Marco Cherubini

Computational physicist with expertise in materials modeling, numerical simulations, development of machine learning potentials and high-performance computing. Skilled in theoretical and computational approaches for investigating the properties of materials. Experienced in managing scientific projects, preparing technical reports, and collaborating with international research teams.

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SKILLS

Programming languages

- **Expert:** Python, Fortran, Bash
- **Proficient:** C++, C, MATLAB, Mathematica

Machine learning for simulations

- Development of ML interatomic potentials
- Integration of MLP in advanced atomistic simulation codes (PIMD,SSCHA)

Data analysis

- Large-scale post-processing automation

High performance computing

- HPC clusters, parallel programming
- HPC grant acquisition

Collaboration & Research Management

- Collaboration with international research teams
- Coordinated HPC simulation tasks across multiple research groups

LANGUAGES

Italian – Native
English – Fluent (C1)
French – Intermediate (B1–B2)

WORK EXPERIENCE

Postdoctoral researcher

Sorbonne University, Paris| Oct 2022 - June 2025

- Developed machine learning-based interatomic potentials to simulate anharmonic and quantum effects in materials, including extensive use of Path Integral Molecular Dynamics techniques
- Designed and automated HPC workflows for large-scale simulations, integrating data pipelines and post-processing tools.
- Collaborated with international academic partners on advanced modeling and simulation projects.
- Co-authored scientific publications and presented results at international conferences
- Developed post-processing tools in Python/Fortran for large-scale simulations.
- Awarded EuroHPC grants to run large-scale simulations

Junior researcher

University of Rome, La Sapienza | Mar 2022 -Sep 2022

- Investigated thermal and vibrational properties of materials using ab initio methods.
- Co-developer of a Python/Fortran based code to investigate vibrational and thermodynamic properties of materials using advanced quantum mechanical methods https://sscha.eu/

EDUCATIONAL BACKGROUND

Ph.D in Physics
University of Rome, La Sapienza| 2022

M.Sc in Physics
University of Rome, La Sapienza| 2018
Final grade: 110/110 cum laude