

Yinzi Shao

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Research Interests

Methodological Areas: Materials-Oriented Machine Learning & Deep Learning, Large Language Model Agents for Materials Discovery, Nanomaterials and Membrane Technology, Density Functional Theory (DFT) Computational Modeling.

Application Areas: Artificial Intelligence for Sustainable Environmental & Living Systems, Membrane Science & Technology (CO₂ Capture, Dielectric Films), Energy Storage Materials (Modeling of Batteries and Supercapacitors).

Education

Xuzhou University of Technology

Aug. 2024 – Present

Saint Petersburg Joint Engineering School: Electronic Science and Technology (Sino-Russian)

- GPA: 83.6/100 CE Rank:1/229
- Research direction: Machine Learning and Deep Learning for Materials, LLMs in Materials Science, DFT, Energy Storage Modeling, Nanomaterials and Membrane Science.

Saint Petersburg Electrotechnical University "LETI"

Aug. 2024 – Present

College of Electrical Engineering and Automation: Electrical Engineering Systems and Technologies (Sino-Russian)

- GPA: 88.5/100 CE Rank:1/229
- Coursework: Semiconductor Devices, Solid State Physics, Electrotechnical Materials, Chemistry, Physics, Electronic and Electrical Apparatus, Information Technology, Mathematical Analysis.

Xuzhou University of Technology

Aug. 2023 – Feb. 2024

Saint Petersburg Joint Engineering School: Environmental Science and Engineering (Sino-Russian)

- GPA: 86.5/100 (**Top 3%**). CE Rank:1/229
- Research direction: Nano-adsorbent materials (Nanobiochar, MOFs, MXene), Pebax 1657 membranes for CO₂ separation.

Publications

- **Y. Shao**, X. Zhang, W. Tan, Y. Zhao, F. Li & B. Gao. (2025). Mixed matrix membrane of Pebax-1657 incorporated with H₂O₂-modified ball-milled biochar for enhanced CO₂ separation. *Environmental Research*, 285, 122302. [SCI Top / JCR Q1]
- W. Chen, **Y. Shao (Co-first author)**, Z. Xu, Z. Bing, S. Cui, Z. Dai, S. Yin, Y. Gao & L. Liu. (2026). Ensemble Machine Learning for Operational Water Quality Monitoring Using Weighted Model Fusion for pH Forecasting. *Sustainability*, 18(3), 1200. [SCI / JCR Q2]
- X. Zhang, W. Xiang, G. Qi, Z. Pan, **Y. Shao**, X. Zhuang & F. Li. (2026). Degradation of pharmaceuticals and personal care products in soils and water. In *Adsorption and Degradation of Emerging Contaminants in Soils and Water* (pp. 45-93). [Book Chapter]
- C. Dai, Z. Xu, H. Luo, T. Zhou, **Y. Shao**, T. Wu, L. Xie & Q. Feng. (2026). Nanoporous materials for isovalent ion separation: Confined transport, chemical recognition and data-guided design. *Science China Materials*. (2nd revision) [SCI Top / JCR Q1]
- C. Cao, X. Zhuang, L. Cao, **Y. Shao**, Y. Zhao & X. Zhang. (2026). Recent Advances in Biochar for CO₂ Capture: Structural Characteristics, Modification Strategies and Influencing Factors. *Water, Air, & Soil Pollution*. (2nd revision) [SCI / JCR Q2]
- **Y. Shao**, X. Zhang, S. Wang, Y. Zhao, C. Cao & B. Gao. (2026). Machine Learning-Driven Design of Amino-Functionalized Biochar/Pebax Mixed Matrix Membranes for Optimal CO₂ Separation. *Journal of Membrane Science*. (Under review) [SCI Top / JCR Q1]
- **Y. Shao**, X. Wu, Y. Gao, Z. Zhou, H. Fei, J. Chang & S. Cui. (2026). A Domain-Adaptive Physics-Augmented Long Short-Term Memory Framework for Extreme Few-Shot Battery Degradation Prediction. *Journal of The Electrochemical Society*. (Under review) [SCI / JCR Q2]
- **Y. Shao**, S. Cui, Y. Gao & S. Sang. (2026). BattField-LLM: An Evidence-Grounded Small Language Model for Structured Extraction of Lithium-Ion and Sodium-Ion Battery Data. *PNAS*. (With Editor) [SCI / JCR Q1]
- S. Cui, **Y. Shao (Co-first author)**, Y. Gao, Y. Yang, S. Liu & Z. Xu. (2026). Adaptive-Gated Ensemble Learning for Lithium-Ion Battery State-of-Health Prediction. *Journal of Power Sources*. (With Editor) [SCI / JCR Q1]

