Dr Mehrdad Asgari

Chemical Engineering (separations, adsorption, Catalysis process translation) | AI and Data-Driven Discovery for Chemistry and Engineering | Materials Science

Address: Cambridge, United Kingdom **Email:** ma2000@cam.ac.uk
Current role: Bye-Fellow, Director of Studies & Tutor, Lucy Cavendish College (University of Cambridge) **Web:** Link
Google Scholar: Link **ORCID:** Link **Cit. / h-index (indicative):** ∼**2,100 / 27**

Profile

I am a chemical engineer and materials scientist working at the interface of **chemical engineering, chemistry, materials science, and data-driven discovery**. My current roles at Lucy Cavendish College, University of Cambridge include **Director of Studies in Chemical Engineering and Biotechnology**, **Tutor**, and **Bye-Fellow**. Alongside academic leadership and teaching, I pursue research and broader academic and industrial initiatives in **AI for chemistry**, **data-driven chemical engineering**, **porous materials**, **adsorption and separation processes**, **catalysis**, **process modelling**, and **structure–property relationships**. My work aims to connect rigorous scientific understanding with practical relevance for both academic and industrial contexts.

Research profile

Main areas

- **AI and data-driven chemistry:** AI-enabled approaches for chemistry and materials problems, including molecular and materials design, chemically informed modelling, and applied chemistry challenges such as dye development.
- **Porous materials and MOFs:** physical, physicochemical, and functional behaviour of porous materials, especially metal–organic frameworks.
- **Adsorption and separation science:** gas adsorption, selective separations, and process-relevant evaluation of sorbent materials.
- **Process modelling:** modelling of adsorption and separation processes, and translation of material-level behaviour into engineering decision-making.
- **Catalysis:** catalytic materials and catalytic phenomena, especially where structure and performance can be interpreted in a mechanistic way.
- **Structure–property relationships:** understanding how composition, topology, defects, morphology, and local chemical environment influence performance in chemical and materials systems.
- **Interpretable scientific machine learning:** trustworthy and interpretable ML methods for chemical engineering and materials science.

Academic appointments

Current

Director of Studies in Chemical Engineering and Biotechnology, Tutor, and Bye-Fellow Apr 2023 – Present
Lucy Cavendish College, University of Cambridge, United Kingdom

- Academic leadership in Chemical Engineering and Biotechnology within the College.
- Teaching, small-group supervision, student guidance, and contribution to the wider academic and collegiate environment.
- Continued development of research and collaborative initiatives spanning chemical engineering, materials science, and AI-enabled scientific discovery.

Previous

Marie Skłodowska–Curie Postdoctoral Fellow (UKRI-funded) Apr 2023 – Mar 2025
Department of Chemical Engineering and Biotechnology, University of Cambridge, United Kingdom

- Developed research at the intersection of advanced materials characterisation, porous materials, and interpretable machine learning.

SNSF Postdoctoral Mobility Fellow Oct 2021 – Mar 2023
Department of Chemical Engineering and Biotechnology, University of Cambridge, United Kingdom

- Worked on porous materials, separation-relevant performance, and translation-minded materials research.

Postdoctoral Researcher Jan 2021 – Sep 2021
LSMO, Institute of Chemical Sciences and Engineering (ISIC), EPFL, Sion, Switzerland

- Worked on computational tools and data analysis for gas adsorption in porous materials.

Postdoctoral Researcher Feb 2020 – Dec 2020
EPFL Valais Wallis, IPESE (SCI-STI-FM), Sion, Switzerland

- Worked on gas capture and separation processes using porous inorganic materials.

Education

Degrees

PhD in Chemical Engineering / Porous Materials 2015 – 2020
EPFL, Switzerland
Thesis: Characterization of metal-organic frameworks for gas adsorption and separation applications
Supervisor: Prof. Wendy Queen

MSc in Chemical Engineering 2011 – 2014
University of Tehran, Iran
Thesis: Core–shell nanoparticles and their impact on chemical gas sensor performance

BSc in Chemical Engineering 2007 – 2011
University of Tehran, Iran
Thesis: Design and construction of an experimental reactor setup for multiphase atmospheric reactions

Funding, prizes, and awards

Selected

- **Marie Skłodowska–Curie Postdoctoral Fellowship (UKRI-funded)** (2023), Sole PI.
- **SNSF Early Postdoctoral Mobility Fellowship** (2021), Sole PI.
- **Swiss Federal Office of Energy Pilot and Demonstration programme** (2022), contribution to proposal preparation.
- **DAAD short-term research grant** (2021).
- Swiss Chemical Society Chemistry Travel Award (2019).
- Ranked **1st** in MSc Chemical Engineering cohort, University of Tehran.
- Ranked **4th** in final stage of Iran National Chemical Engineering Olympiad.

Teaching, supervision, and academic leadership

Teaching and college roles

- Director of Studies in Chemical Engineering and Biotechnology at Lucy Cavendish College, University of Cambridge.
- Tutor at Lucy Cavendish College, contributing to academic support and the wider collegiate environment.
- Small-group Cambridge-style supervisions in core chemical engineering subjects, including process calculations, reaction engineering, heat and mass transfer, process thermodynamics, and fluid mechanics.
- Support for undergraduate learning, academic progression, and problem-solving development.
- Research and project mentoring where relevant at undergraduate, Master's, and doctoral level.

Research and professional activities

Selected themes of activity

- Development of AI and data-driven methods for chemistry, chemical engineering, and materials science.
- Research on porous materials and MOFs for adsorption, separations, and broader functional applications.
- Process-oriented evaluation and modelling of adsorption and separation systems.
- Studies linking physical and physicochemical behaviour of materials to observable performance.
- Work on catalysis and the mechanistic interpretation of catalytic materials behaviour.
- Development of interpretable modelling frameworks for scientific and engineering applications.
- Collaboration across chemistry, chemical engineering, materials science, and computational research.

Selected publication themes

Representative areas

- **Porous materials and MOFs:** adsorption, separation, structural behaviour, stability, and performance.
- **Adsorption and process-relevant modelling:** gas capture, selective separations, and process-facing interpretation.
- **AI and data-driven discovery:** interpretable modelling, anomaly detection, and chemically informed machine learning.
- **Structure–property relationships:** connecting composition, topology, defects, and physicochemical response to performance.
- **Catalysis and functional materials:** catalytic behaviour, active-site interpretation, and advanced materials applications.

Full publication list: Google Scholar (Link)

Service and professional contribution

Selected

- Member, International Scientific Committee, EUROMOF.
- Reviewer for journals across chemical engineering, materials chemistry, and data-driven chemistry.
- Participation in multi-institutional and interdisciplinary research collaborations.

Technical skills

Experimental and engineering

Adsorption and separations: gas adsorption, separation-oriented evaluation, cyclic and condition-sensitive testing, and interpretation of process-relevant metrics.
Materials characterisation: PXRD, spectroscopy-informed analysis, and structure-guided interpretation of material behaviour.
Engineering analysis: process reasoning, modelling perspectives, and performance interpretation for chemical engineering applications.

Computational and data

Python, data analysis, scientific computing, interpretable machine learning, robust validation, and reproducible computational workflows for chemistry, chemical engineering, and materials science.

Last updated: April 22, 2026