Zihao Wang

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Nationality	Chinese
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Main Focus

Energy and Process Systems Engineering

Data-Drive Multiscale Modeling and Optimization

Computer-Aided Molecular, Material, and Process Design

Development of High-Efficient Carbon Capture Technology

Artificial Intelligence for Science (AI4Science)

Education

Since 2020	Ph.D. Student in Process Systems Engineering, International Max Planck Research School for Advanced Methods in Process and Systems Engineering (IMPRS ProEng) / Otto-von-Guericke University Magdeburg, Germany
2017-2020	M.Sc. in Chemical Engineering and Technology, Chongqing University, China
2013-2017	B.Eng. in Chemical Engineering and Technology, Chongqing University, China

Experience

Since 2020	Doctoral Researcher, Max Planck Institute for Dynamics of Complex Technical Systems, Magdeburg, Germany

Teaching Activity

Teaching Assistant, Process Systems Engineering, Otto-von-Guericke University Magdeburg

- Winter Semester 2023

Teaching Assistant, Analysis and Design of Experiments, Otto-von-Guericke University Magdeburg

- Summer Semester 2023
- Summer Semester 2022
- Summer Semester 2021

Journal Article

[J16] **Z. Wang**, T. Zhou, K. Sundmacher. Data-driven integrated design of solvents and extractive distillation processes. ***AIChE Journal***, 2023, e18236.

[J15] T. Zhou, C. Gui, L. Sun, Y. Hu, H. Lyu, **Z. Wang**, Z. Song, G. Yu. Energy applications of ionic liquids: Recent developments and future prospects. ***Chemical Reviews***, 2023.

[J14] **Z. Wang**, T. Zhou, K. Sundmacher. Interpretable machine learning for accelerating the discovery of metal-organic frameworks for ethane/ethylene separation. ***Chemical Engineering Journal***, 2022, 444, 136651.

[J13] **Z. Wang**, Y. Zhou, T. Zhou, K. Sundmacher. Identification of optimal metal-organic frameworks by machine learning: Structure decomposition, feature integration, and predictive modeling. ***Computers & Chemical Engineering***, 2022, 160, 107739.

[J12] **Z. Wang**, H. Wen, Y. Su, W. Shen, J. Ren, Y. Ma, J. Li. Insights into ensemble learning-based data-driven model for safety-related property of chemical substances. ***Chemical Engineering Science***, 2022, 248, 117219.

[J11] H. Qin, **Z. Wang**, Z. Song, X. Zhang, T. Zhou. High-throughput computational screening of ionic liquids for butadiene and butene separation. ***Processes***, 2022, 10(1), 165.

[J10] X. Zhang, S. Sethi, **Z. Wang**, T. Zhou, Z. Qi, K. Sundmacher. A neural recommender system for efficient adsorbent screening. ***Chemical Engineering Science***, 2022, 259, 117801.

[J9] **Z. Wang**, Song, Z., Zhou, T. Machine learning for ionic liquid toxicity prediction. ***Processes***, 2021, 9(1), 65.

[J8] H. Qin, **Z. Wang**, T. Zhou, Z. Song. Comprehensive evaluation of COSMO-RS for predicting ternary and binary ionic liquid-containing vapor–liquid equilibria. ***Industrial & Engineering Chemistry Research***, 2021, 60(48), 17761–17777.

[J7] H. Wen, Y. Su, **Z. Wang**, S. Jin, J. Ren, W. Shen, M. Eden. A systematic modeling methodology of deep neural network-based structure-property relationship for rapid and reliable prediction on flashpoints. ***AIChE Journal***, 2021, e17402.

[J6] A. Yang, Y. Su, **Z. Wang**, S. Jin, J. Ren, X. Zhang, W. Shen, J.H. Clark. A multi-task deep learning neural network for predicting flammability-related properties from molecular structures. ***Green Chemistry***, 2021, 23(12), 4451–4465.

[J5] **Z. Wang**, Y. Su, S. Jin, W. Shen, J. Ren, X. Zhang, J.H. Clark. A novel unambiguous strategy of molecular feature extraction in machine learning assisted predictive models for environmental properties. ***Green Chemistry***, 2020, 22(12), 3867–3876.

[J4] **Z. Wang**, Y. Su, W. Shen, S. Jin, J.H. Clark, J. Ren, X. Zhang. Predictive deep learning models for environmental properties: the direct calculation of octanol-water partition coefficients from molecular graphs. ***Green Chemistry***, 2019, 21(16), 4555–4565.

[J3] Y. Su, **Z. Wang**, S. Jin, W. Shen, J. Ren, M.R. Eden. An architecture of deep learning in QSPR modeling for the prediction of critical properties using molecular signatures. ***AIChE Journal***, 2019, 65(9), e16678.

