Francesco Cosimo Castellucci

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As a Ph.D. student in Physics at Unimore, with a collaboration affiliation with CNR-NANO, specializing in **Condensed Matter Physics**, in my academic course of studies I have acquired deep knowledge in **Solid-State Physics**, **Quantum Many-Body Theory**, and **Phase Transitions**. My research interest lies in theoretical and computational condensed matter, complemented by experience in experimental physics. I have developed skills in **Python** and **Fortran** programming, as well as proficiency with various specialized **first-principle electronic structure software**. In particular, I'm currently interested in the study of **electronic and optical properties** of **nanostructured materials** via density-functional and many body perturbation methods, with the aim of developing and exploiting advanced tools such as **Machine Learning and Deep Learning**.

Education

2024 – 20XX ◇ **Ph.D. Physics and Nanoscience, University of Modena and Reggio Emilia**
- Thesis Title: *Machine Learning methods applied to GW calculations*
- Supervisors: *Prof. Elisa Molinari, Dr. Andrea Ferretti, Dr. Daniele Varsano*

2022 – 2024 ◇ **M.Sc. Physics, University of Modena and Reggio Emilia**
- Final Grade: *110/110 with honors and academic distinction*
- Curriculum: *Theoretical and Computational Physics*
- Thesis Title: *A Machine Learning approach for the screened potential in GW approximation*
- Thesis Supervisors: *Prof. Elisa Molinari, Dr. Andrea Ferretti, Dr. Daniele Varsano, Dr. Giorgia Franchini*
- Content: *Implementation of a Machine Learning model, based on Deep Learning, for accelerating the computations of the linear response functions in GoWo approximation for 2D materials. The new methodology is implemented in the community code Yambo*

2019 – 2022 ◇ **B.Sc. Physics, University of Modena and Reggio Emilia**
- Final grade: *110/110 with honors*
- Thesis Title: *Study of magnetic properties in 2D systems using Monte Carlo methods*
- Thesis Supervisor: *Prof. Marco Gibertini*
- Content: *I performed accurate Monte Carlo simulations, to study magnetic properties and phase transitions in 2D Ising model systems having different lattice symmetries, points and number of layers*

Projects

2026 ◇ **Tutorial: Calculating the Transport Properties (Thermal & Ionic) of v-Li_xSi_{1-x} Glasses via Machine Learning Interatomic Potentials (MLIPs) and Equilibrium Molecular Dynamics (EMD)**: Development of a tutorial and computational workflow (published on GitLab) to simulate and compute the ionic and thermal transport properties of lithium-silicon glasses, combining Machine Learning Interatomic Potentials and Equilibrium Molecular Dynamics.

2025 ◇ **ISCRA B - CoPI**: «Machine Learning methods applied to GW calculations for 2D materials» (acronym: AMALGAMA), PI: Andrea Ferretti, 200k GPU-h, Leonardo-Booster@CINECA

◇ **ISCRA C - PI**: «Enhancing the Computational Efficiency of 2D Materials Simulations via Machine Learning» (acronym: ECE2DvML), PI: Francesco Cosimo Castellucci, 10k GPU-h, Leonardo-Booster@CINECA

Projects (continued)

2023 ◇ **Meta-GGA implementation in the atomic AGWX code**: Implementation of TPSS meta-GGA functional inside the atomic AGWX code; the quality of the results was assessed by comparing the ionization potential for He atom with the one obtained with standard PBE (GGA) functionals with Quantum ESPRESSO. Supervisors: Prof. Alice Ruini, Dr. Andrea Ferretti

◇ **Study of LiH using the Variational Quantum Eigensolver and G_0W_0@PBE**: Study of vertical ionization potential for LiH using the WEST code (with G_0W_0@PBE), using a simulated quantum computer to improve the interatomic distance in the HF approximation. Supervisor: Prof. Marco Govoni

Skills

Languages ◇ - **Italian** (Native)
- **English** (CEFR C1 level in 06/2024 from CLA Unimore; CEFR B2 level in 03/2019 from Cambridge PET)

Programming ◇ - Software development and scripting in **Python**, **Fortran**, **Bash**, and **MATLAB**
- Active developer for the MBPT atomic code **AGWX** (Fortran)

Other ◇ - Design and implementation of **Machine Learning** and **Deep Learning** models applied to computational physics in Python
- Advanced use of first-principles electronic structure software: **Quantum ESPRESSO**, **Yambo**, **WEST**, **Qbox**, and **ASE**
- Parallel computing and code optimization in **HPC** environments (MPI, OpenMP, and debugging/profiling tools)
- Data analysis and scientific writing: **LaTeX**, **Igor Pro**, and **Microsoft Office**

