Nikolaos Patsalidis

Computational Materials Science ▪ Molecular Simulation ▪ Machine Learning

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- Molecular Dynamics ▪ Density Functional Theory ▪ Machine-Learning Potentials
- Active Learning ▪ Scientific Computing ▪ Data Analysis ▪ High-Performance Computing

Work Experience

Postdoctoral Researcher — **Dec 2024 – Present**

Foundation for Research and Technology–Hellas (FORTH), Greece — *Jul 2026 – Present*

The Cyprus Institute, Cyprus — *Dec 2024 – Jun 2026*

- Machine Learning Potentials
- Physics-informed deep learning
- Active Learning
- Data Generation
- Multi-scale workflows
- Molecular Dynamics
- Density Functional Theory
- Liquid/solid, polymer/solid, and gas/solid interfaces

Research Scholar Visitor — **Oct 2023 – Apr 2024**

University of Tennessee, Department of Chemical and Biomolecular Engineering — *Knoxville, USA*

- Elastomer melts
- High-dimensional trajectory processing
- Dynamics and Structure through large scale data analytics

Graduate Research Assistant — **Oct 2020 – Jan 2024**

The Cyprus Institute, Computation-based Science and Technology Research Center — *Nicosia, Cyprus*

- Polymer/solid interface structure and dynamics
- Physics-informed machine learning
- Multi-scale modelling
- High performance computing
- Active learning of gas/solid interfacial potentials

Industry & Research Collaborations

- **Toyota Motor Corporation** — *Sep 2025 – Present*
  Fuel-cell materials ▪ liquid/solid interfaces ▪ physics-informed ML force fields
- **The Goodyear Tire & Rubber Company** — *Oct 2023 – Apr 2024*
  Elastomer compounds ▪ molecular structure and dynamics ▪ tire-compound optimisation
- **AmaDema Ltd, Cyprus** — *Dec 2024 – Jun 2026*
  Nanofibrous membranes ▪ CO_2 permeability ▪ carbon-capture materials
- **NovaMechanics Ltd** — *Oct 2022 – Apr 2025*
  Gas-pollutant sensing ▪ gas/solid interfaces ▪ nanosensor materials

Education

Doctor of Philosophy (PhD) in Computational Sciences — **Oct 2020 – Nov 2024**

The Cyprus Institute — *Nicosia, Cyprus*

- Thesis: Multi-Scale Computational Modelling of Nanostructured Materials

Integrated Master's Degree in Mechanical Engineering — **Sep 2014 – Mar 2020**

National Technical University of Athens — *Athens, Greece*

- Thesis: Development of an Algorithm and Software for Computing Pareto Fronts with a Gradient-Based Method
- Multi-objective optimisation ▪ numerical methods ▪ aerodynamics

Programming & Scientific Software

- **Programming:** Python **(6 years)** ▪ C++ **(1 year)** ▪ Bash **(1 year)** ▪ CUDA **(0.5 years)**
- **Machine Learning:** PyTorch ▪ Graph Neural Networks ▪ Deep Learning
- **Molecular Simulation:** LAMMPS ▪ GROMACS
- **Electronic Structure:** Quantum ESPRESSO ▪ Gaussian

Certificates & Selected Courses

DeepLearning.AI – Deep Learning Specialization — *Oct 2024*

- Neural Networks and Deep Learning
- Improving Deep Neural Networks: Hyperparameter Tuning, Regularization and Optimization
- Structuring Machine Learning Projects
- Convolutional Neural Networks

- Sequence Models

The Cyprus Institute

- Data Visualization
- High Performance Computing
- Modelling and Simulation for Scientific Applications

Selected Software Development

- **FF Develop** *2022 – Present*
  github.com/NikolasPatsalidis/FF_Develop
  Automated DFT data generation ▪ force-field parametrization ▪ active-learning cycles ▪ iterative ML potential training
- **md_pipeline** *2023 – Present*
  github.com/NikolasPatsalidis/md_pipeline
  LAMMPS/GROMACS trajectory processing ▪ feature extraction ▪ structure generation ▪ memory-efficient analysis
- **ReactML** *2024 – Present*
  Private repository
  Reactive machine-learning force fields ▪ graph-based interaction models ▪ learnable interaction channels ▪ PyTorch

Scientific Outreach & Communication

- 5 first-author peer-reviewed publications
- 2 co-authored peer-reviewed publications
- 1 authored book chapter
- 10+ international conference presentations
- Trainer: Density Functional Theory ▪ atomistic modelling

Selected Awards

- Seal of Excellence – Marie Skłodowska-Curie Actions Postdoctoral Fellowship, 2025
- Best Poster Presentation – European Materials Modelling Council International Workshop, 2025
- Best Young Researcher Oral Presentation – 37th Panhellenic Conference on Solid State Physics and Materials Science, 2023
- Journal Cover – *Journal of Chemical Information and Modeling*
- Journal Cover – *Journal of Physical Chemistry C*

Soft Skills

- Scientific Communication
- Complex Concept Understanding
- Team work
- Presentation Skills
- Technical Reporting
- Cross-Functional Collaboration
- Problem Solving
- Industry Collaboration
- Interdisciplinary Research