Fan Yao PhD Candidate

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Research Profile

PhD researcher specializing in heterogeneous catalysis with a strong focus on understanding catalyst evolution under realistic reaction conditions. My research combines catalyst design, operando spectroscopy, and mechanistic analysis to reveal how structural dynamics—including oxygen vacancies, metal exsolution, and surface reconstruction—govern catalytic performance.

Rather than viewing catalysts as static materials, my long-term goal is to directly visualize catalyst evolution by integrating operando spectroscopy with advanced chemical imaging.

Key Research Highlights

- One-year Visiting PhD Researcher at the Paul Scherrer Institute (PSI), Switzerland
- Research on Cu exsolution and dynamic catalyst evolution during CO_2 hydrogenation
- Extensive experience in operando XPS, in situ XRD and in situ DRIFTS
- Designed transition-metal oxide and perovskite catalysts through defect engineering
- Specialized in oxygen-vacancy chemistry, catalyst reconstruction and structure–activity relationships
- First-author publications in *Journal of Environmental Chemical Engineering* and *ACS ES&T Engineering*; additional manuscripts under review in *Applied Catalysis B: Environment and Energy* and *Journal of Colloid and Interface Science*

Education

Zhe Jiang University, China | Sep 2023 – Present
PhD | School of Energy Engineering

Paul Scherrer Institute (PSI), Switzerland | Dec 2025 – Present
Visiting PhD | Group of Prof. Jeroen A. van Bokhoven

South China University of Technology, China | Sep 2020 – Jul 2023
Master | School of Environment and Energy

China Jiliang University, China| Sep 2016 – Jul 2020
Bachelor | Environmental Engineering

Current & Future Research Interests

- Dynamic Catalyst Evolution
- Operando Characterization
- Chemical Imaging for Catalysis
- Oxygen Vacancy Chemistry
- CO_2 Conversion

Research Experience

Environmental Catalysis and Reaction Mechanisms | ZJU

• Synergistic multi-pollutant (NOx & CVOC) catalysis over Ru/Mn-based oxide catalysts.

• Oxygen circulation and oxygen-vacancy-mediated catalytic pathways.

• In situ DRIFTS studies of surface intermediates and dynamic surface evolution.

• Sulfur-resistant catalytic mechanisms and structure–activity relationships.

CO_2 Hydrogenation and Exsolution Catalysis | PSI

• Designed Cu/$SrTiO_3$ catalysts for CO_2 hydrogenation.

• Investigated hydrogen-driven catalyst evolution using operando XPS and in situ XRD.

• Studied dynamic oxygen-vacancy formation and surface reconstruction.

• Participated in synchrotron-based catalyst characterization.

Representative Research Contributions

Catalyst Design

Designed Ru/Mn oxide catalysts and Cu-doped perovskite catalysts for environmental catalysis and CO_2 hydrogenation.

Operando Mechanistic Studies

Combined operando XPS, in situ XRD and DRIFTS to investigate how catalyst surfaces dynamically reconstruct under realistic reaction conditions

Understanding Dynamic Catalyst Evolution

Revealing the cooperative roles of oxygen vacancies, metal exsolution and surface reconstruction.

Research Expertise

Operando Characterization
• Operando XPS.
• In situ XRD.
• DRIFTS.
• Auto chem

Catalyst Design
• Transition Metal Oxides.
• Perovskites.
• Oxygen Vacancy Engineering.
• Mechanochemical Synthesis

Advanced Characterization
• TEM/SEM
• BET
• Raman

Computational Tools
• Basic DFT (VASP)
• AiiDA Workflow
• Data Analysis (Python)

Selected Publications

First-Author Publications

1. **F. Yao**, Y. Peng*, A. Cao, B. Zhou, S. Lu, J. Yan, Mechanochemical Force–Electron–Chemical Coupling at MnCe/$BaTiO_3$ Interfaces for Synergistic Multi-Pollutant Catalysis, Journal of Colloid and Interface Science, 2026.
2. **F. Yao**, Y. Peng*, A. Cao, B. Zhou, S. Lu, J. Yan, Dynamic Oxygen Circulation at Mn-Ov-Ce Interfaces Enables Low-Temperature Synergistic Removal of NOx and Chlorinated VOCs, Applied Catalysis B: Environment and Energy, under review.
3. **F. Yao**, Y. Peng, Z. Gong, et al., Degradation of o-DCB and Dioxins by MnCe Catalysts Prepared via the Mechanochemical Method, Journal of Environmental Chemical Engineering, 2025.
4. **F. Yao**, X. Wang, Y. Zhao, et al., Nitrogen-Doped Porous Biochar via Azotobacter chroococcum-Based Nitrogen Fixation for Improved VOC Adsorption, ACS ES&T Engineering, 2024.
5. **F. Yao**, G. Ye, W. Peng, et al., Preparation of Activated Biochar with Adjustable Pore Structure for Efficient VOC Adsorption, Journal of Environmental Chemical Engineering, 2023.

Additional co-author publications in Chemical Engineering Journal, Journal of Environmental Sciences, Environmental Science and Pollution Research, etc.

Research Funding & Projects

1. National Key R&D Program of China | Participant | 2022–Present
- Research on sulfur-resistant catalysts for VOC removal.
- Responsible for catalyst synthesis, characterization, catalytic evaluation.

2. National Natural Science Foundation of China | Key Participant | 2023–Present
- Mechanochemical regulation of Mn–Ce catalysts for synergistic NOx/VOC removal.
- Responsible for catalyst preparation, performance evaluation and characterization.

3. Industrial VOC Control Project | Key Participant | 2020
- Field investigation, emission analysis and VOC monitoring

Honours & Awards

2025.06 CSC Scholarship for PhD students

2023.09-2024.12 Outstanding Graduate Student*2.

2024.12 Inspirational Scholarship for PhD Students.

2021.11 Hualu environmental protection innovation scholarship.

2019.12 National Inspirational Scholarship

Academic Activities

- Reviewer for Journal of Hazardous Materials
- Oral Presentation, The 15th International Symposium on Catalytic Science and Technology Guangzhou, China | Nov. 2025
- Oral Presentation, The 18th Forum on Persistent Organic Pollutants and Chemical Product Environmental Safety | Chongqing, China | May 2025
- Oral Presentation, The 14th National Conference on Environmental Catalysis and Materials Kunming, China | Nov 2024