Conferences/Workshops/Schools/External courses

8 - 11 June 2026 ◇ **Recent Advances in Computer-Aided Spectroscopy 2026**, CNR-NANO & Unimore, Modena, Italy

16 - 19 March 2026 ◇ **Debugging and Optimization of Scientific Applications**, CINECA Academy, Casalecchio di Reno, Bologna, Italy

09 - 13 June 2025 ◇ **School on Machine Learning for Molecules and Materials Research**, Zadar, Croatia (poster contribution)

05 - 06 June 2025 ◇ **CNR-NANO Institute 4th workshop**, Modena, Italy (poster contribution)

19 - 23 May 2025 ◇ **Yambo School on Many-Body Perturbation Theory and Excited-State Simulations**, CNR-NANO, Modena, Italy (tutoring activities)

5 - 7 March 2025 ◇ **Introduction to Parallel Computing with MPI and OpenMP**, CINECA Academy, Casalecchio di Reno, Bologna, Italy

8 - 10 January 2025 ◇ **22nd International Workshop on Computational Physics and Materials Science: Total Energy and Force Methods**, ICTP, Trieste, Italy

26 - 28 November 2024 ◇ **YAMBO developers' meeting 2024**, Modena, Italy (oral contribution)

Teaching Activities

2024 - 20xx ◇ **University of Modena and Reggio Emilia**, tutoring activities in General Physics for Bachelor's Degree in Physics students, from Mechanics to Thermodynamics, theory and exercises (40 hours)

Teaching Activities (continued)

2023 - 2024 ◇ **University of Modena and Reggio Emilia**, tutoring activities in General Physics for Bachelor's Degree in Automotive Engineering students, from Mechanics to Electromagnetism, theory and exercises (60 hours)

PhD Internal Courses

2026 ◇ **Ab initio spectroscopy**, Prof. Cocchi

◇ **An introduction to Python: from fundamentals to data and HPC**, Dr. Spallanzani and Prof. Govoni

2025 ◇ **Theory and numerical simulation of mass, charge and heat transport**, Prof. Baroni and Dr. Grasselli

◇ **Introduction to random variables and complex systems**, Dr. Petri

◇ **Introduction to the renormalization group and critical phenomena**, Prof. Trancanelli

◇ **Management of scientific projects**, Unimore

2024 ◇ **Elements of quantum technologies**, Prof. Affronte

◇ **Publish or perish**, Unimore

Public Engagement

25 February 2025 ◇ **Unimore Orienta 2025**: Participation to the Open Day for the FIM department in Unimore as a testimonial of B.Sc., M.Sc. and Ph.D. programs in Physics; activities consisted of a presentation, Q&A and poster sessions

2024 - 2025 ◇ **La ricerca in Fisica**: Participation to the poster session organized by Physics dept. about research topics for B.Sc. and M.Sc. students

References

Ph.D. Project Supervisors

◇ **Prof. Elisa Molinari** - elisa.molinari@unimore.it
Department of Physics, University of Modena and Reggio Emilia

◇ **Dr. Andrea Ferretti** - andrea.ferretti@nano.cnr.it
Center S3, CNR Institute of Nanoscience, Modena

◇ **Dr. Daniele Varsano** - daniele.varsano@nano.cnr.it
Center S3, CNR Institute of Nanoscience, Modena

Seminars

◇ "A tale of quantum science and simulations: Quantum Espresso past and future", Stefano Baroni

◇ "Molecular defects in N-based systems: Common threads and future directions", Jonathan Pelliciari

◇ "Ion transport in battery materials: Computational methodology and applications", Yoshitaka Tateyama

◇ "Many-body interactions in photo-excited lead-free perovskites", Costanza Borghesi

◇ "Challenges and Opportunities for Electronic Structure Calculations at Exascale", William Dawson

◇ "From first-principles to ML-accelerated molecular dynamics: Quantitative predictive modelling of disordered materials for memory and energy applications", Guido Ori

Seminars (continued)

- "Superconducting Electronics with Indium Arsenide On Insulator (InAsOI)", Giovanni Paghi
- "Quantum information processing with hole-spin qubits in silicon", Gaia Forghieri
- "Functional theory of the occupied spectral density", Andrea Ferretti
- "A personal journey through the middle earth between quantum and classical physics: gas phase synthesis and studies of nanoparticles", Sergio D'Addato
- "Nanostructured and Functionalized Surfaces for Single-Molecule Detection", Gaetano Scamarcio
- "How to Design an Award-Winning Scientific Poster" webinar, ECOSISTER PILLAR TRAINING
- "Grany Graphics Masterclass: Visuals That Win Fundings" webinar, ECOSISTER PILLAR TRAINING
- "Modeling Molecular Crystals with Machine Learning Interatomic Potentials", Ivor Lončarić
- "Permanent condensation of excitons in two dimensions", Massimo Rontani