



LORENZO GOTTARDI

Date of birth: 12/10/2000

Nationality: Italian

Gender: Male

CONTACT

 Italy (Home)

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EDUCATION AND TRAINING

01/09/2024 – CURRENT Modena, Italy

Phd student in Physics and Nanosciences Università degli Studi di MODENA e REGGIO EMILIA

Main activities and responsibilities:

- Research in computational materials science and solid-state physics under the supervision of Prof. Marco Govoni.
- Benchmarking of Time-Dependent Density Functional Theory (TDDFT) and Δ SCF methodologies for excited-state calculations.
- Investigation of zero-phonon lines (ZPL) of point defect complexes in diamond for quantum technology applications.
- Utilization of large-scale electronic structure codes (Quantum ESPRESSO, WEST, GPAW) on High-Performance Computing (HPC) architectures.
- Development of computational scripts and workflows (Python, Fortran, Bash, CMake).
- Physics tutor for undergraduate students (Biology course).

Level in EQF EQF level 8

05/10/2022 – 18/10/2024 Modena, Italy

Corso di Laurea Magistrale in Scienze Chimiche Università degli Studi di MODENA e REGGIO EMILIA

Master's Degree

- **Title of qualification awarded:** Master's Degree in Chemistry (2nd cycle degree)
- **Final degree mark:** 110/110 cum laude
- **Thesis Title:** Determination of the structure-crystallization relationship in aluminoboron silicate glasses
- **Thesis Supervisor:** Prof. A. Pedone
- **Thesis Opponent:** Prof. G. Malavasi
- **Main subject / occupational skills covered:**
 - Application of classical molecular dynamics to amorphous materials.
 - Investigation of crystallization processes and the formation of crystal embryos through molecular dynamics simulations.

Level in EQF EQF level 7

10/09/2019 – 20/09/2022 Modena, Italy

Chimica Università degli Studi di MODENA e REGGIO EMILIA

Bachelor's Degree:

- **Thesis Title:** Computational Study of the Decomposition of Polyethylene Oxide (PEO) in Lithium Batteries.
- **Thesis Supervisor:** Prof. F. Faglioni
- **Final degree mark:** 110/110 cum laude
- **Main subject / occupational skills covered:**
 - Application of computational chemistry methods to model energy storage materials.
 - Investigation of polymer electrolyte degradation mechanisms in lithium-ion batteries.
 - User of the Gaussian quantum chemistry software package for electronic structure calculations.

Level in EQF EQF level 6

01/05/2018 – 31/05/2018

Extracurricular Course on Ceramic Materials IIS A.VOLTA

Study of the properties, application, and practical use of ceramic materials.

PUBLICATIONS

2026

Integrating artificial intelligence with experimental and computational materials science to predict crystallization in multicomponent glasses

Authors Marco Bertani, Matilde Benassi, Lorenzo Gottardi, Gianluca Malavasi, Ashutosh Goel, Alfonso Pedone |

Journal Name Acta Materialia | **Volume, Issue and Pages** Volume 311, Article 122216 | **Publisher** ELSEVIER

WORK EXPERIENCE

University of Modena and Reggio Emilia / CECAM IT-SIMUL node Modena, Italy

Organizing Committee Member (YRM 2027)

17/05/2026 – Current

Main activities and responsibilities:

- Organization and logistical planning of the international scientific conference YRM 2027.
- Drafting of the CECAM funding proposal and coordination of node outreach alongside fellow committee members.

SKILLS

perform scientific research | Parallel computing in HPC environment

CONFERENCES AND SEMINARS

12/12/2024 – 13/12/2024 Bologna

High Performance Computing and Quantum Computing – 7th Edition

Link <https://www.hpc.cineca.it/newsletter/seventh-edition-hpcqc-workshop/>

07/04/2025 – 17/04/2025 Benasque- Spain

Time dependent density functional theory prospects and applications

Participated as a student in the school and in the workshop

Link <https://benasque.org/2025tdfft/>

18/05/2025 – 24/05/2025 Turin

Quantum 2025

Participated with a poster entitled "Excited state properties of defects in diamond "

Link <https://www.quantum2025.unito.it/>

15/12/2025 – 16/12/2025 Bologna

High Performance Computing and Quantum Computing – 8th Edition

Link <https://www.quantumcomputinglab.cineca.it/en/hpcqc-2025/>

11/05/2026 – 15/05/2026 Zaragoza - Spain

Young Researchers' Meeting - 22nd edition

Participated with a Talk entitled " When Does Δ SCF Fail? A TDDFT Benchmark of Excited-state Forces and Zero-Phonon Lines for Defects in Diamond"

Link <https://sites.google.com/view/ym-2026>

08/06/2026 – 11/06/2026 Modena

Recent Advances in Computer-aided Spectroscopy 2026 workshop

Participated as a student

Link <https://racs2026.nano.cnr.it/>

26/08/2026 – 28/08/2026 Brixen - Italy

CMT@BRIXEN

Participated with a poster entitled "TDDFT FORCES REVEAL THE LIMITS OF Δ SCF FOR DIAMOND DEFECTS"

Link <https://cmtconference.it/>

LANGUAGE SKILLS

MOTHER TONGUE(S): Italian

Other language(s):

English

Listening B2

Reading B2

Writing B2

Spoken production B2

Spoken interaction B2

Levels: A1 and A2: Basic user; B1 and B2: Independent user; C1 and C2: Proficient user

HPC SKILLS

Programming & Software Development

Languages: Python, Fortran.

Build & Version Control: Implementation of CMake build systems for WEST-code

Electronic Structure & Molecular Dynamics Codes

1. **DFT & Excited-State Methods:** Quantum ESPRESSO (expert user), WEST (expert user), GPAW.
2. **Molecular Dynamics & Classical Simulations:** DL_POLY, GULP.
3. **Quantum Chemistry & Solid State:** Gaussian (proficient user), Materials Studio (CASTEP for NMR calculations)..

High-Performance Computing (HPC) & Environments

Specialty: Large-scale simulations in condensed matter theory and code optimization.

Environments & Schedulers: Advanced proficiency in Linux environments, Bash scripting, and the Slurm workload manager.

Parallel Computing: Experience with MPI, OpenMP, and GPU-accelerated architectures.

HPC PROJECTS & COMPUTATIONAL GRANTS

07/01/2026 – CURRENT

Machine learning accelerated Study of Defects for Quantum Technologies [ML-DEFQT]

- **Role:** Principal Investigator (ISCRA-B Project)
- **System:** CINECA Leonardo (LEONARDO_B)
- **Allocation:** 998,400 standard compute hours
- **Science domain:** Condensed matter physics

02/01/2025 – 02/10/2025

Excited State Properties with Time-Dependent Density Functional Theory [TDDFT-3D]

- **Role:** Principal Investigator (ISCRA-C Project)
- **System:** CINECA Leonardo (LEONARDO_B)
- **Allocation:** 73,728 standard compute hours
- **Science domain:** condensed matter physics

08/01/2026 – CURRENT

WEST BENCHMARK

- **Role:** Principal Investigator (ISCRA-C Project)
- **System:** CINECA Leonardo (LEONARDO_B)
- **Allocation:** 80,000 standard compute hours
- **Science domain:** condensed matter physics