

OMID BARATI FARIMANI

Graduate Student Research Assistant – Carnegie Mellon University
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PROFESSIONAL SUMMARY

Ph.D. student in Mechanical Engineering at Carnegie Mellon University with expertise in **machine learning, molecular simulations, and AI-driven materials discovery**. Experienced in developing deep learning pipelines, retrieval-augmented LLMs, and graph neural networks for molecular and polymer design. Proven record of high-impact publications in leading journals and active manuscripts on cutting-edge AI-materials frameworks. Eager to apply computational and AI expertise to industrial R&D and innovation.

EDUCATION

Carnegie Mellon University, Pittsburgh, PA.

PhD candidate in Mechanical Engineering, Developing AI Agents for Materials and Mechanical Systems, 2022 – Present.

CORE SKILLS

- **Machine Learning & AI:** Deep learning (PyTorch, TensorFlow), Graph Neural Networks, Retrieval-Augmented Generation (RAG), XGBoost
- **Data Analysis & Modeling:** Molecular dynamics simulations, desalination modeling, polymer performance prediction
- **Programming:** Python, PyTorch Geometric, RDKit, NumPy, Pandas, Scikit-learn
- **Big Data & Pipelines:** Dataset preprocessing, feature extraction, high-performance computing workflows
- **Research & Communication:** Peer-reviewed publications, technical reporting, presentations, collaboration across disciplines

WORKING EXPERIENCE

Graduate Student Research Assistant

Carnegie Mellon University – AI-ML Lab | Jan 2022 – Present

- Designed and implemented deep learning pipelines to predict water flux and ion rejection in nanomaterials.
- Developed retrieval-augmented LLM systems (*NanoGPT*) for nanotechnology research.
- Constructed large-scale molecular datasets and fingerprint descriptors for desalination membranes.
- Applied graph neural networks and advanced ML models to accelerate polymer discovery.
- Authored and co-authored publications in *Nano Letters* and *ACS Applied Materials & Interfaces*.
- Collaborated with interdisciplinary teams bridging mechanical engineering, chemistry, and computer science.

PUBLICATIONS

Peer-Reviewed

- *Machine learning in membrane design: From property prediction to AI-guided optimization* – *Nano Letters*, 2024.
- *Fast Water Desalination with a Graphene–MoS₂ Nanoporous Heterostructure* – *ACS Applied Materials & Interfaces*, 2024.
- *NANO-GPT: A Query-Driven Large Language Model Retrieval-Augmented Generation System for Nanotechnology Research* – *arXiv*, 2025.

Manuscripts Under Review / In Preparation

- *Desalination LLM: Large Language Model Agents Design Efficient Graphene Membranes for Water Desalination.*
- *A Generalizable Computational-to-Experimental Framework Agent for Polymer Design Optimization in Separation Technologies.*

RELEVANT COURSEWORK

- Machine Learning for Engineers – CMU
- Deep Learning for Engineers – CMU
- Mechanical Project Management – CMU
- AI Agents for Engineering- CMU