



# Chiara Corapi

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Date of birth: 11 Aug 1999 Nationality: Italian

## EDUCATION AND TRAINING

[ 1 Nov 2025 – Current ]

### PhD student in Nanoscience for Medicine and the Environment

#### University of Bologna

City: Bologna | Country: Italy | Field(s) of study: Physical Chemistry ; Computational Chemistry ; Photochemistry

"Computational and experimental investigation of photoactive molecular materials"

#### Main project

- **Research Focus:** Development of piezochromic smart coatings constituted by mechanoluminochromic Cu-based compounds dispersed in a polymer binder.
- **Characterization:** Investigation of the relationship between the microstructure of Cu-based compounds and their mechanoluminochromic behavior within the polymer matrix, with a focus on correlating mechanical force with optical signal changes.
- **Modeling:** Elucidation of the atomistic mechanisms governing mechanoluminochromic properties via first-principles simulations.

[ 1 Sep 2021 – 26 Jan 2024 ]

### M.Sc. Physical Chemistry (LM-54)

#### University of Pisa <https://www.dcci.unipi.it/>

City: Pisa | Country: Italy | Field(s) of study: Physical Chemistry ; Theoretical Chemistry | Final grade: Cum laude | Level in EQF: EQF level 7 | Type of credits: ECTS | Number of credits: 120 | Thesis: Simulation of intersystem crossing dynamics of benzophenone upon excitation in the  $\pi\pi^*$  band (translated). Supervisor: Prof. Giovanni Granucci

[ 1 Sep 2018 – 28 Jul 2021 ]

### B.Sc. Chemistry and Chemical Technologies (L-27)

#### Unical - University of Calabria <https://ctc.unical.it/>

City: Rende, Cosenza | Country: Italy | Field(s) of study: Chemistry | Final grade: Cum laude | Level in EQF: EQF level 6 | Type of credits: ECTS | Number of credits: 180 | Thesis: 'Chiral Symmetry Breaking' and the origin of life: simple treatment and simulation of a mathematical model describing the evolution of a racemic system towards homochirality (translated). Supervisor: Prof. Giorgio Celebre

## WORK EXPERIENCE

#### University of Bologna

City: BOLOGNA | Country: Italy

[ 1 May 2024 – 31 Oct 2025 ]

### University research assistant

Modelling ground and excited-state properties of mechano-luminochromic copper halide-based coordination polymers.

## CONFERENCES AND SEMINARS

[ 5 Feb 2026 ]

### "NextGenCHEM - New Frontiers in Chemistry: Research by PhD Candidates"

Bologna

[ 27 Jan 2026 – 1 Feb 2026 ]

### Winter Workshop on Materials for Energy – wWME 2026 Bressanone

## High Performance Computing to Enhance Efficiency of Scientific Simulations -

[ 15 Sep 2025 – 19 Sep 2025 ]

**CINECA**

Bologna

[ 7 Sep 2025 – 12 Sep 2025 ]

**Summer School "Ab Initio Modelling in Solid State Chemistry"** Torino

[ 9 Jun 2025 – 12 Jun 2025 ]

**X Ciamician Photochemistry School** Bologna

[ 15 Apr 2025 ]

**Workshop on Raman Spectroscopies for Materials Science - RaMS** Milano

## HONOURS AND AWARDS

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[ 15 Apr 2025 ]

**Second best poster award in Raman spectroscopies for materials science (RaMS) workshop**

**Awarding institution:** Politecnico di Milano

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## INTERNSHIPS AND RE-SEARCH TRAINING

[ 14 Mar 2023 – 14 Jan 2024 ]

**Curricular Internship – Department of Chemistry and Industrial Chemistry, University of Pisa**

Computational simulations of the excited-state dynamics of benzophenone following excitation in the  $\pi\pi^*$  band were carried out using the Surface Hopping method with semi-empirical electronic wave functions. Since intersystem crossing plays a key role in this system, spin-orbit coupling was included in the nonadiabatic dynamics simulations.

Additionally, the transient photoionization spectrum of benzophenone was simulated and compared with available experimental data from the literature. This comparison aimed both to validate the computational approach—particularly the quantum decoherence algorithm used in the simulations—and to provide insights into the decay mechanisms of benzophenone.

[ 20 Apr 2021 – 30 Jun 2021 ]

**Curricular Internship – Department of Chemistry and Chemical Technologies, University of Calabria**

Homochirality, i.e., the predominance of a single enantiomer in chiral biological molecules, is one of the most intriguing characteristics of life on Earth. During the internship, a simple mathematical model based on Frank's hypothesis was developed, describing an autocatalytic mechanism between D and L enantiomers that promotes deviation from the racemic state and leads to the dominance of one species.

[ Apr 2018 – May 2018 ]

**Pre-collegiate A-level Math course, Department of Math e Informatics, University of Calabria**

## LANGUAGE SKILLS

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**Mother tongue(s):** Italiano

**Other language(s):**

**English**

**LISTENING B2 READING B2 WRITING B2**

**SPOKEN PRODUCTION B2 SPOKEN INTERACTION B2**

**Spanish**

**LISTENING B1 READING B1 WRITING B1**

**SPOKEN PRODUCTION B1 SPOKEN INTERACTION B1**