

Education

University of Cambridge

PHD IN CHEMICAL ENGINEERING

Cambridge, United Kingdom

2023 - Present

- Areas of Research: Machine Learning; Generative Deep Learning; Molecular Simulations; Nanoporous Materials.

University of Cambridge

M.RES IN PHYSICAL SCIENCES (NANOSCIENCE AND NANOTECHNOLOGY) (GRADE: 81/100 - DISTINCTION)

Cambridge, United Kingdom

2022 - 2023

- Thesis: Guiding the rational design of biocompatible metal-organic frameworks for drug delivery using interpretable machine learning.

Indian Institute of Technology Gandhinagar

B.TECH (WITH HONOURS) IN MATERIALS SCIENCE AND ENGINEERING (GPA: 9.11/10.00 - DEPARTMENT RANK 1)

Gandhinagar, India

2018 - 2022

- Institute Gold Medal, Director's Silver Medal, Gold Medal for Outstanding Research (Undergraduate)

Awards

- 2025 **Winton Cambridge - Berkeley Exchange Award.** Awarded a research fellowship at University of California, Berkeley under the supervision of Professor **Omar Yaghi (Nobel Prize in Chemistry, 2025)** to work on the “*generative design of metal-organic framework (MOF) water harvestors*”. California, US
- 2022 **Gold Medal for Outstanding Research (B.Tech).** Awarded for the best overall undergraduate research at IIT Gandhinagar. Gandhinagar, India
- 2022 **Institute Gold Medal (Materials Science and Engineering).** Awarded for the highest overall GPA in the B.Tech program in Materials Science and Engineering at IIT Gandhinagar. Gandhinagar, India
- 2022 **Director's Silver Medal (Materials Science and Engineering).** Awarded for the best overall performance in the B.Tech program in Materials Science and Engineering at IIT Gandhinagar. Gandhinagar, India
- 2022 **Engineering and Physical Sciences Research Council (EPSRC) PhD Award.** Awarded a fully-funded integrated MRes/PhD studentship at the Department of Physics, University of Cambridge. Cambridge, UK
- 2022 **Trinity-Henry Barlow (Honourary) Scholarship 2022-23.** Awarded on the recommendation of the Trinity-Henry Barlow electors at Trinity College, Cambridge. Cambridge, UK
- 2022 **American Society of Materials (ASM) International India National Council Award.** Awarded for performing outstanding materials research as an undergraduate student. India
- 2020 **Summer Undergraduate Research Fellowship (SURF), Caltech.** Awarded a research fellowship at California Institute of Technology under the guidance of Professor **Austin Minnich** to work on the “*reduction of electronic noise in semiconductors*.” [held virtually due to COVID-19] California, US
- 2020-22 **Scholarship for Academic Excellence, IIT Gandhinagar.** Awarded for securing the highest GPA in Materials Science and Engineering in the respective years. Gandhinagar, India
- 2019-22 **Dean's List for Excellence in Academics, IIT Gandhinagar.** Felicitated for academic excellence (securing over 8.5 GPA) in semesters III, V and VI of my undergraduate studies. Gandhinagar, India

Manuscripts Under Review

1. **Menon, D.**, Bhadane, P., Mahato, P., Goyal, P., Lynch, I., Chakraborty, S., and Misra, S.K., **Selective heavy-metal sequestration and rare-earth element recovery using metal-organic frameworks.** *Nature Protocols (revisions underway)*.
2. Zhao, Q.†, Li, B.†, **Menon, D.†**, Alizadeh Kiapi, M.R., Chen, X., Fairen-Jimenez, D., Zang, H-Y., and Xuan, W., **V-Shaped Cationic Tectons Direct Anion Templated Assembly of Superprotonic Polyanion-Organic Frameworks for High-Power Fuel Cells.** *Nature Chemistry (revisions underway)*.
3. Yang, S-L., Shi, M-H., Chen, X., Alizadeh Kiapi, M.R., **Menon, D.**, Huang, Y-B., Si, D-H., Zou, L., Fairen-Jimenez, D., Zang, and Cao, R., **Solar-driven tandem catalysis for sustainable ethylene glycol production from CO₂ and water.** *Nature Catalysis (revisions underway)*.
4. Chen, X., Wee, L.H., Alizadeh Kiapi, M.R., Tampaxis, C., Zheng, Y., Asgari, M., **Menon, D.**, Willhammar, T., Keenan, L.L., Charalambopolou, G., Cui, Y., Steriotis, T., and Fairen-Jimenez, D., **Topology-driven design of an ultraporous red MOF for high-performance hydrogen and methane storage.** *Nature Synthesis (under review)*.
5. Le, T-H. T., Alizadeh Kiapi, M.R., **Menon, D.**, Fairen-Jimenez, D., and Ortuno, M.A., **Oxidative Ring-Opening of Dimethylfuran in Zeolitic-Imidazolate Frameworks through Computational Design.** *The Journal of Physical Chemistry C (revisions underway)*.

