



Department: School of Chemical Engineering

Professional field: Chemical Engineering, Process Systems Engineering

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### Profile

Prof. Zhen Song received the bachelor's degree in chemical engineering and technology from Shandong University in 2011, and the PhD degree from East China University of Science and Technology (ECUST) in 2017. From June 2017 to April 2019, he worked as a Postdoc supported by the Max Planck Society at Max Planck Institute for Dynamics of Complex Technical Systems, and from April 2019 to June 2021, he worked as a Researcher funded by the German Research Foundation at Otto von Guericke University Magdeburg. Since July 2021, he has become a senior research fellow and doctoral supervisor at the school of Chemical Engineering, ECUST. He has been selected for the High-Level Talents Plan of Shanghai (Overseas) and received the National Natural Science Fund for Excellent Young Scientists Fund Program (Overseas).

### Research Field

Design of functional solvents/materials, Chemical Process Intensification, Artificial Intelligence in Chemical Engineering

### Research results and selected published papers

Published over 40 peer-reviewed journal articles with more than 900 citations and h-index of 20 by Dec. 2021, 10 representative papers in the past five years are listed as follows.

1. Chen GZ, Song Z\*, Qi ZW\*, Sundmacher K. Neural recommender system for the activity coefficient prediction and UNIFAC model extension of ionic liquid-solute systems. *AIChE Journal*. 2021; 67: e17171.
2. Chen G, Song Z\*, Qi ZW\*. Transformer-convolutional neural network for surface charge density profile prediction: Enabling high-throughput solvent screening with COSMO-SAC. *Chemical Engineering Science*. 2021; 246: 117002.
3. Qin H, Wang ZH, Zhou T, Song Z\*. Comprehensive evaluation of COSMO-RS for predicting ternary and binary ionic liquid-containing vapor-liquid equilibria. *Industrial & Engineering Chemistry Research*. 2021; 60: 17761-17777.
4. Hu XT, Wang JW, Mei MC, Song Z\*, Cheng HY, Chen LF\*, Qi ZW. Transformation of CO<sub>2</sub> incorporated in adducts of N-heterocyclic carbene into dialkyl carbonates under ambient conditions: An experimental and mechanistic study. *Chemical Engineering Journal*. 2021; 413: 127469.
5. Song Z, Zhou T, Qi ZW, Sundmacher K. Extending the UNIFAC model for ionic liquid-solute systems by combining experimental and computational databases. *AIChE Journal*. 2020; 66: e16821.
6. Song Z, Shi HW, Zhang X, Zhou T. Prediction of CO<sub>2</sub> solubility in ionic liquids using machine learning methods. *Chemical Engineering Science*. 2020; 223: 115752.
7. Song Z\*, Hu, XT, Wu HY, Mei MC, Linke S, Zhou T, Qi ZW, Sundmacher K. Systematic screening of deep eutectic solvents as sustainable media of separations exemplified by the CO<sub>2</sub> capture process. *ACS Sustainable Chemistry & Engineering*. 2020; 8: 8741-8751.
8. Wang JW, Song Z\*, Li X, Cheng HY, Chen LF, Qi ZW\*. Towards rational functionalization of ionic liquids for enhanced extractive desulfurization: computer-aided solvent design and molecular dynamics simulation. *Industrial & Engineering Chemistry Research*. 2020; 59: 2093-2103.
9. Song Z, Hu XT, Zhou YG, Zhou T, Qi ZW, Sundmacher K. Rational design of double salt ionic liquids as extraction solvents: Separation of thiophene/n-octane as example. *AIChE Journal*. 2019; 65: e16625.
10. Song Z, Zhang CY, Qi ZW, Zhou T, Sundmacher K. Computer - aided design of ionic liquids as solvents for extractive desulfurization. *AIChE Journal*. 2018; 64: 1013-1025.