- S. Liu, Y. Gao, **Y. Shao** & S. Yin. (2026). Improving NAO Left-Arm Inverse Kinematics via Rotation Matrix Encoding, Chained Kernel Regression, and Non-Negative Least Squares Ensemble Stacking. *2026 International Conference on Sensor-Cloud and Edge Computing System*. [EI Conf]
- W. Duan, Q. Zhang, **Y. Shao** & F. Xue. (2026). Machine Learning-Based Toxicity Prediction of Industrial Chemicals Using Tox21 Database: Toward Applications in Epichlorohydrin, Acrylonitrile, and Styrene-Based Polymers. *2026 9th International Conference on Advanced Algorithms and Control*. [EI Conf]
- **Y. Shao**, X. Zhuang, X. Fei, Y. Huang, J. Yu & X. Zhang. (2025). CO₂ separation performance of corn stalk biochar-doped Pebax 1657 mixed matrix membranes. *Open Journal of Natural Science*, 13(2), 329-337. [Core Journal]
- S. Liu, **Y. Shao (Co-first author)**, Z. Yao & Y. Gao. (2026). Learning-based inverse dynamics compensation with online adaptation for high-precision trajectory tracking of robotic manipulators. *Artificial Intelligence and Robotics Research*. (Accept) [Core Journal]
- X. Zhuang, **Y. Shao**, S. Zhang, Y. Tao, Z. Jiang, Y. Chen, Y. Huang & C. Cao. (2026). Microbial pretreatment and microwave pyrolysis enhance CO₂ adsorption performance of bamboo biochar. *Advances in Environmental Protection*, 16, 304. [Core Journal]
- X. Zhuang, Y. Chen, **Y. Shao**, S. Zhang, Z. Jiang, Y. Zhu & C. Cao. (2026). Effect of microbial treatment time on CO₂ adsorption performance of biochar. *International Journal of Ecology*, 15, 9. [Core Journal]
- Y. Gao, Y. Sun, R. Ge, **Y. Shao**, Y. Chen & J. Wei. (2025). Impact of digital transformation on the sustainability innovation effect of the emergency industry: Evidence from A-share listed companies. *Sustainable Development*, 15, 151. [Core Journal]
- **Y. Shao**, X. Fei, Y. Huang, X. Zhuang, J. Yu & X. Zhang. (2025). CO₂ separation performance of mixed matrix membranes enhanced by microporous biochar. *Sustainable Energy*, 15(1), 1-8. [Journal]
- **Y. Shao** & B. Zhang. (2025). The Accountability Paradox: How Generative AI Challenges Our Notions of Responsibility. *ICCK Transactions on Emerging Topics in Artificial Intelligence*, 2(3), 169-172. [Journal]
- Y. Luo, **Y. Shao**, B. Zhang, K. Liu, S. Liu, Z. Yuan & S. Sang. (2025). Forecasting China's Nuclear Power Generation to 2030: An ARIMA Model-Based Trend Analysis. *Engineering Frontiers*, 1(1), 3. [Journal]
- J. Yu, X. Zhuang, **Y. Shao**, T. Wang, W. Xiang & X. Zhang. (2025). Enhanced CO₂ adsorption characteristics of distiller's grains biochar by anaerobic fermentation. *Bioprocess*, 15, 92. [Journal]

Funding & Grants

- National Innovation and Entrepreneurship Training Program for College Students (XCX2024117/ Excellent Completion) (**PI**)
- National Key R&D Program of China (2024YFB3612600) (**Participant**)
- National Natural Science Foundation of China (22375100, 22275098 and 62288102) (**Participant**)
- Basic Research Program of Jiangsu (BK20243057) (**Participant**)
- Open Fund, Zhejiang Key Lab of Pollution Control for Port-Petrochemical Industry (Y202502) (**Participant**)
- Open Fund, Zhejiang Key Lab of Petrochemical Environmental Pollution Control (2024Z02) (**Participant**)
- Jiangsu Province College Students' Innovation Training Program (202610293144Y) (**Participant**)

Project & Research Experience

Performance Optimization of Pebax 1657 Mixed Matrix Membranes (MMMs) Using Machine Learning, Large Language Models, and Nanomaterials (Nanobiochar, MXene, and MOFs) Jun. 2023 – Present

Advisors: [Prof. Xueyang Zhang](#) (Vice Dean, CN) and [Prof. Bin Gao](#) (AAAS Fellow, SSSA Fellow, USA).