† - equal contribution.

Research Articles

1. Chakraborty, S., Mikulska, I., Dhupal, P., Langford, N., Nehzati, S., Boseley, R., Pham, S., Pfrang, C., Kaur, M., Valsami-Jones, E., Ignatyev, K., **Menon, D.**, Misra, S.K. and Lynch, I., 2025. **Mapping the Hierarchical Environmental Transformations of Nanoscale UiO-66 Metal-organic Framework.** Environmental Science & Technology.
2. Chakraborty, S., Dhupal, P., Mikulska, I., Pham, S., Ellis, L.J., **Menon, D.**, Misra, S.K. and Lynch, I., 2025. **Biotic Transformation of Abiotically Stable Nanoscale UiO-66 Metal-Organic Framework by Daphnia magna Results in Chronic Reproductive Toxicity.** ACS Nano.
3. Kumar, A., Satpathy, B.K., Goyal, P., Upadhyay, R., Alizadeh Kiapi, M.R., Jasuja, K., **Menon, D.** and Misra, S.K., 2025. **Bimetallic MOF-derived CuO-Co₃O₄ heterostructures as high-capacity electrodes for asymmetric supercapacitors.** Chemical Engineering Journal, 520, p.165685.
4. Zhuang, Y., Mendes, B.B., **Menon, D.**, Oliveira, J., Chen, X., Duman, F.D., Coniot, J., Mercado, S., Liu, X., Zhang, S.Y. and Conde, J., 2025. **Multiscale Profiling of Nanoscale Metal-Organic Framework Biocompatibility and Immune Interactions.** Advanced Healthcare Materials, 14(29), p.e01809.
5. Liu, B., Chen, X., Yang, Y., Alizadeh Kiapi, M.R., **Menon, D.**, Zhao, Q., Yuan, G., Keenan, L., Fairen-Jimenez, D., and Xia, Q., 2025, **Engineering Bodipy-based Metal-Organic Frameworks for Efficient Full-Spectrum Photocatalysis in Amide Synthesis.** Angewandte Chemie, e202505405.
6. Melle, F., **Menon, D.**, Coniot, J., Ostolaza-Paraiso, J., Mercada, S., Oliveira, J., Chen, X., Mendes, B.B., Conde, J., and Fairen-Jimenez, D., 2024. **Rational Design of Metal-Organic Frameworks for Pancreatic Cancer Therapy: From Machine Learning Screening to *In Vivo* Efficacy.** Advanced Materials, p.2412757.
7. **Menon, D.** and Fairen-Jimenez, D., 2025. **Guiding the rational design of biocompatible metal-organic frameworks for drug delivery.** Matter
8. Chen, X.†, **Menon, D.**†, Wang, X., He, M., Alizadeh Kiapi, M.R., Asgari, M., Lyu, Y., Tang, X., Keenan, L.L., Shepard, W., Wee, L.H., Yang, S., Farha, O.K., and Fairen-Jimenez, D., 2024. **Flexibility-frustrated porosity for enhanced selective CO₂ adsorption in an ultramicroporous metal-organic framework.** Chem‡
9. Bhadane, P.†, **Menon, D.**†, Goyal, P., Alizadeh Kiapi, M.R., Satpathy, B.K., Lanza, A., Mikulska, I., Scatena, R., Michalik, S., Mahato, P., Asgari, M., Chen, X., Chakraborty, S., Mishra, A., Lynch, I., Fairen-Jimenez, D., and Misra, S.K. 2024. **A Two-Dimensional Metal-Organic Framework for Efficient Recovery of Heavy and Light Rare Earth Elements from Electronic Wastes.** Separation and Purification Technology, 360, p.130946.
10. Bhadane, P., Mahato, P., **Menon, D.**, Satpathy, B.K., Wu, L., Chakraborty, S., Goyal, P., Lynch, I. and Misra, S.K., 2024. **Hydrolytically stable nanosheets of Cu-imidazolate MOF for selective trapping and simultaneous removal of multiple heavy metal ions.** Environmental Science: Nano.‡
11. Goyal, P.†, **Menon, D.**†, Jain, P., Prakash, P. and Misra, S.K., 2023. **Linker mediated enhancement in reusability and regulation of Pb(II) removal mechanism of Cu-centered MOFs.** Separation and Purification Technology, 318, p.123941.
12. Chakraborty, S., **Menon, D.**, Akhil, V.V.S., Sahoo, M., Ranganathan, R., Zhang, P. and Misra, S.K., 2023. **Does the doping strategy of ferrite nanoparticles create a correlation between reactivity and toxicity?** Environmental Science: Nano.‡
13. Goyal, P., Paruthi, A., **Menon, D.**, Behara, R., Jaiswal, A., Keerthy, V., Kumar, A., Krishna, V. and Misra, S.K., 2021. **Fe doped bimetallic HKUST-1 MOF with enhanced water stability for trapping Pb(II) with high adsorption capacity.** Chemical Engineering Journal, p.133088.

