



## 王梓豪

出生年月 1995 年 7 月

籍贯 湖南省衡阳市

电话 182 2527 8255

邮箱 zwang@mpi-magdeburg.mpg.de

求职意向 重庆大学化学化工学院化学工程系、弘深青年教师岗、申威峰教授智能化工团队



## 研究方向

- 化学工业数字化、数字孪生与智能化
- 数据驱动多尺度建模与智能优化算法
- 溶剂与化工分离过程协同优化设计
- 高效多孔材料与变压吸附工艺开发

## 教育背景

- 2020.10 至今 德国马克斯普朗克学会 复杂技术系统动力学研究所  
工学博士（过程系统工程） 导师：Kai Sundmacher 教授（柏林勃兰登堡科学院院士）  
合作导师：周腾教授（香港科技大学）
- 2017.09–2020.07 重庆大学 化学化工学院  
工学硕士（化学工程与技术） 导师：申威峰教授（国家优青）
- 2013.09–2017.07 重庆大学 化学化工学院  
工学学士（化学工程与工艺） 导师：魏顺安副教授

## 教学经历

- 2023 年至今 助教 过程系统工程（硕士课程，马格德堡大学，德国）
- 2020–2023 年 助教 化工实验分析与设计（硕士课程，马格德堡大学，德国）

## 可讲授课程

- 化工专业课程：《化工原理》、《化工分离工程》、《化工设计》、《化工热力学》
- 交叉学科课程：《过程系统工程》、《机器学习在化学化工中的应用》

## 研究成果：已发表 SCI 论文 17 篇（其中 7 篇为第一作者）及书籍章节 2 篇，论文被引次数 459 次（Web of Science）

- [1] Wang Z, Zhou T, Sundmacher K. Data-driven integrated design of solvents and extractive distillation processes. *AIChE Journal*, 2023, 69(12), e18236. (化学工程顶刊、SCI)
- [2] Wang Z, Shen W\*, et al. Insights into ensemble learning-based data-driven model for safety-related property of chemical substances. *Chemical Engineering Science*, 2022, 248, 117219. (化学工程三大刊、SCI)
- [3] Wang Z, Zhou Y, Zhou T, et al. Identification of optimal metal-organic frameworks by machine learning: Structure decomposition, feature integration, and predictive modeling. *Computers & Chemical Engineering*, 2022, 160, 107739. (化工系统工程顶刊、SCI)



