Dhruv Menon

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Building generative deep learning models and autonomous, end-to-end discovery pipelines to design novel materials. Research focuses on transformer architectures, flow matching, diffusion models, variational autoencoders, and LLM-based agentic AI for closed-loop molecular design, from computational screening and simulation to experimental validation.

EDUCATION

University of Cambridge Cambridge, UK
PhD in Chemical Engineering *Sept. 2023 – Jan. 2027 (Expected)*

- Research: Generative deep learning, chemical language models, molecular simulation, and inverse design of nanoporous materials.

University of Cambridge Cambridge, UK
M.Res. in Physical Sciences (Nanoscience and Nanotechnology); Grade: 81/100 (Distinction) *2022 – 2023*

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

Indian Institute of Technology Gandhinagar Gandhinagar, India
B.Tech. with Honors in Materials Science and Engineering; Grade: 9.11/10.00 *2018 – 2022*

- Institute Gold Medal; Director's Silver Medal; Gold Medal for Outstanding Research; Dean's List and academic excellence scholarships.

EXPERIENCE

Generative Molecular Design for Reticular Materials 2023 – Present
Doctoral Research, University of Cambridge; Supervisor: Prof. David Fairen-Jimenez *Cambridge, UK*

- Developed **Nexerra**, a generative molecular design framework combining transformer-based chemical language models, variational autoencoders, and conditional flow matching for inverse molecular design.
- Built scalable data-generation and preprocessing pipelines for $\sim$1 million molecular structures, including molecular augmentation, tokenization, canonicalization, filtering, and automated quality control.
- Developed representation learning methods for molecular embeddings, latent-space optimization, and conditional molecular generation under chemical validity, synthesizability, and physical design constraints.
- Integrated learned molecular representations with automated crystal structure assembly, molecular simulation, and high-throughput virtual screening for end-to-end AI-guided materials discovery for adsorption, gas storage, water harvesting, and drug delivery.

Generative Design of Water Harvesting Materials Jul. 2025 – Sept. 2025
Winton Cambridge–Berkeley Exchange Fellow, UC Berkeley; Supervisor: Prof. Omar M. Yaghi *Berkeley, CA*

- Extended the **Nexerra** framework by developing application-specific objective functions and multi-objective optimization strategies for atmospheric water-harvesting materials.
- Investigated molecular design criteria balancing chemical validity, synthesizability, hydrophobicity, adsorption-relevant features, and structural constraints.
- Worked with synthetic chemists to prioritize machine-learning-generated candidates for high-throughput synthesis and characterization workflows.

Computational Drug Delivery & Nanomedicine 2023 – 2025
Doctoral Research, University of Cambridge; Supervisor: Prof. David Fairen-Jimenez *Cambridge, UK*

- Developed interpretable machine learning models to predict the biocompatibility of drug delivery systems, enabling high-throughput screening of 86,000+ experimentally reported materials for nanomedicine applications.
- Built a hierarchical virtual screening workflow combining machine learning toxicity prediction with Grand Canonical Monte Carlo simulations to identify optimal drug carriers for multiple chemotherapeutics prior to experimental validation.
- Applied the computational framework to discover **PCN-222** as a promising drug delivery platform, which was subsequently synthesized, characterized, and evaluated experimentally.
- Collaborated with experimental researchers to translate computational predictions into in vitro and mouse models of pancreatic cancer, where the optimized MOF formulation demonstrated reduced tumour growth and metastatic spread, validating the practical utility of the computational screening strategy.

Molecular Simulations of Confined Proton Transport 2024 – 2026
Doctoral Research, University of Cambridge; Supervisor: Prof. David Fairen-Jimenez *Cambridge, UK*

- Developed multiscale simulation workflows integrating Grand Canonical Monte Carlo and molecular dynamics to investigate molecular transport, and proton-conduction mechanisms in functional porous materials.