† - equal contribution; ‡ - cover.

Reviews, Perspectives and Commentaries

1. Asgari, M., Albacete, P., **Menon, D.**, Lyu, Y., Chen, X., and Fairen-Jimenez, D., 2025, **The structuring of porous reticular materials for energy applications at industrial scales.** Chemical Society Reviews.‡
2. **Menon, D.** and Fairen-Jimenez, D., 2025. **Response to “feature assessment of MOF biocompatibility should consider statistical approaches beyond machine learning models”.** Matter, 8(6).
3. Chakraborty, S., **Menon, D.**, Mikulska, I., Pfrang, C., Fairen-Jimenez, D., Misra, S.K. and Lynch, I., 2025. **Make metal-organic frameworks safe and sustainable by design for industrial translation.** Nature Reviews Materials, pp.1-3.
4. **Menon, D.*** and Chakraborty, S., 2023. **How safe are nanoscale metal-organic frameworks?** Frontiers in Toxicology, 5, p.1233854.
5. **Menon, D.**, Singh, R., Joshi, K.B., Gupta, S. and Bhatia, D., 2022. **Designer, Programmable DNA-peptide hybrid materials with emergent properties to probe and modulate biological systems.** ChemBioChem, p.e202200580.
6. **Menon, D.** and Ranganathan, R., 2022. **A Generative Approach to Materials Discovery, Design and Optimization.** ACS Omega, 7(30), pp.25958-25973.
7. **Menon, D.** and Bhatia, D., 2022. **Biofunctionalized metal-organic frameworks and host-guest interactions for advanced biomedical applications.** Journal of Materials Chemistry B.

† - equal contribution; * - corresponding author; ‡ - cover.

Book Chapters

1. **Menon, D.**, Chakraborty, S., Goyal, P., Valsami-Jones, E. and Misra, S.K., 2023. **Nano Metal-Organic Frameworks as a Promising Candidate for Biomedical Applications.** in *Nanomaterials in Healthcare* (pp. 115-131). CRC Press.

Presentations and Conferences

1. **De novo design of metal-organic frameworks using generative deep learning**, Kavli ENSI Seminar, UC Berkeley, September 2025. Φ
2. Goyal, P.[†], **Menon, D.**[†], Jain, P., Prakash, P. and Misra, S.K., 2022. **Linker mediated improvement in stability of Cu-centered Metal-Organic Frameworks for enhanced Pb(II) removal from water.** 7th International Conference on Multifunctional, Hybrid and Nanomaterials, Genoa, Italy[#]
3. Goyal, P., Paruthi, A., **Menon, D.**, Kumar, A., Krishna, A., and Misra, S.K., 2021. **Improving hydrolytic stability of HKUST-1 metal organic framework by doping Fe(III), and its consequence of Pb(II) removal.** 7th Nano Today Conference, Guangzhou, China. [#]

† - equal contribution; # - poster presentation; \$ - oral presentation; Φ - seminar/talk

Research Experiences

A summary of key research projects. I work at the intersection of deep learning, computational materials science, and computational chemistry. My research focuses on: (i) the discovery, design, and optimization of nanoporous materials, and (ii) developing mechanistic insights into their performance. While most of my work since starting my PhD has been computational, my undergraduate and master's research also involved substantial experimental work.

