

Riccardo Dal Molin

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Date of Birth: 21/08/1999

Citizenship: Italy

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Research Interests

Theory and computational methods in solid-state physics, *Ab initio* and classical molecular dynamics, *Machine learning*.

Education

International School for Advanced Studies (SISSA)

Trieste, Italy

PhD in Theory and Numerical Simulation of Condensed Matter
in collaboration with ENI s.p.a

10/2024 – Present

Thesis: *Machine Learning Wannier Functions Properties for Functional Materials: from Piezoelectricity to Superconductors*

Advisor: Professor A. Marrazzo

Industrial co-advisor : Dr. B. Tirri

University of Trieste

Trieste, Italy

Master's Degree in Physics, *110/110 cum laude*

08/2022 – 10/2024

Thesis: *Drag properties of graphene coatings: Atomistic simulations*

Advisors: Professors M. Peressi, E. Smargiassi, Dr. D. Bidoggia

University of Trieste

Trieste, Italy

Bachelor's Degree in Physics

08/2018 – 05/2022

Thesis: *Development of an interatomic potential based on deep neural networks for single layers of tungsten ditelluride*

Advisor: Professor A. Marrazzo

Research Experience

Master's Thesis Work

Supervisor: Prof. M. Peressi

05/2024 – 10/2024

Developed an atomistic simulation protocol (molecular dynamics) to calculate the aerodynamic drag coefficient between a single graphene layer and water at low velocities. The work relies on non-equilibrium molecular dynamics using semi-empirical potentials to construct steady water flows and determine the hydrodynamic properties of the graphene-water interface at the nanoscale.

Report Collaboration: *Protocols and preliminary tests for drag coefficient calculations through MD simulations*, part of the ASGARD project (*Atomistic simulations of damage, adhesion and drag reduction of graphene-based coatings*) in collaboration with Leonardo S.p.A, Ferrovie dello Stato, and ICSC.

Software Used: LAMMPS, OVITO

Bachelor's Thesis Work

Supervisor: Prof. A. Marrazzo

08/2021 – 05/2022

Developed an interatomic potential for single layers of tungsten ditelluride (WTe_2) using deep neural networks. By training a neural network on *ab initio* molecular dynamics trajectories, an interatomic potential capable of predicting *ab initio* dynamics of tungsten ditelluride was created. Special attention was paid to constructing a protocol for verifying the network's generalization and extrapolation capabilities.

Software Used: DeepMD, Nequip, LAMMPS, Quantum ESPRESSO

Internship at Elettra Sincrotrone - Trieste

Supervisor: Professor D. Fausti

06/2021 – 09/2021

Bachelor's internship (9 ECTS), where I worked with a research group in an optical spectroscopy laboratory. I analyzed data related to fluctuation correlation spectroscopy and calibrated lasers for *pump-and-probe* measurements.

Conferences

Young Researchers' Workshop on Machine Learning for Materials

05/2022

Poster titled: *Development of a DeepMD potential for monolayer WTe_2*

International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods

01/2025

Poster titled: *Slip properties of graphene-water interfaces: atomistic simulations*

MARVEL-ICTP College: Materials simulations in the age of AI

06/2026

Poster titled: *Equivariant Machine Learning of Berry-Phase Polarization*

T.I for tutorial: *Berry-phase electric polarization with Quantum ESPRESSO*

Summer School on Molecular Dynamics for Materials Science, Nanotechnology, and Biophysics

06/2026

T.I for tutorial: *AiiDA tutorials: automated active learning of a neural-network interatomic potential with AiiDA-TrainsPot*

Skills

Programming

Advanced: Python, Fortran

Familiar: C, Mathematica, f2py

Experience in High-Performance Computing: HPC Cineca - Leonardo/Marconi100

Experience with Quantum ESPRESSO ab-initio code, and with AiiDA ecosystem

Languages

Italian (Native), English (B2)