Hossein Tahmasbi, Ph.D.

Curriculum Vitae

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Personal Information

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Work Experience

11/2021–now **Postdoctoral Researcher**, *Center for Advanced Systems Understanding (CASUS), Helmholtz-Zentrum Dresden-Rossendorf e.V. (HZDR)*, Görlitz, Germany.
Mentors Dr. Attila Cangi and Prof. Dr. Thomas D. Kühne
11/2019–11/2021 **Postdoctoral Researcher**, *Theoretical Chemistry, Leiden Institute of Chemistry, Leiden University*, Leiden, The Netherlands.
Mentor Dr. Jörg Meyer

Academic Education

09/2014–07/2019 **Ph.D. in Hard Condensed-Matter Physics**, *Institute for Advanced Studies in Basic Sciences (IASBS)*, Zanjan, Iran.
Thesis title *Interatomic Potentials based on Artificial Neural Network: Structural and Thermal Properties of Matters*
Supervisors Dr. S. Alireza Ghasemi and Dr. Maximilian Amsler
Advisor Dr. Jörg Meyer
8/2017–5/2018 **Visiting Ph.D. Researcher**, *Theoretical Chemistry, Leiden Institute of Chemistry, Leiden University*, Leiden, The Netherlands.
Supervisor Dr. Jörg Meyer
09/2005–01/2008 **M.Sc. in Solid-State Physics**, *Iran University of Science and Technology (IUST)*, Tehran, Iran.
Thesis title *Gain in a free-electron laser with coaxial wiggler and guide magnetic field*
Supervisor Prof. Dr. Mahdi Esmaeilzadeh
09/2001–06/2005 **B.Sc. in Applied Physics**, *Arak University*, Arak, Iran.

Publications

Research

2026 **H. Tahmasbi**, A. Knüpfer, T. D. Kühne, H. Mirhosseini, "*Benchmarking Universal Machine Learning Interatomic Potentials on Elemental Systems*", submitted.
2025 **H. Tahmasbi**, M. Beerbaum, B. Brzoza, A. Cangi, and T. D. Kühne, "*Scalable machine learning model for energy decomposition analysis in aqueous systems*", J. Chem. Phys. 163, 214115 (2025)
2024 **H. Tahmasbi**, K. Ramakrishna, M. Lokamani, and A. Cangi, "*Machine Learning-Driven Structure Prediction for Iron Hydrides*", Phys. Rev. Mater. 8, 033803 (2024).

2023 S. Kumar, **H. Tahmasbi**, K. Ramakrishna, M. Lokamani, S. Nikolov, J. Tranchida, M. A. Wood, and A. Cangi, "*Transferable Interatomic Potentials for Aluminum from Ambient Conditions to Warm Dense Matter*", Phys. Rev. Res. 5, 033162 (2023).

2021 O. V. Lushchikova, M. Szalay, **H. Tahmasbi**, L. Juurlink, J. Meyer, T. Höltzl, and J. M. Bakker, "*IR spectroscopic characterization of the co-adsorption of CO_2 and H_2 onto cationic Cu_n^+ clusters*", Phys. Chem. Chem. Phys. 23, 26661 (2021).

2021 **H. Tahmasbi**, S. Goedecker and S. A. Ghasemi, "*Large-Scale Structure Prediction of Near-Stoichiometric Magnesium Oxide Based on a Machine-Learned Interatomic Potential: Crystalline Phases and Oxygen-Vacancy Ordering*", Phys. Rev. Mater. 5, 083806, (2021).

2021 H. Mirhosseini, **H. Tahmasbi**, S. R. Kuchana, S. A. Ghasemi, and T. D. Kühne, "*An automated approach for developing neural network interatomic potentials with FLAME*", Computational Materials Science, 197, 110567 (2021).

2021 O. V. Lushchikova, **H. Tahmasbi**, S. Reijmer, R. Platte, J. Meyer, and J. M. Bakker, "*IR Spectroscopic Characterization of H_2 Adsorption on Cationic Cu_n^+ (n=4-7) Clusters*", J. Phys. Chem. A, 125, 2836 (2021).

2020 M. Amsler, S. Rostami, **H. Tahmasbi**, E. Rahmatizad, S. Faraji, R. Rasoulkhani, and S. A. Ghasemi, "*FLAME: a library for atomistic modeling environments*", Computer Physics Communications, 256, 107415 (2020).

2017 H. A. Eivari, S. A. Ghasemi, **H. Tahmasbi**, S. Rostami, S. Faraji, R. Rasoulkhani, S. Goedecker and M. Amsler, "*Two-Dimensional Hexagonal Sheet of TiO_2*", Chemistry of Materials, 29, 8594 (2017).

2017 R. Rasoulkhani, **H. Tahmasbi**, S. A. Ghasemi, S. Faraji, S. Rostami and M. Amsler, "*Energy landscape of ZnO clusters and low density polymorphs*", Phys. Rev. B, 96, 064108 (2017).

Book

2016 **Hossein Tahmasbi**, Mohammad Behtaj, Solutions to Problems for "*Statistical Mechanics, R. K. Pathria and Paul D. Beale (3rd Edition)*", Hampa Press.

Software Projects

2014–2021 `FLAME`: a library for atomistic modeling environments, `https://github.com/flame-code/FLAME`

2020–2024 `PyFLAME`: An automated workflow for developing neural network interatomic potentials with FLAME, `https://github.com/flame-code/PyFLAME`

2021–2024 `MALA`: Materials Learning Algorithms, `https://mala-project.github.io/mala/index.html`

Awards

2018 Research Award, *Iran Science Elites Federation*

2017 Sabbatical Research Fellowship, *Ministry of Science, Research and Technology of I.R. Iran*

Skills

- **Operating Systems:** Linux/Unix, Windows
- **Programming & Scripting:** Python, Shell Script (Bash), FORTRAN
- **Computational Modeling & Simulation:** FHI-aims, VASP, LAMMPS, PHONOPY, Sheng/almaBTE
- **Data Visualization:** VESTA, V_Sim, VMD
- **Version Control:** Git, GitHub
- **Technical Documentation:** LaTeX, Microsoft Office

Languages

Persian **Native**

English **Professional working proficiency**

German **Limited working proficiency**

References

1 **Prof. Dr. Thomas D. Kühne**.
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- Homepage

2 **Dr. Attila Cangi**.
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3 **Dr. Hossein Mirhosseini**.
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- Homepage

4 **Dr. Jörg Meyer**.
Leiden Institute of Chemistry, Leiden University, Leiden, The Netherlands
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