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

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

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

Projects (continued)

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

Skills

Languages	- Italian (mother's tongue) - English (CEFR B2 level in 03/2019 from Cambridge PET, CEFR C1 level in 06/2024 from CLA Unimore)
Programming	- Intermediate programmer in Python, Fortran, Bash and MATLAB - Experience in development in MBPT atomic code AGWX (Fortran)
Other	- Intermediate User in Machine Learning and Deep Learning main topics and models, from theory to laboratories in Python - Intermediate User in first principle electronic structure codes: Quantum ESPRESSO, Yambo, WEST, Qbox - Intermediate User in HPC topics and tools (MPI, OpenMP and debugging/optimization tools) - LaTeX, Microsoft Office, Igor and other post-processing software

Conferences/Workshops/Schools/Courses

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)
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)

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

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
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