Liquid Crystals Using Topological Descriptors. *Under Review*, 2022.

Journal Publications

[J1] S. Qin, **S. Jiang**, 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. *RSC Digital Discovery*, 2022. doi:10.26434/chemrxiv-2022-3tq4c.

[J2] 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*, 2022. doi:10.1021/acssuschemeng.2c06052.

[J3] N. Bao, **S. Jiang**, A. D. 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.

[J4] 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.

[J5] **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.

[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.

[J7] **S. Jiang**, J. Noh, C. Park, A. D. Smith, N. L. Abbott, and V. M. Zavala. Endotoxin Detection Using Liquid Crystal Droplets and Machine Learning. *RSC Analyst*, 146 (4), 1224-1233, 2021. doi:10.1039/D0AN02220A.

[J8] 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. *RSC Chemical Science*, 11 (46), 12464-12476, 2020. doi:10.1039/D0SC03261A.

[J9] 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.

[J10] 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.

[J11] 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

[C1] **S. Jiang** and P. Balaprakash. Graph Neural Network Architecture Search for Molecular Property Prediction. *IEEE International Conference on Big Data*, 1346-1353, 2020. doi:10.1109/BigData50022.2020.9378060.

Book Chapters

[B1] **S. Jiang**, S. Qin, J. L. Pulsipher, and V. M. Zavala. Convolutional Neural Networks: Basic Concepts and Applications in Manufacturing. *Artificial Intelligence in Manufacturing: Concepts and Methods*, 2022. Accepted. arXiv:2210.07848.

SOFTWARE PRODUCTS

[S1] DeepHyper: Scalable Neural Architecture and Hyperparameter Search for Deep Neural Networks. https://github.com/deephyper, 2020-Present (Contributor)

[S2] Convolutional Neural Nets in Chemical Engineering: Foundations, Computations, and Applications. https://github.com/zavalab/ML/tree/master/ConvNet

[S3] Accurate Characterization of Mixed Plastic Waste Using Machine Learning and Fast Infrared Spectroscopy. https://github.com/zavalab/ML/tree/master/Plastic_FastIR

[S4] Using ATR-FTIR Spectra and Convolutional Neural Networks for Characterizing Mixed Plastic Waste. https://github.com/zavalab/ML/tree/master/CNN_Plastic

[S5] Graph Neural Network Architecture Search for Molecular Property Prediction. https://github.com/sjiang87/tutorials/tree/develop/tutorials/notebooks/08_NAS_GNN

[S6] Fast Predictions of Liquid-Phase Acid-Catalyzed Reaction Rates Using Molecular Dynamics Simulations and Convolutional Neural Networks. https://zenodo.org/record/4460617

PRESENTATIONS

[P1] **S. Jiang**, S. Zinchik, S. Friis, F. Long, L. Høgstedt, Z. Xu, M. Kamran, S. Paheding, A. G. McDonald, E. Bar-Ziv, and V. M. Zavala. Real-Time Characterization of Mixed Plastic Waste Using Machine Learning and Infrared Spectroscopy. *2023 FOCAPO-CPC*, San Antonio, TX. [link]

[P2] **S. Jiang**, S. Qin, P. Balaprakash, R. C. Van Lehn, and V. M. Zavala. Molecular Property Uncertainty Quantification Using Automatic Graph Neural Architecture Search. *2022 AIChE Annual Meeting*, Phoenix, AZ. [link]

[P3] **S. Jiang**, N. Bao, A. D. Smith, J. J. Schauer, M. Mavrikakis, R. C. Van Lehn, N. L. Abbott, and V. M. Zavala. Characterization of Chemoresponsive Liquid Crystals Using Topological Descriptors and Machine Learning. *2022 AIChE Annual Meeting*, Phoenix, AZ. [link]

[P4] **S. Jiang**, S. Zinchik, S. Friis, F. Long, L. Høgstedt, Z. Xu, M. Kamran, S. Paheding, A. G. McDonald, E. Bar-Ziv, and V. M. Zavala. Rapid and Real-Time Mixed-Plastic Waste Analysis Using Infrared Spectroscopy and Machine Learning. *2022 TWCCC Fall Meeting*, Virtual. [link]

[P5] **S. Jiang**, S. Zinchik, S. Friis, F. Long, L. Høgstedt, Z. Xu, M. Kamran, S. Paheding, A. G. McDonald, E. Bar-Ziv, and V. M. Zavala. Rapid and Real-Time Mixed-Plastic Waste Analysis Using Infrared Spectroscopy and Machine Learning. *2021 AIChE Annual Meeting*, Boston, MA. [link]

[P6] **S. Jiang**, S. B. Fain, K. Carey, L. Denlinger, N. Jarjour, M. Schiebler, R. Sorkness, A. Hahn, and V. M. Zavala. Ensemble Machine Learning Using Quantitative Chest CT and Clinical Biomarkers to Predict Asthma Severity and Outcomes. *ATS 2021 International Conference*, Virtual. [link]

[P7] **S. Jiang**, A. K. Chew, W. Zhang, R. C. Van Lehn, and V. M. Zavala. Characterizing Complex Solvent Environments in Acid-Catalyzed Reactions Using Molecular Dynamics Simulations and 3D Convolutional Neural Nets. *2020 AIChE Annual Meeting*, Virtual. [link]

[P8] **S. Jiang**, N. Bao, A. D. Smith, J. J. Schauer, M. Mavrikakis, R. C. Van Lehn, N. L. Abbott, and V. M. Zavala. Color As a Source of Information in Liquid Crystal Sensors. *2020 AIChE Annual Meeting*, Virtual. [link]

[P9] **S. Jiang**, J. Noh, C. Park, A. D. Smith, N. L. Abbott, and V. M. Zavala. Endotoxin Sensors Using Liquid Crystals and Machine Learning. *2019 AIChE Annual Meeting*, Orlando, FL. [link]

COMPUTER SKILLS & COURSES TAKEN

Skills

- Machine Learning (PyTorch, TensorFlow)
- High-Performance Computing (C/C++)
- Data Analysis (Julia, Matlab, R)
- Other (Aspen, OriginLab, Blender)

Courses

- CS 760 (Machine Learning)
- CS 759 (High-Performance Computing)
- CS 639 (Computational Learning Theory)
- CS 532 (Matrix Method Machine Learning)
- CS 838 (Advanced Computer Vision)
- CS 524 (Introduction to Optimization)
- CS 726 (Nonlinear Optimization)
- CBE 620 (Transport Phenomena)
- CBE 660 (Advanced Mathematics)
- CBE 710 (Advanced Thermodynamics)
- CBE 735 (Kinetics and Catalysis)

COLLABORATORS

- UW-Madison: Sean B. Fain (Medical Physics); James J. Schauer (Civil and Environmental Engineering); Manos Mavrikakis, Reid C. Van Lehn, Sean P. Palecek, Marcel Schreier, George W. Huber (Chemical and Biological Engineering).
- External: Tyler A. Soderstrom (ExxonMobil); Zhenyu Wang, Ivan Castillo (Dow); Ezra Bar-Ziv (Michigan Tech); Nicholas L. Abbott (Cornell); Prasanna Balaprakash (Argonne); Darren J. Lipomi, Shyue Ping Ong (UCSD); Nelly Ramírez-Corona (Universidad de las Américas Puebla).