- Designed reproducible analysis pipelines for diffusion, radial distribution functions, hydrogen-bond networks, velocity correlations, spatial distributions, and transport behaviour.
- Integrated molecular simulations with structural and experimental evidence to identify the mechanisms governing transport under nanoconfinement.

KEY PUBLICATIONS

20+ peer-reviewed publications across materials chemistry, molecular simulation, and AI-guided materials design, including Nature Chemistry, Advanced Materials, Chem, Matter, and Chemical Society Reviews. **800+ citations; h-index 16**. Full list on Google Scholar. ϕ denotes co-first authorship.

- **Menon, D.**, Singh, V., Chen, X., Alizadeh Kiapi, M.R., Zyuzin, I., Macleod, H.W., Rampal, N., Shepard, W., Yaghi, O.M., and Fairen-Jimenez, D., 2026. **A chemical language model for reticular materials design.** arXiv preprint arXiv:2603.20389 [Link] *(JACS, Under Revision)*
- Zhao, Q.$^{\phi}$, Li, B.$^{\phi}$, **Menon, D.**$^{\phi}$, Zhu, C.$^{\phi}$, Alizadeh Kiapi, M.R., Chen, X., Long, D.-L, Liu, J., Xiao, Z., Yang, D., Fairen-Jimenez, D., Zang, H-Y., and Xuan, W., 2026. **Cation-directed assembly and sequential functionalization enable superprotonic polyanion-organic frameworks for high-power fuel cells.** Nature Chemistry. [Link]
- Melle, F., **Menon, D.**, Conniot, J., Ostolaza-Paraiso, J., Mercado, 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. [Link]
- **Menon, D.** and Fairen-Jimenez, D., 2025. **Guiding the rational design of biocompatible metal-organic frameworks for drug delivery.** Matter [Link]
- Chen, X.$^{\phi}$, **Menon, D.**$^{\phi}$, 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 CO_2 adsorption in an ultramicroporous metal-organic framework.** Chem [Link]

SKILLS

- **Machine Learning**: Transformers; Attention; Variational Autoencoders; Flow Matching; Diffusion Models; Equivariant Models; Representation Learning; Graph Neural Networks; Chemical Language Models.
- **Programming**: Python; HPC; SLURM; Docker; Git; Latex; RDKit; NumPy; pandas; automated simulation and data pipelines
- **Modelling and Simulation**: Molecular dynamics; Grand Canonical Monte Carlo; LAMMPS; RASPA; Classical Force Fields; Statistical Mechanics; Adsorption; Molecular Transport; and High-Throughput Virtual Screening.
- **Molecular Design**: Inverse molecular design; molecular representations; structure-property analysis; synthetic accessibility; porous materials; drug-delivery materials; gas adsorption; water harvesting.

AWARDS AND FUNDING

- **Winton Cambridge-Berkeley Exchange Scholar** – awarded a research fellowship at University of California Berkeley under the supervision of Prof. Omar Yaghi (Nobel Laureate, 2025) to work on the "generative design of metal-organic framework water harvesters", **2025**.
- **Gold Medal for Outstanding Research, IIT Gandhinagar** – awarded for best overall undergraduate research at IIT Gandhinagar, **2022**.
- **Institute Gold Medal, Materials Science and Engineering** – highest overall GPA in B.Tech. program, IIT Gandhinagar, **2022**.
- **EPSRC PhD Award** – awarded a fully-funded integrated MRes/PhD studentship at the Department of Physics, University of Cambridge, **2022**.
- **Summer Undergraduate Research Fellowship, 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), **2020**.

SELECTED INVITED TALKS

- **De novo design of metal–organic frameworks using generative deep learning**, Kavli ENSI Seminar, University of California Berkeley, 2025.

SELECTED SERVICE & MENTORING

Reviewer for *Chemical Society Reviews*, *Advanced Science*, *Journal of Chemical Theory and Computation*, *Materials Horizons*, and *Nature Communications*. Supervised undergraduate and MPhil projects in adsorption, nanoporous materials, and machine learning for materials. Supervisor for advanced nanomaterials and undergraduate materials science courses.