

# Luca Leoni

# Curriculum Vitae – April 5, 2025

	Personal details
Birth	1999. August the 16th. Faenza (Italy)
Languages	Italian (mothertongue). English (fluent)
Website	www.unibo.it/sitoweb/luca.leoni12
ORCiD	0009-0007-5648-0719
Scholar	Google Scholar
Github	Luca-Leoni
	Accademic experience
	Education
2023–present	<b>Doctorate in physics</b> , University of Bologna (Italy).
2021–2023	<b>Master degree in condensed matter physics</b> , <i>University of Bologna (Italy)</i> . 110/110 cum laude
2018–2021	<b>Bachelor degree in physics</b> , <i>University of Bologna (Italy)</i> . 110/110 cum laude
	Academic internships
2022–2023	<b>Research internship</b> , <i>University of Vienna (Austria)</i> . Master thesis development
July 2022	Summer school, University of Vienna (Austria).
	Machine learning for materials hard and soft
	Teaching activities
2024–present	Supervisor of bachelor students (University of Bologna, Italy)
2023–present	Teaching assistant of statistical mechanics (University of Bologna, Italy)
2022–present	Teaching assistant of Computational Material physics (University of Bologna, Italy)
	Doctorate project
Title	Data-Driven study of quasiparticle in materials
Supervisor	Cesare Franchini
Description	Research of novel Machine Learning models able to enhance first-principle estimates of quasiparticle properties in condensed matter systems.

#### Master Thesis

Title Enhancing diagrammatic Monte Carlo via machine learning

Supervisor Cesare Franchini

Description Study on the possible strategies to enhance the statistical properties of the diagrammatic Monte Carlo algorithm. Two approaches have been found successful to achieve such task: an analytical one that grants the minimum correlation possible in the Markov Chain, and a more general neural network protocol based on the Normalizing Flow architecture.



Programming projects

- 2023 **NF-DiagMC**, *Normalizing Flow guided Diagrammatic Monte Carlo*, (C++). Library for the training and integration of Normalizing Flows model for Feynman diagram sampling inside Diagrammatic Monte Carlo algorithm. Completely written in C++ using Pytorch C++ API and with a stand-alone module to perform Diagrammatic Monte Carlo simulation that can be used also without Normalizing Flows.
- 2024 **LEOPOLD**, *LEarning Of POLaron Dynamics*, (Python/JAX), in release. Python library for training and using the LEOPOLD Machine Learning interatomic potential. Written completely using JAX and JAX-MD to perform highly optimized molecular dynamics natively on GPU without the need of a LAMMPS plugin.

#### Analytical skills

#### Condensed matter physics

- High Feynman diagrams, polaron physics, Spin-Boson model, perturbation theory
- Good Non-adiabatic approaches, surface science, electron-phonon coupling

#### Computational physics

- High Density Functional Theory, Diagrammatic Monte Carlo, Molecular Dynamics, Nudge Elastic Band
- Good Kinetic Monte Carlo, Ehrenfest dynamic

#### Machine Learning

- High Interatomic potentials, Equivariant networks, Normalizing Flows
- Good Singular Value Decomposition, auto-encoders



\* = corresponding author  $\dagger =$  coauthorship

- Angeletti, A.<sup>†</sup>, <u>Luca Leoni</u><sup>†</sup>, Massa, D., Pasquini, L., Papanikolaou, S. & Franchini, C. Hydrogen diffusion in magnesium using machine learning potentials: a comparative study. *npj Computational Materials* **11.** ISSN: 2057-3960. http://dx.doi.org/10.1038/s41524-025-01555-z (Mar. 2025).
- Luca Leoni<sup>\*</sup> & Franchini, C. Global sampling of Feynman's diagrams through normalizing flow. *Phys. Rev. Res.* 6, 033041. https://link.aps.org/doi/10.1103/PhysRevResearch.6.033041 (3 July 2024).
- 3. Viktor C. Birschitzky<sup>†</sup>, <u>Luca Leoni</u><sup>†</sup>, Reticcioli, M. & Franchini, C. *Machine Learning Small Polaron Dynamics*, in review Sept. 2024. arXiv: 2409.16179 [cond-mat.mtrl-sci]. https://arxiv.org/abs/2409.16179.

## Conferences and Workshops

- March 2025 March Meeting, Anaheim (California), poster. Global sampling of Feynman digrams through Normalizing Flows
- March 2025 **March Meeting**, *Anaheim (California)*, contributed talk. Machine Learning small polaron dynamics
  - Feb 2025 **TACO PhD Meeting**, *Schladming (Austria)*, contributed talk. Small Polaron dynamics with Machine-Learned Force Fields
  - Sep 2024 **NIS Colloquia: EX-MACHINA**, *University of Torino (Italy)*, contributed talk. Hydrogen Diffusion in Magnesium Using Machine Learning Potentials
  - July 2024 **CECAM workshop: Frontiers in many-body excited-state dynamics from first principles**, *CECAM-HQ-EPFL, Lausanne (Switzerland)*, contributed talk. Machine learning small polaron dynamics
  - July 2024 **CECAM workshop: Machine Learning of First Principles Observables**, *Zuse Institute Berlin* (*Germany*), contributed talk. Machine learning small polaron dynamics
  - May 2024 **CECAM workshop: MLM4MS**, *Joef Stefan Institute (Slovenia)*, poster. Global sampling of Feynamn digrams through Normalizing Flows
  - May 2022 **MANO Spring workshop**, *University of Bologna (italy)*, presentation. Multiscale simulation of phenomena governed by rare events: kinetic Monte Carlo combined with firstprinciples calculation
  - Dec 2021 **MANO Winter workshop**, *University of Bologna (italy)*, poster. Application of Machine Learning to force flied based molecular dynamics

# Collaborations

- Bologna **Hydrogen Transport**, *Luca Pasquini*, University of Bologna, (Italy). Collaborated with experimentalist to study Hydrogen diffusion inside Magnesium by benchmarking firstprinciple calculation with experimental results.
  - WienSFB-TACO, Technische Universität Wien, (Austria).External collaborator of the TACO: TAming COmplexity in Materials Modeling project
  - Roma **NF-SCHA**, *Lorenzo Monacelli*, Università la Sapienza, (Italy). Currently collaborating to apply Normalizing Flows inside the non-linear self consistent harmonic approximation

### **Recognitions and Awards**

2024 Prize for the 12 best Master thesis in Physics (University of Bologna, Italy)