Arsalan Hashemi

GitHub

Residence/domicile: Espoo, Finland

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LinkedIn

I am a computational materials scientist with more than 9 years experience, including six years in engineering physics and three years in chemistry. Expertise in **density functional theory calculations**, **molecular dynamics simulations**, and **machine learning** for high-throughput virtual screening. I have a proven track record as a **Python** programmer and big data analyst. [Google Scholar] [ORCiD]

Academic Background: Research Experience

PostDoc in "Computational Material Science" *Sept. 2025 - Present*
Department of Physics, Prof. M. Karttunen *Eastern University of Finland, Finland*

- My mission is to develop machine learning models to study macromolecules for applications in water purification and drug delivery.

PostDoc in "Computational Physics" *Apr. 2024 - Aug. 2025*
Department of Applied Physics, Prof. T. Ala-Nissilä *Aalto University, Finland*

- Conducting ab-initio molecular dynamics simulations and deep learning to study the interactions between NaCl electrolytes and graphene (EU-funded GreenDiGi project).
- Exploring novel two-dimensional heterostructure platforms for hosting single-atom catalysts.

PostDoc in "Computational Electrochemistry" *Feb. 2023 - Mar. 2024*
Department of Chemistry and Materials Science, Prof. K. Laasonen *Aalto University, Finland*

- Developing an outlier detection algorithm to enhance predictability in general, with a specific focus on organic molecule solubility. [Manuscript]
- Leveraging high-throughput virtual screening to predict the redox potential and solubility of organic molecules. [Article]
- Collaborating with experimentalists and providing computational support for their findings on battery technology. [Article]

Research Assistant in "Computational Electrochemistry" *Aug. 2020 - Jan. 2023*
Department of Chemistry and Materials Science, Prof. K. Laasonen *Aalto University, Finland*

- Exploring electrode-electrolyte interactions through molecular dynamics simulations. [Article]
- Delivering data-driven presentations and reports at annual CompBat EU-project meetings.

Doctoral Candidate in "Engineering Physics" *Jun. 2016 - Jul. 2020*
Department of Applied Physics, Emeritus Prof. M. Puska *Aalto University, Finland*

- Developing computational methods for advancing Raman and PL spectroscopies. [Thesis]
- Employing machine learning molecular dynamics to compute lattice thermal conductivity. [Article]

Academic Background: Education

PhD in Computational Engineering Physics *June 2016 - Jan. 2023*
Aalto University, Finalnd
Thesis title: Modeling Raman and Photoluminescence Spectra of Defective Materials

MSc in Solid-State Physics *September 2012 - September 2014*
Isfahan University of Technology, Iran
Thesis title: The Role of Temperature and Magnetic Effects on the Stacking-fault Energy in Iron

BSc in Solid-State Physics *September 2007 - September 2011*
Mazandaran University, Iran

Research Interests

Machine Learning in Materials Science
Applying ML techniques to predict potential energy surfaces of solids and molecules and to accelerate the discovery of new materials.

Electrochemical Energy Storage
Investigating the mechanisms of electron transfer and ion transport in next-generation batteries.

Interfacial Electron Transfer and Electrode-Electrolyte Interactions
Developing approaches to uncover interfacial electron transfer and solidification processes on surfaces.

Light-Matter Interactions for Defect Characterization and Catalytic Development
Exploring solids and surfaces for characterization (Raman/PL), quantum applications (single-photon emitters, qubits), and catalytic electrochemical reactions (e.g., CO_2 reduction).

Quantum Computing Algorithms in Materials Modelling
Applying quantum computing algorithms to accelerate traditional computational modeling for drug discovery and materials science applications.

Technical Skills

- **Material Science:** VASP, CP2K, Gaussian, GPUMD, GROMACS, PHONOPY, ASE, RDkit
- **Machine Learning & Data Analysis:** Pandas, Matplotlib, Numpy, SciKit-Learn, SQL, PyTorch
- **Software Development:** React Native, GitHub Actions (CI/CD), Version Control systems (Git)
- **Programming:** Python, Javascript, Bash
- **HPC Tools:** Experience with SLURM, OpenMP, MPI, and Linux

Research Fundings

Marie Skłodowska-Curie Actions: COFUND Programme (Talent4Iberia-101128265) *2025*
Short-listed (12 out of 70); 10 fellows were awarded

Marie Skłodowska-Curie Actions PF (HORIZON-MSCA-2024-PF-01-01) *2025*
Received the European Commission's Seal of Excellence

HPC-Europa3, Transnational Access programme *Nov. 2020*
Fund and computational resources support to collaborate with Dr. Mahdi Ghorbani-Asl in Germany.

Condensed Matter and Materials Physics *Apr. 2018*
Financial assistance of 2000 euros for collaboration with Prof. Paul Erhart at Chalmers University in Sweden.

Condensed Matter and Materials Physics *Dec. 2016*
Financial assistance of 2000 euros for collaboration with Dr. Arkady Krasheninnikov of HZDR Institute in Germany.

Teaching and Mentoring Experience

PhD Thesis Advising
2023-2024

- "A paper has been submitted to PCCP and archived on arXiv." [Manuscript]

M.Sc. Thesis Mentoring
2019

- "An empirical potential study of first-order Raman scattering in defective MoS_2" [Article]

Teaching Assistant in Solid-State Course *taught by Dr. Hannu-Pekka Komsa*
2018, 2019

Open-Source Contributions

Angle-Dependent Raman Spectroscopy (Python package, [GitHub])

Optical Absorption Analysis (Python package, [GitHub])

Machine Learning for Organic Molecule Solubility (Python package, [GitHub])

Certifications

World-class Software Engineer (Project-based) *Mar. 2024*
YouNovel Oy, Finland

- "3-month program to cover clean code, testing practices, CI/CD strategies, and web development"

Python for Scientific Computing (Assignment-based) *Nov. 2023*
Aalto University School of Science

- "4-day course in NumPy, SciPy, Matplotlib, Pandas, and Python projects packaging"