

Amir Mahdi Zardoshti, MSc.

✉ mahdi.zardoshti02@sharif.edu

🌐 zardoshtgroup.org

🌐 linkedin.com/in/amir-mahdi-zardoshti-678a2a363

☎ +98 (0)992-6104387



Education

- 2020 – 2024 **Bachelor of Science in Applied Chemistry** Chemistry Faculty, School of Chemistry, University of Tehran, Tehran, Iran.
- 2024 – **Master of Science in Physical Chemistry** Chemistry Department, Sharif University of Technology, Tehran, Iran.

Subjects of Interest

- Neural Networks,, Geometric Deep Learning, Active Learning, Transfer Learning**
- Bayesian optimization, Gaussian Process Regression**
- Computational Chemistry**
- Molecular Dynamics (MD), Ab Initio Molecular Dynamics (AIMD), and Multi-Configurational Time-Dependent Hartree (MCTDH), Ring-polymer instanton theory**
- Computational Drug Design**
- De novo protein design: AlphaFold**
- Organic Synthesis**

Research Experience

- 2023 – 2024 **Industrial Intern.** Tarmim Darou Behavar Company (brand name: “Behrokh”). Worked on the synthesis of nanomaterials (e.g. MOFs), and small molecules.
- 2022 – 2024 **Undergraduate Researcher.** Artificial Intelligence in Drug Design, IBB Institute, University of Tehran, Tehran, Iran. Worked under the supervision of **Dr Mohammad Taheri-Ledari** and **Dr Kaveh Kavousi**, conducting research on the application of machine learning techniques to drug discovery pipelines.
- 2024 – Present **MSc Thesis Research.** Using Machine Learning to Model Potential Energy Surfaces and Explore Their Applications in Spectroscopy — supervised by **Prof Zahra Jamshidi**, Department of Chemistry, Sharif University of Technology, Tehran, Iran. Applied deep learning models to predict quantum chemical properties from molecular structures.

Selected Projects

Computational Projects

- Geometric Deep Learning Based on Local Molecular Properties: Integrating Quantum Mechanics-Driven 3D-QSAR with Deep Learning-Based Point Cloud to Predict Drug Efficacy.** (Feb. 2024, 3rd International and 12th Iranian Conference on Bioinformatics. Poster presentation)

Selected Projects (continued)

- **Generative point-cloud models combined with transformer-based SMILES captioning for de novo drug design.** (Independent ongoing project since February 2025)
- **Learning Potential Energy Surfaces for Quantum-Accurate Molecular Dynamics and Spectroscopy.** (MSc thesis project)

Laboratory Projects

- **Synthesis of Metal–Organic Frameworks (MOFs): UiO-66(Zr) and derivatives.** Explored applications in catalysis and drug delivery.
- **Heterocyclic Compounds Synthesis & Nucleotide Chemistry.** Preparation and characterisation of: – **Oxazole derivatives** as a novel class of VEGFR2 kinase inhibitors. – **2-Arylbenzimidazoles** via copper-catalysed condensation of anilines with benzoic acids.

Current Research

- **Learning Potential Energy Surfaces for Quantum-Accurate Molecular Dynamics and Spectroscopy — MSc Thesis Research** Under the supervision of **Prof. Zahra Jamshidi**, Sharif University of Technology.

Research focused on integrating **Machine Learning Interatomic Potentials (MLIPs)** with **quantum chemistry methods** to predict molecular properties with high accuracy and computational efficiency. To generate a sufficiently diverse ensemble of molecular structures, techniques such as **normal mode sampling** and **active learning** were employed. Furthermore, to achieve high-level quantum-chemical precision, **transfer learning** was applied.

The main applications of this work include:

- *Finding minimum-energy structures of molecules and small metal clusters using Neural Networks and Gaussian Process Regression.*
- *Enhanced Molecular Dynamics simulations for Infrared (IR) spectral prediction.*
- *Excited-State Non-Adiabatic Molecular Dynamics.*
- *Tunneling splitting calculations.*

Skills

Programming Languages

- Python (advanced), C++ (basic), Bash scripting

Deep Learning

- Model development using PyTorch and TensorFlow; Applied advanced methods including **geometric deep learning, point cloud-based deep learning, graph neural networks, interatomic potential neural networks, message passing neural network, Gaussian processes regression, generative models, LSTM, and Transformer architectures**, with emphasis on chemistry-related AI tasks.

Quantum Chemistry

- DFT and *ab initio* molecular dynamics using ORCA, Gaussian, CP2K, SHARC and MCTDH.

Skills (continued)

Computational Drug Design	■ Molecular docking with AutoDock, pharmacophore modelling using MOE, molecular dynamics simulations with GROMACS.
Visualisation Tools	■ PyMOL, VMD.
Languages	■ Fluent in Persian (native) and English (British academic proficiency — reading, writing, and speaking.)

Miscellaneous Experience

Awards and Achievements

2014–2020	■ Exceptional Talents School , Tehran — Studied at a nationally recognized school for gifted students.
2020	■ Top Rank in National University Entrance Exam , admitted to the University of Tehran for BSc in Applied Chemistry.
2024	■ 16th Rank Nationwide in Iran's Master's Entrance Exam — Admitted to Sharif University of Technology.
2015–2024	■ Iranian National Chemistry Olympiad Finalist — Qualified three times (twice in high school, once in university).
2015	■ Member of Iran National Youth Football Team.

Teaching Experience

2025	■ Teaching Assistant — Mathematics I , Faculty of Chemistry, School of Chemistry, University of Tehran, Tehran, Iran.
	■ Teaching Assistant — Analytical Chemistry I , Faculty of Chemistry, School of Chemistry, University of Tehran, Tehran, Iran.
	■ Teaching Assistant — Computational Chemistry , Department of Chemistry Sharif University of Technology Tehran, Iran.

Certification

Feb. 2024	■ Poster Presentation Certificate — Presented research at the 3rd International and 12th Iranian Conference on Bioinformatics: <i>Enhancing Drug Design for VEGFR2: Integrating Quantum Mechanics-Driven 3D-QSAR with Deep Learning to Predict Drug Efficacy.</i>
Feb. 2025	■ Executive Committee Certificate — Recognized for active participation in organising the 5th Winter School of Computational Chemistry, Sharif University of Technology, under the supervision of Prof Zahra Jamshidi.

References

Dr. Zahra Jamshidi

Assistant Professor, Department of Chemistry
Sharif University of Technology
Email: njamshidi@sharif.edu