Study plan in

# Computational Materials Physics

UNIMORE
UNIVERSITÀ DEGLI STUDI DI MODENA E REGGIO EMILIA
Dipartimento di Scienze Fisiche, Informatiche e Matematiche

*M.Sc. program in Physics – Curriculum Theoretical and Computational physics*

## Overview

This study plan is designed to train students in the most advanced **principles** and **methods** of computational materials modeling. Teachings on the **quantum theory of condensed matter** combine with courses on the most recent **computational techniques**. Coupling fundamental equations and atomistic descriptions of matter with **machine learning**, **data-driven methods** and **high-performance computing** techniques, allows to study *in silico* innovative materials and their interaction with radiations, or screen for specific application-oriented properties vast classes of materials before being synthesized in the lab.

## Goal

At the end of this program students will be able to understand the physics and functioning **principles of material simulations** and their interaction with **external probes**. They will perform quantitative predictions of material properties using **state-of-the-art codes** and master **advanced computational methods** and protocols for the investigation of material properties and engineering with the most advanced computer architectures.

### More info and suggestions from

Study plan coordinator
Prof. Alice Ruini

Program director
Prof. Paolo Bordone

Program website
`www.fim.unimore.it/LM/FIS`

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## Fist year

### Advanced quantum mechanics (M) – M Gibertini

A self-contained course addressing several aspects of quantum mechanics relevant to modern developments of physics, from condensed-matter theory to particle physics and their fundamental interactions. Emphasis will be given to the concept of Berry phase, the path integral formulation, and scattering theory.

### Quantum field theory (M) – D Trancanelli, E Bertuzzo

An introductory course on QFT providing the quantization of scalar, spinor and vector fields, and covering the computation of scattering processes and decay rates in 4, Yukawa and QED theory. The course also provides a first discussion of radiative correction and renormalization.

### Statistical mechanics and phase transitions (M) – G Goldoni

An advanced course in statistical mechanics, from theoretical foundations to phase transitions and critical phenomena, including quantum condensates (BEC, superfluids, superconductors). Attendees are introduced to modern theoretical methods, from the Ginzburg-Landau theory to the statistical field theory and the renormalization group approach.

### Quantum physics of matter (M) – R Magri

An advanced course on matter-light and matter-electron interactions, using quantum linear response theory to discuss elementary excitations of material systems and their spectral features: electronic and phonon excitations, excitons, plasmons, polaritons.

### Laboratory of Quantum Simulation of Materials (D) – A Ruini

Frontal lectures and hands-on tutorial sessions introduce attendees to theoretical/computational techniques for the electronic structure simulation of condensed matter systems. Special emphasis is given to Density Functional Theory, the present state-of-the-art, parameter-free and atomistic scheme for the predictive description of materials.

### Solid state physics (D) – G Goldoni, F Grasselli

A course on the quantum theory of solid matter which is behind modern material science and semiconductor technology which shape the technological world. From electronic properties and transport phenomena to interaction with radiation, topological properties and advanced phenomena like superconductivity.

### Nanoscience and quantum materials (D) – E Molinari

Nanosystems are both quantum worlds with astonishingly new properties and the basis of new nanodevices. The course provides a conceptual and practical framework dealing with the physics and description of a set of prototype nanosystems, from nanotubes and graphene structures to nanocrystals, quantum wells, wires and dots.

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## Fields of specialization

- quantum processes in materials
- quantum matter
- material design & discovery
- computational modelling
- machine learning
- high-performance computing

## Opportunities

We have a tradition of **development** and **exploitation** of advanced computational methods to simulate innovative materials and predict their spectroscopic properties. We participate in large networks of **worldwide collaborations**, supported e.g. by **EU projects** and **Marie-Curie networks**, with computational and experimental groups which drive **thesis projects** on topics at the forefront of research, which will be conducted on **high-end computing infrastructures**. Students may also opt for the **Double Degree program** and spend the 2nd year on a research project at the Radboud University (NL).

## Employment

The acquired skills will enable the attendee to pursue employment in research on advanced new materials at international **private and public laboratories**, at Computing facilities like CINECA, in industrial R&D sectors, or to proceed for a PhD, both within the **Graduate School in Physics and Nanoscience** in Modena and worldwide.

## Notes

Ask the Master coordinator for further suggestions on other available courses to tailor the program to your interests.

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### Machine learning for scientific applications (R) – F Grasselli

An introduction to key ideas and techniques in machine learning for applications in physics, from basic principles to advanced topics in supervised and unsupervised learning, including worked hands-on examples. Subjects include Gaussian Process Regression, Bayesian Inference, Kernel methods, Deep Neural Networks, Convolutional Neural Networks, and Encoder-Decoder models.

### High Performance Computing for physical sciences (R) – P Bonfà

A course which combines lectures and hands-on projects to exploit modern computers in diverse fields, from high-throughput material screening to climate modeling to black holes formation, introducing to general concepts of parallel computing and practical approaches based on OpenMP, MPI, and GPU programming.

### Theory and simulation of excitations in materials (R) – M Govoni

A course to master the fundamental techniques to simulate excitations in materials and molecules from first principles, with focus on interrogating materials with light: molecular dynamics for simulating vibrational spectroscopies (Infrared & Raman), time-dependent density functional theory, many-body perturbation theory, and quantum embedding methods for simulating photoelectron spectroscopies, optical absorption and excited states phenomena occurring in materials for energy and quantum information science.

## Second year

### Laboratory of nanostructures (D) – F Rossella

The course covers the entire nanotechnology chain, from raw nanomaterials (semiconductor nanowires, 2D materials, nanotubes) to device fabrication (lithography techniques) to electrical and thermal transport measurements and in manufactured nanodevices. Classical and quantum transport experiments will be discussed.

### Quantum information processing (F) – P Bordone

An introduction to the theory behind quantum computers and QIP in general. Topics range from the basic concepts of QIP such as quantum entanglement and generalized quantum dynamics, to fundamental QIP algorithms, such as Shor's factoring, and quantum cryptography.

### Chemical physics of biomolecules (F) – G Brancolini

A unique, multidisciplinary course to acquire advanced theoretical understanding of chemical physics, with emphasis on biomolecules, colloids and their application to nano-biophysics and nano-medicine.

**Legend:** (M) mandatory course for this curriculum; (D) chosen within distinctive (*caratterizzanti*) courses; (R) chosen within related (*affini*) courses; (F) selected as a free choice course

This study plan is a suggested set of courses, chosen within the curriculum, to ensure an in-depth professional training combined with the broad spectrum of skills required to modern scientists. Mandatory, distinctive and related courses provide the natural background of this study plan. However, the study plan can also be tailored to the students' scientific interests. Ask the study plan coordinator for further indications.