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- [4] **Wang Z**, Zhou T, Sundmacher K. Interpretable machine learning for accelerating the discovery of metal-organic frameworks for ethane/ethylene separation. *Chemical Engineering Journal*, 2022, 444, 136651. (中科院一区 TOP、IF = 13.3)
- [5] **Wang Z**, **Shen W\***, et al. A novel unambiguous strategy of molecular feature extraction in machine learning assisted predictive models for environmental properties. *Green Chemistry*, 2020, 22(12), 3867–3876. (中科院一区 TOP、IF = 9.3)
- [6] **Wang Z**, **Shen W\***, et al. 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. (中科院一区 TOP、IF = 9.3)
- [7] **Wang Z**, Song Z, Zhou T. Machine learning for ionic liquid toxicity prediction. *Processes*, 2021, 9(1), 65. (中科院四区、IF = 2.8)
- [8] **Wang Z**, Shen W. Automated extraction of molecular features in machine learning-based environmental property prediction. In: *Applications of Artificial Intelligence in Process Systems Engineering*, 2021, 67–92. (书籍章节)
- [9] **Wang Z**, Shen W. Predictive deep learning models for environmental properties. In: *Applications of Artificial Intelligence in Process Systems Engineering*, 2021, 39–66. (书籍章节)
- [10] Qin H, **Wang Z**, Ruan J, et al. Integrating machine learning model and computer-aided molecular design toward rational ionic liquid selection for separating fluorinated refrigerants. *Separation and Purification Technology*, 2024, 129796. (中科院一区 TOP、IF = 8.1)
- [11] Zhou T, Gui C, Sun L, Hu Y, Lyu H, **Wang Z**, Song Z, Yu G. Energy applications of ionic liquids: Recent developments and future prospects. *Chemical Reviews*, 2023, 123(21), 12170–12253. (中科院一区 TOP、IF = 51.4)
- [12] Qin H, **Wang Z**, Song Z, et al. High-throughput computational screening of ionic liquids for butadiene and butene separation. *Processes*, 2022, 10(1), 165. (中科院四区、IF = 2.8)
- [13] Wen H, Su Y, **Wang Z**, et al. A systematic modeling methodology of deep neural network-based structure-property relationship for rapid and reliable prediction on flashpoints. *AIChE Journal*, 2022, 68(1), e17402. (化学工程顶刊、SCI)
- [14] Zhang X, Sethi S, **Wang Z**, et al. A neural recommender system for efficient adsorbent screening. *Chemical Engineering Science*, 2022, 259, 117801. (化学工程三大刊、SCI)
- [15] Qin H, **Wang Z**, Zhou T, et al. 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. (化学工程三大刊、SCI)
- [16] Yang A, Su Y, **Wang Z**, et al. A multi-task deep learning neural network for predicting flammability-related properties from molecular structures. *Green Chemistry*, 2021, 23(12), 4451–4465. (中科院一区 TOP、IF = 9.3)
- [17] Su Y, **Wang Z**, Jin S, et al. An architecture of deep learning in QSPR modeling for the prediction of critical properties using molecular signatures. *AIChE Journal*, 2019, 65(9), e16678. (化学工程顶刊、SCI)
- [18] Zhao S, Zhang M, **Wang Z**, Xian X. Enhanced high-rate performance of  $\text{Li}_4\text{Ti}_5\text{O}_{12}$  microspheres/multiwalled carbon nanotubes composites prepared by electrostatic self-assembly. *Electrochimica Acta*, 2018, 276, 73–80. (中科院三区、IF = 5.5)
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- [19] Zhao S, Zhang M, Xian X, Ka O, **Wang Z**, Wang J. Insight into the formation mechanism of  $\text{Li}_4\text{Ti}_5\text{O}_{12}$  microspheres obtained by a CTAB-assisted synthetic method and their electrochemical performances. *Journal of Materials Chemistry A*, 2017, 5(26), 13740–13747. (中科院二区 TOP, IF = 10.7)

## 学术报告/墙报

- **Wang Z**. Integrated molecular and process design using Bayesian optimization. *15th International Max Planck Research School Workshop*, 德国 Schkopau, 2024.04.15, 墙报.
- **Wang Z**, Zhou T, Sundmacher K. Data-driven integrated design of solvents and extractive distillation processes. *2023 AIChE Annual Meeting*, 美国 奥兰多, 2023.11.08, 口头报告.
- **Wang Z**, Zhou T, Sundmacher K. Molecular property targeting for optimal solvent design in extractive distillation processes. *33rd European Symposium on Computer-Aided Process Engineering*, 希腊 雅典, 2023.06.19, 墙报.
- **Wang Z**. Data-driven integrated solvent and process design. *14th International Max Planck Research School Workshop*, 德国 Naumburg, 2023.03.14, 口头报告.
- **Wang Z**, Zhou T, Sundmacher K. A novel machine learning-based optimization approach for the molecular design of solvents. *32nd European Symposium on Computer-Aided Process Engineering*, 法国 图卢兹, 2022.06.13, Keynote 口头报告.
- **Wang Z**. Machine learning for solvent design in chemical processes. *13rd International Max Planck Research School Workshop*, 德国 Wernigerode, 2022.08.29, 口头报告.

## 所获奖项

- 2024 年            国家优秀自费留学生奖学金
- 2020–2024 年    国际马克斯普朗克研究学校 (IMPRS) 博士奖学金
- 2020 年            重庆大学优秀毕业研究生
- 2019 年            重庆大学优秀研究生
- 2018–2020 年    重庆大学研究生 A 等学业奖学金
- 2016 年            第十届全国大学生化工设计竞赛全国二等奖

## 学术兼职

担任 Chemical Engineering Journal、Engineering Applications of Artificial Intelligence、Digital Chemical Engineering、Separation and Purification Technology、Chemical Engineering Research and Design、Current Opinion in Chemical Engineering 等 SCI 期刊审稿人