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Curriculum Vitae

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Education

2024 – present
- **Master of Science in Physical Chemistry** Chemistry Department, Sharif University of Technology, Tehran, Iran.

2020 – 2024
- **Bachelor of Science in Applied Chemistry** Chemistry Faculty, School of Chemistry, University of Tehran, Tehran, Iran.

Research of Interest

- Research interests centre on the application of **machine learning methods** and **artificial intelligence techniques** in computational chemistry and molecular modelling. The initial motivation arose from studies in **Quantitative Structure–Activity Relationship (QSAR)** analysis, employing methods such as **Principal Component Analysis (PCA)**, **Support Vector Machines (SVMs)**, and **voxel-based convolutional neural network**. Further work has explored the representation of molecular structures as **point clouds**, leading to the use of **point cloud–based neural network architectures**. During the master's programme, attention expanded to **Message Passing Neural Networks (MPNNs)**, which are capable of accurately modelling **potential energy surfaces (PESs)** and benefit from **transfer learning**.
- Current research interests also include data preparation and sampling strategies, with particular emphasis on uncertainty estimation through **query-by-committee frameworks**, and the use of **Gaussian Process Regression (GPR)** as a probabilistic approach to energy-surface prediction and uncertainty quantification.
- A long-term objective is the development of **machine learning interatomic potentials (MLIPs)** that integrate the advantages of MPNNs and GPR to provide accurate, transferable models for quantum-chemical systems and molecular dynamics; I also aim to represent molecules via point-cloud sampling of their **electrostatic potential around the molecular surface (ESP)**, and leverage point-cloud-based deep learning to enable the design and discovery of new molecules for **de novo** drug design.

Research Experience

2023 – 2024
- **Industrial Intern.** Tarmim Darou Behavar Company (brand name: "Behrokh"). 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.

Research Experience (continued)

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; represented molecular structures as **point clouds** and applied **point cloud–based deep learning** to predict **drug efficacy**.

Current Research

- MSc proposal research: **Learning Potential Energy Surfaces for Quantum-Accurate Molecular Dynamics and Spectroscopy** Under the supervision of **Prof. Zahra Jamshidi**, Sharif University of Technology.
  Research applies MLIPs with quantum-chemistry methods to predict molecular properties accurately and efficiently, using uncertainty-guided **Bayesian sampling** and **active-learning** loops to prioritize informative configurations, reduce dataset-generation cost, and minimize training data requirements. The main applications of this work include:
  - *Learning the PES of molecules and small metal clusters, with a particular focus on* Ag_{20}.
  - *Enhancing Molecular Dynamics simulations for Infrared (IR) spectral prediction.*
  - *I would like to learn and work in the area of Excited-State Non-Adiabatic Molecular Dynamics in the future.*

- **Generative point-cloud models combined with transformer-based SMILES captioning for de novo drug design.** Conceived and currently developing this project independently (since February 2025); the core idea is to translate a molecule's **point-cloud representation**—derived from its **electrostatic potential energy surface**—into a **SMILES format**. The work involves employing the **FoldingNet architecture** as a point cloud auto-encoder , integrated with a **Transformer-based molecular captioning model**.

Skills

Programming Languages
- **Python** (intermediate), **C++** (beginner)

Deep Learning
- Experienced with **PyTorch** and **TensorFlow 1.x**; worked with **point cloud–based deep learning** models such as **PointNet**, **PointNet++**, and **Point Cloud Auto-encoder (FoldingNet)**, as well as **message passing neural networks** including **SchNet**, **PhysNet**, and **PAINN**; with some additional experience in **Transformer** architectures and **LSTM** models.

Quantum Chemistry
- Experienced with geometry optimization, vibrational frequency, and TDDFT calculations using **Gaussian** and **ORCA**; performed Born–Oppenheimer AIMD simulations in **CP2K** using KS-DFT; currently learning **SHARC** and **MCTDH** for excited-state dynamics.

Skills (continued)

Cheminformatics & Molecular Tools	• Experienced with **RDKit** for molecular featurization, property evaluation, and dataset preparation; proficient with the **Atomic Simulation Environment (ASE)** for building structures, running atomistic workflows, and interfacing with quantum-chemistry/MD codes.
Visualisation Tools	• Avogadro, VMD, PyMOL, Multiwfn.
Languages	• Native in Persian; fluent in English; interested in learning French and German.

Miscellaneous Experience

Awards and Achievements

2024	• **16th Rank Nationwide** in Iran's Master's Entrance Exam — Admitted to Sharif University of Technology.
2018, 2019, 2024	• **Iranian National Chemistry Olympiad Finalist** — Qualified three times (twice in high school, once in university).
2020	• **Top Rank in National University Entrance Exam**, admitted to the University of Tehran for BSc in Applied Chemistry.
2014–2020	• **Exceptional Talents School**, Studied at a nationally recognized school.
2015	• **Member of Iran National Youth Football Team**.

Teaching Experience

Fall 2025	• **Teaching Assistant — Computational Chemistry,** Department of Chemistry Sharif University of Technology Tehran, Iran.
Spring 2025	• **Teaching Assistant — General Mathematics I,** Faculty of Chemistry, School of Chemistry, University of Tehran, Tehran, Iran. View Teaching Certificate
	• **Teaching Assistant — Analytical Chemistry I,** Faculty of Chemistry, School of Chemistry, University of Tehran, Tehran, Iran. View Teaching Certificate

Certification

February 2024	• **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. View Certificate

Miscellaneous Experience (continued)

Publications

- Zardoshti, Amir Mahdi; Zarvani, Maral; Taheri-Ledari, Mohammad; Kavousi, Kaveh. *Enhancing Drug Design for VEGFR2: Integrating Quantum Mechanics-Driven 3D QSAR with Deep Learning to Predict Drug Efficacy.* The 12th National Conference and the 3rd International Bioinformatics Conference, Behshahr. Proceedings link

References

- **Prof. Zahra Jamshidi** (M.Sc. Supervisor)
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