- Fabricated Pebax-1657 mixed matrix membranes incorporating ball-milled H₂O₂-modified nanobiochar, corn stalk biochar, and bamboo biochar, and evaluated CO₂ permeability and CO₂/N₂ selectivity under varying filler loadings and surface-modification conditions.
- Prepared, characterized, and screened multiple nanomaterials (MXene, MOFs, CNTs, and graphene) for incorporation into Pebax-1657 membranes to investigate their effects on CO₂ separation performance.
- Performed density functional theory (DFT) calculations to investigate the electronic structure and CO₂ adsorption behavior of biochar-based fillers, providing mechanistic insights complementary to the experimental permeation results.
- Developed machine learning and large language model (LLM)-based workflows to correlate membrane composition and fabrication parameters with gas separation performance, enabling data-driven optimization of filler selection and processing strategies.
- **Outcome:** Authored 4 first-author works on this project, including one published SCI Top Q1 paper (Environmental Research, 2025) and a second SCI Top Q1 paper under review (Journal of Membrane Science); co-authored 6 further group papers on biochar-based CO₂ capture and related environmental degradation research, including a book chapter led by Prof. Bin Gao.

Battery system optimization modeling based on machine learning and LLM fine-tuning

Jan. 2024 – Present

Advisor: *Sijing San* (Xuzhou, CN) and *Zhongyuan Yuan* (Xuzhou, CN)

- Developed a domain-adaptive physics-augmented Long Short-Term Memory (LSTM) framework for battery degradation prediction under extreme few-shot conditions, embedding electrochemical aging mechanisms as physical constraints to improve prediction accuracy when cycling data is scarce.
- Built BattField-LLM, an evidence-grounded large language model for structured extraction of lithium-ion and sodium-ion battery data, fine-tuned to ground its outputs in electrochemical evidence for tasks such as capacity fade, state-of-health, and electrode material property extraction.
- Designed and implemented an adaptive-gated ensemble learning framework for lithium-ion battery state-of-health prediction, integrating multiple base learners through an adaptive gating mechanism to capture nonlinear degradation behavior across different aging stages and operating conditions.
- **Outcome:** 3 (co-)first-author manuscripts led by BattField-LLM submitted to SCI Top Q1 journal; two other battery papers under review. Contributed to 3 collaborative works on robotics, sustainability and power forecasting.

Data-Guided Design of Nanoporous Materials for Isovalent Ion Separation

Jan. 2025 – Present

Advisors: *Prof. Linghai Xie* (Excellent Young Scholars, CN)

- Investigated how confined pore geometries govern ion transport and chemical recognition selectivity across membrane and framework materials, as part of a collaborative study on nanoporous materials for isovalent ion separation.
- Synthesized and organized structure-performance data across reported nanoporous systems, establishing data-guided design principles linking pore architecture to isovalent ion selectivity.
- Constructed a curated database of nanoporous materials by extracting structural descriptors, transport properties, and ion selectivity metrics from published literature.
- **Outcome:** Co-authored review article in Science China Materials (2nd revision, SCI Top / JCR Q1) on confined transport, chemical recognition and data-guided design of nanoporous materials for isovalent ion separation.

Working & Teaching Experience

China Architecture & Culture Press

Jul. 2024 – Present

Assistant Editor

Kowloon, Hong Kong

- Assisted in manuscript revision, proofreading and academic formatting.
- Supported journal promotion and academic event organization.

Nanyang Technological University

Jul. 2018 – Aug. 2018

Exchange Scholar

Singapore, SG

- English Proficiency Training & Engineering Education.

Open DFT Team

Jun. 2025 – Present

Team Leader

GitHub Open-source Project

- Led a 5-member team to build open-source LLM-assisted DFT computing workflow system.
- Promoted the project on Xiaohongshu (RedNote), earning 1,000+ combined likes and favorites.

