

Setayesh Pardis



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Summary

Materials scientist and engineer, currently conducting PhD research at Wetsus in collaboration with the Universities of Twente and Maastricht, with a strong background in computational modeling, simulations, and data-driven analysis of complex systems. Experienced in developing custom Python-based workflows for scientific calculations, data analysis, and visualization. Passionate about computational chemistry and integrating physics-based and machine learning methods to investigate structure–property relationships in materials.

Education

Ph.D. Candidate Universities of Twente & Maastricht, Netherlands *Sep 2026 – Present*

Research Focus: *Data-Driven deterioration Assessment of Aging PVC Drinking Water Mains*

Developing a quantitative failure risk parameter by integrating non-destructive testing (NDT) signals, machine learning models, and physical degradation mechanics. Promoters: Prof Richard Leendersloot, prof Inna Gitman

Master of Science in Materials Science University of Turin, Italy *July 2025*

Thesis: *Machine Learning for Modeling Hydrogen Energy Storage Materials*

Developed machine learning models (SVR, Random Forest, XGBoost, DNN) to predict hydrogen PCT curves and hysteresis behavior, combining data-driven workflows with thermodynamic interpretations.

Bachelor of Science in Materials Science and Engineering Bu-Ali University, Iran *September 2021*

Thesis: *Analysis of Deformation Behavior of Triplex Steels*

Studied phase transformations and Mn effects on mechanical properties using XRD and FESEM analysis.

Academic Experience

PhD Researcher Wetsus *Sep 2026 – Present*

- Developing a data-driven framework combining ultrasonic NDT signals and machine learning to model structural degradation and assess failure risk in aging PVC water mains.
- Integrating physics-based failure mechanics with environmental markers to establish quantitative decision-support models for asset management.

Research Fellow Politecnico di Torino – DISAT *Aug 2025 – Jul 2026*

- Conducted large-scale molecular dynamics simulations (LAMMPS, GROMACS) to study atomic-scale phase evolution in monocrystalline and polycrystalline copper under Prof. Giovanni M. Pavan.
- Developed automated Python workflows for trajectory-based data labeling, structural clustering, and local entropy mapping (Dyngsight-based Shannon/KL entropy).
- Derived multi-descriptor correlations for order–disorder transitions, resulting in two manuscripts (one under review, one in prep).

Research Assistant (MSc Project) University of Turin – Materials Science Department *2024 – 2025*

- Conducted machine-learning-driven modeling of hydrogen energy storage materials.
- Applied data preprocessing, feature engineering, and performance benchmarking ($R^2=0.9$).
- Investigated the relationship between composition, microstructure, and thermodynamic properties.
- Supervised by Prof. Mauro Palumbo.

Research Assistant (BSc Project) Bu-Ali Sina University – Engineering Department, Hamedan, Iran *2020 – 2021*

- Conducted experimental research on the hot deformation behavior of triplex steels under the supervision of Dr. Yousef Mazaheri.
- Performed metallurgical characterization using XRD, FESEM, and optical microscopy to study phase evolution and mechanical response.
- Assisted in data collection, mechanical testing, and analysis of strain-induced phase transformations.
- Contributed to project reporting and literature review as part of the undergraduate research group in Materials Engineering.

Teaching Assistant – Fundamentals of Ceramics Engineering and Composites Bu-Ali 2021 – 2022
Sina University, Hamedan, Iran

- Assisted laboratory and tutorial sessions focused on ceramic processing, sintering, and composite microstructure analysis.
- Helped students understand phase formation, toughening mechanisms, and the relationship between composition and mechanical properties.
- Supported practical demonstrations on ceramic powder preparation and microstructural characterization.
- Supervised by Prof. Shahab Kazemi.

Programming and Method Development Experience

Languages: Python, Bash

Libraries: NumPy, Pandas, SciPy, Scikit-learn, TensorFlow, PyTorch, MDAnalysis, Dynsight, Matplotlib, Seaborn

Systems: Linux/Unix, Git, SLURM job scripting

Method Development Highlights:

- Implemented Python modules for computing **Shannon and KL entropy** from simulation data.
- Designed unsupervised learning pipelines (**DBSCAN, PCA, K-means**) for atomic environment classification.
- Developed automated **trajectory refinement and visualization tools** for entropy and population analysis.
- Integrated **machine learning models** into MD workflows for property prediction.
- Analyzed how structural and thermodynamic descriptors respond to deformation and temperature changes.

Software & Tools: LAMMPS, GROMACS, OVITO API (introductory)

Technical Skills

- **Computational Methods:** Molecular Dynamics, Machine Learning, Entropy Analysis
- **Materials Characterization:** XRD, SEM, FTIR, UV-Vis, Raman, Mechanical Analysis
- **Software Tools:** ANSYS, LAMMPS, GROMACS, OVITO, FreeFEM, SolidWorks, CATIA
- **Soft Skills:** Analytical Thinking, Collaboration, Research Communication, Independent Problem Solving
- **Languages:** English (Fluent), Italian (Intermediate), Persian (Native)

Projects

Michelin x University of Turin – Sustainable Solutions for Energy and Water Reduction – 2025
Designed an industrial water purification system aligned with Michelin's 2030 sustainability goals.

Design and Optimization for Sustainability – University of Turin– 2024

Developed finite element heat conduction models and performed LCA-based energy efficiency evaluations.

Certificates

- Machine Learning Specialization – DeepLearning.AI (Coursera, 2024)
- Python for Everybody – University of Michigan (Coursera, 2023)
- Introduction to Computational Chemistry – University of Turin (2024)