Hossein Tahmasbi, Ph.D.

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GitHub
GitLab
Google Scholar
LinkedIn

SKILLS

Programming

Python
(Numpy, Scipy, Matplotlib, Pandas)

FORTRAN

Pytorch

Git, GitHub/GitLab

Jupyter Notebooks

AI Agent Workspaces (Terok / LLM development tools)

Technical Skills

High-Performance Computing (HPC) (Slurm, GPU acceleration/computing)

Automated & High-Throughput Workflows (AiiDA, MongoDB)

LaTeX

Linux/Unix/Windows, Bash Scripting

Computational Materials Science

Density Functional Theory (DFT)

Machine Learning Interatomic Potentials (MLIPs)

Molecular Dynamics (MD), *Ab Initio* MD

Software: FHI-aims, VASP, LAMMPS

VESTA, V-Sim, VMD, ...

EDUCATION

2014–2019 **Ph.D. in Condensed-Matter Physics**
Institute for Advanced Studies in *Basic Sciences (IASBS), Zanjan, Iran*

2005–2008 **M.Sc. in Solid-State Physics**
Iran University of Science and *Technology (IUST), Tehran, Iran*

2001–2005 **B.Sc. in Applied Physics**
Arak University, Arak, Iran

PROFESSIONAL EXPERIENCE

Postdoctoral Researcher
Center for Advanced Systems Understanding (CASUS),
Helmholtz-Zentrum Dresden-Rossendorf e.V. (HZDR), Germany 2021-current

- Conducted high-throughput calculations utilizing a MongoDB/AiiDA database to train machine learning interatomic potentials for Aluminium and iron hydride.
- Developed a multi-layer perceptron model using a custom Python implementation based on PyTorch for water molecules.
- Benchmarked and validated leading universal Machine Learning Interatomic Potentials, generating critical data that guided selection of the most stable and accurate models.
- Collaborated with interdisciplinary teams, presenting research findings at international conferences and publishing in leading journals.

Postdoctoral Researcher
Theoretical Chemistry,
Leiden Institute of Chemistry, Leiden University, Netherlands 2019-2021

- Collaborated with experimentalists at Leiden and Radboud University to explore IR spectroscopic characterization of H_2 and CO_2 on cationic Cu clusters.
- Utilized automated methods with ASE packages to investigate the energy landscape and identify stable structures.
- Conducted a systematic study that aligned theoretical findings with experimental IR spectra, demonstrating strong agreement.

Visiting Ph.D. Researcher
Theoretical Chemistry,
Leiden Institute of Chemistry, Leiden University 2017-2018

- Conducted in-depth research on long-wavelength phonons in dissociative chemisorption, specifically focusing on N_2 on Ru.
- Utilized state-of-the-art Neural Network Potentials to perform large-scale, high-fidelity atomic simulations, effectively overcoming the size and timescale limitations of traditional ab initio methods.
- Performed extensive data analysis using Python, supporting and validating research findings.

Ph.D. Candidate
Institute for Advanced Studies in Basic Sciences 2014-2019

- Developed interatomic potentials using Artificial Neural Networks to analyze structural and thermal properties of materials.
- Contributed to the implementation of the FLAME code (Fortran and Python), enhancing features like structure prediction and neural network methods.
- Explored energy landscapes of TiO_2, ZnO and non-stoichiometric MgO, leading to the discovery of novel structures.
- Supported graduate students in developing computational methods, including optimization techniques for atomistic systems using Fortran.