Generative design of metal-organic framework water harvestors

University of California Berkeley

SUPERVISOR: PROFESSOR OMAR YAGHI; WINTON - BERKELEY EXCHANGE, 2025

July - September, 2025

- Developed a generative deep learning platform - **Nexerra^{R1}** - comprising a chemical language model coupled with flow models for the inverse design of metal-organic frameworks for water harvesting applications.

Generative modeling and computational design in reticular chemistry

University of Cambridge

SUPERVISOR: PROFESSOR DAVID FAIREN-JIMENEZ; PHD PROJECT

Ongoing

- Developing machine learning and generative deep learning methods for the discovery, design and optimisation of metal-organic frameworks. Using computational chemistry methods such as grand canonical Monte Carlo simulations and molecular dynamics for the high-throughput screening of large databases to inform materials selection and unravel mechanistic insights into material performance in applications such as drug delivery, gas storage and proton conductivity.

Defect engineering of Cu(II) metal-organic frameworks to enhance applicability for water remediation applications

IIT Gandhinagar

SUPERVISOR: PROFESSOR SUPERB MISRA; UNDERGRADUATE RESEARCH

2021-23

- Devised strategies - such as doping and linker exchange - for significantly enhancing the water stability of Cu(II) metal-organic frameworks. This drastically improved the performance of the frameworks for the selective capture of a wide-range of toxic heavy metal contaminants from water.

Enhancing the efficiency of plasmonic nanostructures for nanophotonic devices

University of Cambridge

SUPERVISOR: PROFESSOR JEREMY BAUMBERG; M.RES RESEARCH

2023

- Developed strategies - such as nanoparticle dimer formation and ion-beam milling - for enhancing the plasmonic efficiency (coupling) of plasmonic nano-antennae.

Floating catalyst bio-hybrids for artificial photosynthesis

University of Cambridge

SUPERVISOR: PROFESSOR ERWIN REISNER; M.RES RESEARCH

2023

- Devised a novel strategy using adaptive laboratory evolution for the direct interfacing of syngas fermenting bacteria as a bio-catalyst onto electrodes for an enhanced bio-photoelectrochemical performance.

Generative approaches to materials discovery, design and optimisation

IIT Gandhinagar

SUPERVISOR: PROFESSOR RAGHAVAN RANGANATHAN; UNDERGRADUATE RESEARCH

2021-22

- Studied and developed algorithms such as variational autoencoders and generative adversarial networks for the discovery and design of materials.

Peer Review

Peer reviewer for: **RSC Advances** (Royal Society of Chemistry); **Journal of Chemical Theory and Computation** (American Chemical Society); **Chemical Society Reviews** (Royal Society of Chemistry); **Digital Discovery** (Royal Society of Chemistry)

Supervision & Teaching

1. **Course Supervisor:** Adsorption and Advanced Nanoporous Materials (University of Cambridge, 2025). *Course supervisor for the final year (IIB) undergraduate course.*
2. **Course Supervisor:** Materials Science (University of Cambridge, 2025). *Course supervisor for the 1st-year (IA) undergraduate course.*

3. **Co-supervision:** Anthony Ortega (University of Cambridge, 2024). *Supervised Anthony for an **MPhil** project on the development of machine learning based approaches for the high-throughput screening of CO₂ sorbents.*
4. **Co-supervision:** Aron Alagaraj (University of Cambridge, 2023-24). *Supervised Aron for a **Part IIB** project on the development of machine learning based approaches for predicting and understanding the ecotoxicology of metal-organic frameworks.*
5. **Teaching Assistant:** ES202 - Introduction to Materials (IIT Gandhinagar, 2021). *Made instructional experimental and theoretical videos for the better understanding of course concepts. Conducted discussion and doubt sessions to address the academic concerns of over 170 students.*

Technical Knowledge

Core Skills: Machine Learning; Deep Learning; Molecular Simulations (Grand Canonical Monte Carlo Simulations & Molecular Dynamics)

Tools: Python; RASPA; LAMMPS; Materials Studio; Adobe Illustrator

Additional

Football Player

IIT Gandhinagar

IIT GANDHINAGAR FOOTBALL TEAM

2018-22

- Represented the institute at the 54th Inter-IIT Sports Meet at IIT Kharagpur in 2019 in Men's Football and various district- and state-level college tournaments.