Honors & Awards

- 2025 National Scholarship (**Academic Exception, First Case in Jiangsu Province**)
- 2025 7th "Jisi Cup" National College Students' Research-Oriented Academic Achievement Competition, **Special Prize (1st Author)**
- 2025 2nd Youth Green Technology Innovation Competition, **Bronze Award (1st Author)**
- 2025 18th National College Students' Innovation Annual Conference, **Selected for Presentation (1st Author)**
- 2025 Mathematical Contest in Modeling (MCM), United States, International, **2nd Prize (Ranking not in order)**
- 2025 18th "CMB Cup" National College Students' Energy Conservation and Emission Reduction Social Practice and Science & Technology Competition, National Finals, **2nd Prize (1st Author)**
- 2025 18th "CMB Cup" National College Students' Energy Conservation and Emission Reduction Social Practice and Science & Technology Competition, National Finals, **3rd Prize (Team Member)**
- 2025 China International College Students' Innovation Competition, National Finals, **3rd Prize (2nd Team Leader)**

- 2025 15th "CP Cup" National College Students' Market Research and Analysis Competition, National Finals, Undergraduate Group, **3rd Prize (1st Author)**
- 2025 National College Students' Innovation Training Program, **Excellent Project Completion (Principal Investigator)**
- 2025 5th Jiangsu Province Energy Conservation and Emission Reduction Social Practice and Science & Technology Competition, **1st Prize (1st Author)**
- 2025 China Undergraduate Mathematical Contest in Modeling, Jiangsu Provincial Round, **1st Prize (1st Author)**
- 2025 National College Students' Statistical Mathematical Modeling Competition, Jiangsu Provincial Round, **1st Prize (1st Author)**
- 2025 15th "CP Cup" National College Students' Market Research and Analysis Competition, Jiangsu Provincial Round, Undergraduate Group, **1st Prize (1st Author)**
- 2025 China International College Students' Innovation Competition, Jiangsu Provincial Round, **2nd Prize (1st Author)**
- 2025 Asia and Pacific Mathematical Contest in Modeling, Certificate of Achievement, International, **2nd Prize (1st Author)**
- 2026 6th Jiangsu Province College Students' Energy Conservation and Emission Reduction Social Practice and Science & Technology Competition, **2nd Prize (1st Author)**
- 2026 6th Jiangsu Province College Students' Energy Conservation and Emission Reduction Social Practice and Science & Technology Competition, **2nd Prize x2 (Team Member)**
- 2025 "Poetry and Painting Fluid Mechanics" Creative Competition, **2nd Prize (1st Author)**
- 2025 7th Jiangsu Province College Students' Water Creative Design Competition, **2nd Prize (Team Member)**
- 2025 "Poetry and Painting Fluid Mechanics" Creative Competition, **3rd Prize (Team Member)**
- 2025 IODA International Original Design Award, **Gold Award (Team Member)**
- 2025 11th National Youth Science Popularization Innovation Experiment and Works Competition, Jiangsu Provincial Round, **3rd Prize (1st Author)**
- 2025 11th National College Students' Energy Economics Academic Creativity Competition, Jiangsu Provincial Round, **3rd Prize (Team Member)**
- 2024 Asia and Pacific Mathematical Contest in Modeling, Certificate of Achievement, International, **1st Prize (1st Author)**
- 2024 4th Jiangsu Province College Students' Energy Conservation and Emission Reduction Social Practice and Science & Technology Competition, **2nd Prize (1st Author)**
- 2024 4th Jiangsu Province College Students' Energy Conservation and Emission Reduction Social Practice and Science & Technology Competition, **1st Prize (Team Member)**
- 2024 National College Students' Mathematical Modeling Competition, Jiangsu Provincial Round, **3rd Prize (1st Author)**

Skills & Certificates

Programming Languages: C++, Python, PHP, SQL.

Data Processing & Plotting Software: Origin, LaTeX, Visio, SPSS.

Numerical Calculation & Machine Learning Software: MATLAB, Mathematica, Scikit-learn, PyTorch, TensorFlow, CUDA.

DFT & Material Simulation Software: VASP, Materials Studio (CASTEP), VESTA, Pymatgen.

Experimental Instruments Mastered: Hitachi SU8600 SEM (Master theoretical principle, operated with supervisor guidance), Rigaku Ultima IV XRD, Mettler-Toledo TGA/DSC3+, TA DSC Q20 DSC, KuboX1000 gas sorption analyzer, Agilent 7890B GC, Elementar Vario Macro cube elemental analyzer, HORIBA Xplora Plus confocal Raman spectrometer, PerkinElmer Spotlight 400 FTIR spectrometer, Anton Paar Litesizer 500 nanoparticle & zeta potential analyzer, SMT-275 gas permeability tester, XQM-2 planetary ball mill.

Hobbies and Activities: Hiking, Running, Biking, Cooking, Baking.