[J2] S. Zhao, M. Zhang, **Z. Wang**, X. Xian. Enhanced high-rate performance of $Li_4Ti_5O_{12}$ microspheres/multiwalled carbon nanotubes composites prepared by electrostatic self-assembly. ***Electrochimica Acta***, 2018, 276, 73–80.

[J1] S. Zhao, M. Zhang, X. Xian, O. Ka, **Z. Wang**, J. Wang. Insight into the formation mechanism of $Li_4Ti_5O_{12}$ microspheres obtained by a CTAB-assisted synthetic method and their

electrochemical performances. ***Journal of Materials Chemistry A***, 2017, 5(26), 13740–13747.

Conference Paper

[C3] **Z. Wang**, T. Zhou, K. Sundmacher. (2023). Molecular property targeting for optimal solvent design in extractive distillation processes. In: *33rd European Symposium on Computer Aided Process Engineering*, 1247–1252. ISBN: 9780443152757. DOI: 10.1016/B978-0-443-15274-0.50199-2.

[C2] **Z. Wang**, T. Zhou, K. Sundmacher. (2022). A novel machine learning-based optimization approach for the molecular design of solvents. In: *32nd European Symposium on Computer Aided Process Engineering*, 1477–1482. ISBN: 9780323958790. DOI: 10.1016/B978-0-323-95879-0.50247-2.

[C1] T. Zhou, **Z. Wang**, K. Sundmacher. (2022). A new machine learning framework for efficient MOF discovery: Application to hydrogen storage. In: *14th International Symposium on Process Systems Engineering*, 1807–1812. ISBN: 9780323851596. DOI: 10.1016/B978-0-323-85159-6.50301-8.

Conference Talk

[T2] **Z. Wang**, T. Zhou, K. Sundmacher. *Data-driven integrated design of solvents and extractive distillation processes*. Presented at: 2023 AIChE Annual Meeting. Orlando, USA, November 08, 2023.

[T1] **Z. Wang**, T. Zhou, K. Sundmacher. *A novel machine learning-based optimization approach for the molecular design of solvents*. Keynote presented at: 32nd European Symposium on Computer-Aided Process Engineering (ESCAPE-32). Toulouse, France, June 13, 2022.

Conference Poster

[P3] **Z. Wang**, T. Zhou, K. Sundmacher. *Molecular property targeting for optimal solvent design in extractive distillation processes*. Presented at: 33rd European Symposium on Computer-Aided Process Engineering (ESCAPE-33). Athens, Greek, June 19, 2023.

[P2] T. Zhou, **Z. Wang**, K. Sundmacher. *A new machine learning framework for efficient MOF discovery: application to hydrogen storage*. Presented at: 14th International Symposium on Process Systems Engineering (PSE 2021+). Kyoto, Japan, June 21, 2022.

[P1] Z. Ayaz, **Z. Wang**, A. Lieb, K. Sundmacher, F. Scheffler. *Synthesis and characterisation of CALF-20/GO nanocomposites for microwave assisted adsorbate regeneration*. Presented at: 8th International Conference on Metal-Organic Frameworks and Open Framework Compounds. Dresden, Germany, September 5, 2022

Master's Thesis Supervision

[M1] S.D. Sreedhar. *Surrogate-based optimization of extractive distillation processes using active learning*. Otto-von-Guericke University Magdeburg, Germany.

Award/Honor

Since 2020	IMPRS PhD Financial Support from the Max Planck Society
2019, 2020	Outstanding Graduate Student of Chongqing University
2019, 2020	Class A, Chongqing University Scholarship
2016	Second Prize, 10th China Undergraduate Chemical Engineering Design Competition

Book Contribution

[B2] **Z. Wang**, W. Shen. (2021). Automated extraction of molecular features in machine learning-based environmental property prediction. In: Ren, J., Shen, W., Man, Y., & Dong, L. (Eds.) *Applications of Artificial Intelligence in Process Systems Engineering*, 67–92. Elsevier.

[B1] **Z. Wang**, W. Shen. (2021). Predictive deep learning models for environmental properties. In: Ren, J., Shen, W., Man, Y., & Dong, L. (Eds.) *Applications of Artificial Intelligence in Process Systems Engineering*, 39–66. Elsevier.

Journal Reviewer

Separation and Purification Technology (IF = 8.6)

Current Opinion in Chemical Engineering (IF = 6.6)

Environment, Development and Sustainability (IF = 4.9)

Scientific Reports (IF = 4.6)

Frontiers of Chemical Science and Engineering (IF = 4.5)

Flexible and Printed Electronics (IF = 3.1)

Inverse Problems (IF = 2.1)