

Mohan Guo

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Education

University of Amsterdam *MSc in Artificial Intelligence* *Amsterdam, Netherlands*
Sept 2023 – Present

- **Cum Laude**
- GPA: **8.70/10**
- Thesis: Frame-based Equivariant Diffusion Models for 3D Molecular Generation (SOTA performance)
- Coursework: Computer Vision (9.35/10), Machine Learning, Deep Learning, Natural Language Processing, Reinforcement Learning

Southeast University *MEng in Communication Engineering* *Nanjing, China Sept 2020*
– June 2023

- Grade: 88.9/100
- Coursework: Algorithm Design and Analysis, Engineering Matrix Theory

Nanjing University of Science and Technology *BEng in Communication Engineering* *Nanjing, China Sept 2016*
– Apr 2020

- Grade: 91/100
- Awards: **National Scholarship Recipient** (Top 0.2%), **Principal's Medal** (Highest Honor for Bachelor's Degree)
- Coursework: Engineering Mathematics (97), Linear Algebra (98), Probability and Statistics (98)

Projects

Frame-based Equivariant Diffusion Models for Molecular Generation *Amsterdam, Netherlands*
Jan 2025 – Present

- Developed a novel **frame-based equivariant diffusion framework** for 3D molecule generation that decouples $E(3)$ symmetry constraints from backbone architectures.
- Systematically studied **geometric representation learning** through multiple canonicalization schemes to encode symmetry-aware molecular structures.
- Adapted and optimized **Diffusion Transformer (DiT)** with edge-aware geometric attention, enhancing sample quality and inference efficiency.
- Achieved **SOTA or comparable performance across all metrics** (e.g. test NLL of -137.97) while maintaining high molecular stability (89.39%) and 50% faster sampling compared to EDM on QM9 dataset.
- **Supervisors:** Cong Liu and Prof. Patrick Forré (AMLab, AI4Science Lab)
- Published at **Frontiers in Probabilistic Inference: Sampling Meets Learning (FPI)@NeurIPS2025**

AI Engineer Intern *HAVAS Media* *Amsterdam, Netherlands*
Nov 2024 – May 2025

- Independently developed an **LLM-powered agent system** that interfaces with structured tabular data to answer domain-specific financial queries with high accuracy.
- Designed a semantic integration pipeline for **embedding financial terminology and mathematical expressions** into language model prompts, enabling precise querying over internal databases.
- Implemented **hallucination mitigation strategies** including response filtering and retrieval grounding, enhancing system reliability and factual correctness.
- **Tech Stack:** Python, PyTorch, SQL, Google Cloud Platform, NLP, Graph Neural Networks

E(n) Equivariant Diffusion Model Optimization *Amsterdam, Netherlands*
Apr – May 2024

- Implemented equivariant diffusion models in JAX for 3D molecular generation with **60% performance improvement**

- Explored **consistency model** for accelerated molecular sampling and enhanced synthetic accessibility prediction
- **Published at GRaM Workshop @ ICML 2024**

Neural-symbolic Causal Representation Learning

Amsterdam, Netherlands

Jun – Aug 2024

- Investigated **causal representation learning under few-shot settings**, aiming to align learned latent factors with **human-interpretable causal concepts**.
- Integrated **neural-symbolic semantic constraints** into BISCUIT’s loss function to improve interpretability and structure-grounded generalization.
- Applied and evaluated the model on iThor embodied scenes, demonstrating improvements in **concept-level alignment and causal consistency**.
- **Supervisor:** Prof. Sara Magliacane

Reproducibility Study of Equal Improvability Fairness

Amsterdam, Netherlands

Feb – May 2024

- This research focuses on the Equal Improvability (EI) framework, a theoretical model designed to equalize acceptance rates across different groups by quantifying the required efforts for improvement. This framework aims to enhance long-term fairness in decision-making processes.
- We reproduced the results and validated the claims. We also conducted extended experiments. Unlike the original study that used a Gaussian distribution dataset, we introduced non-parametric updates and a Chi-square fit to generalize the dataset. This approach allowed us to test the EI framework’s adaptability and performance under different distribution scenarios.

ASIC Design & Algorithm Developer Intern *Purple Mountain Laboratory*

Nanjing, China Sep 2021

– Jun 2023

- Led the design and development of a **real-time FMCW radar baseband chip** for autonomous driving applications during a two-year research internship.
- Successfully completed **tape-out and mass production**, with the chip deployed in commercial use.
- Developed and optimized signal processing algorithms in C++ and MATLAB, ensuring real-time performance on embedded hardware.
- **Tools:** C++, MATLAB, Signal Processing, Real-time Systems, Algorithm Optimization

Technical Skills

Code Python (PyTorch, JAX, NumPy, Scikit-learn, Pandas), C++, MATLAB, Bash, Git
AI 3D Generation, Diffusion Models, Flow Matching, Score Matching, Equivariant Networks, Geometric Deep Learning, Representation Learning, Graph Neural Network, Group Theory, Causality, Transformer
Tools SQL, Linux, HPC, Docker, Google Cloud Platform, Real-time Systems, FPGA Prototyping

Publications

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- **Guo, M.**, Liu, C., Forré, P. (2025). Frame-based Equivariant Diffusion Models for 3D Molecular Generation. arXiv preprint arXiv:2509.19506. (Earlier version published at **Frontiers in Probabilistic Inference: Sampling Meets Learning (FPI)@NeurIPS2025**), extensive version on [Arxiv](#)
 - Sedlacek, M., Vozikis, A., Bartak, P., Cadigan, L., **Guo, M.** *Equivariant Diffusion for Molecule Generation in 3D using Consistency Models*. GRaM Workshop @ ICML 2024.
 - Yang, M., Zhao, D., Xu, C., Gu, P., Yi, Y., **Guo, M.**, Yan, X., Liu, L., Chai, Y., Liu, H., You, X. *K/Ka-Band Hybrid-Packaged Four-Element Four-Beam Phased-Array Transmitter and Receiver Front-Ends with Optimized Beamforming Passive Networks*. IEEE JSSC, 59(11), 3142–3155. (2024)
 - Yang, M., Xu, C., Gu, P., Yi, Y., **Guo, M.**, Liu, L., Yan, X., You, X., Zhao, D. *K/Ka-Band 4-Element 4-Beam Hybrid Phased-Array Transmitter and Receiver Front-Ends with Compact Layout Floor-Plans and Fault-Tolerant Digital Circuits*. IEEE A-SSCC, 2023.
 - **Guo, M.**, Zhao, D., Wu, Q., Wu, J., Li, D., Zhang, P. *An Integrated Real-Time FMCW Radar Baseband Processor in 40-nm CMOS*. IEEE Access, 11, 36041–36051. (2023)