PERSONAL INFORMATION   Daniele Bondi

Male | 13/11/2001 | Italian nationality

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CURRENT POSITION

Current position: First-year PhD student in "Chemistry" at the University of Bologna (UNIBO), member of the International PhD College of Bologna and member of the Collegio Superiore of Bologna expected to obtain the II level Master linked to its five-year program by May 2026.

TITLE OF QUALIFICATION AWARDED

Academic qualification: Master's Degree in "Photochemistry and Molecular Materials" obtained from UNIBO in September 2025 with final grade: 110/110 cum laude.

EXTRACURRICOLAR EXPERIENCES

Participation to Eurocamp 2018, an activity promoted by the town of Formigine in cooperation with the European municipalities twinned with it and consisting in requalifying an area in a foreign city together with people from all over Europe. This edition took place in the French city of Saumur

WORK-SCHOOL EXPERIENCES

Experiences undertook in the school year 2017/2018

Model European Parliament (School, local and regional phases).
Simulation of the European Parliament for a total of 70 hours (Regional phase of 30 hours at the A. Rotti high school in Ferrara).

Volunteering at the "La Porta Bella" association.
After-school activities at the Magreta headquarters of the association for 27 hours.

Course to become a chess teacher organized by the cultural association "Club 64".
Lessons organized by a "Club 64" teacher at the "A. Tassoni" high school (30 hours).

Experiences undertook in the school year 2018/2019

Model European parliament (School and local phases as commission coordinator).
The activity lasted a total of 40 hours.

Work-school activity at the engineering department of Unimore.
Lessons on the various courses of studies proposed by the engineering department of the University of Modena and Reggio-Emilia (25 hours).

Project for the San Carlo foundation of Modena.
Activity, based on the theme of the environment, consisting in coming up with an initiative to requalify an urban area of Modena (50 hours).

EDUCATION AND TRAINING

School year 2024/2025	Victory of the thematic PhD scholarship "Computational strategies for luminescent molecular materials", XLI cycle, at the University of Bologna
School year 2024/2025	Master's degree in "Photochemistry and Molecular Materials" at UNIBO (final grade 110/110 cum laude).
School year 2022/2023	Bachelor's degree in "Chimica e Chimica dei Materiali" at UNIBO (final grade: 110/110 cum laude).
School year 2019/2020	Scientific high school diploma achieved at the "Alessandro Tassoni" high school of Modena (final grade: 100/100 cum laude).
Academic year 2014/2015	Title of qualification awarded: Lower secondary school diploma (final grade: 10/10 cum laude).

PERSONAL SKILLS AND COMPETENCES

Mother tongue	Italian

Other languages

	UNDERSTANDING		SPEAKING		WRITING
	Listening	Reading	Interaction	Oral production	
English	C1	C1	C1	C1	C1
	PET of the Cambridge University. Level B1. CAE of the Cambridge University. Level C1.				
French	Scholastic knowledge	Scholastic knowledge	Scholastic knowledge	Scholastic knowledge	Scholastic knowledge

Grades for the three years of middle school in French: 10. Additional practice on the language was made during the six months period I spent in Paris for the Erasmus+ internship connected to my Master's internship and thesis.

Social skills and competences	I Possess excellent communication skills, further developed through the experience as a delegate in the MEP, the Eurocamp project and my six months long Erasmus+ internship at the Sorbonne Université of Paris.
Organisational skills and competences	Leadership: achieved through various expereinces. In particular, serving as captain of the main team of the "Adriano Fiori" middle school in the "Coppa Ruffini" mathematics games in 2014/2015 (the team then placed third) and as captain of a team in the national tennis tournament in Albarella (the team then placed fourth).

Computer skills and competences

Excellent knowledge of the **Microsoft Office** Suite softwares (Word, PowerPoint, Excel, Outlook), of **AutoCAD**, of the **Linux** environment and of **MATLAB.**

Ability to program in **Julia**, and good competences with the programming languages **Fortan** and **Python** too.

I carried out a computational internship in Professor Fabrizia Negri's laboratory at the University of Bologna for my Bachelor's degree in "Chemistry and Chemistry of Materials" focused on the calculation of properties related to charge transport in crystals of cumulenic molecules (my Bachelor's thesis is entitled: "Calculation of Electronic Interactions in Molecular Crystals of Conjugated Cumulenic Systems"). Thanks to this experience, I acquired skills in the use of the **Gaussian16** software for performing quantum-chemical calculations, in the use of the in-house software **Pandora Suite**, useful for studying charge transport in crystalline structures, and in the use of several graphical software tools for visualizing molecules or molecular orbitals, such as **IQMOL, Avogadro, Chimera, gmolden, VMD, Mercury, and Tinker.**

I subsequently completed my final internship for the Master's degree in "Photochemistry and Molecular Materials", focused on the **theoretical and computational development** of a mathematical framework and on its software implementation for molecular systems of different sizes.

I personally developed a **Julia** program to study the 1D H_2^+ system using exact methods, both stationary and time-dependent. I went beyond the Born–Oppenheimer approximation by including non-adiabatic coupling coefficients and I investigated laser-induced excitations.

In parallel, I applied non-exact methods (e.g., **surface hopping molecular dynamics** using the **SHARC** software) to larger molecules, verifying the ESIPT (excited state intramolecular proton transfer) phenomenon in a triazole-based molecule. This experience significantly strengthened my skills in theoretical-mathematical development and programming.

In May 2025, I participated in a mathematics school focused on machine learning, structured into two 12-hour courses:

1. "(Un)supervised learning with applications to molecular dynamics" held by Professor Gabriel Stoltz (École des Ponts ParisTech);

2. "From machine-learned wavefunctions to interatomic potentials" held by Professor Geneviève Dusson (CNRS and Université Franche-Comté).

In June 2025, I participated in the tutorial sessions of the ORCA 6.0.1 software at the "Workshop on Computational Chemistry and Machine Learning for Chemical Physics" (CY Cergy Paris Université), held by Professor Chamil Sameera Wickramarachchi Millawalage.

In October 2025, after completing my Master's degree, I carried out the internship related to my Collegio Superiore final thesis in the laboratory of my academic tutor, Professor Ivan Rivalta. The central topic of this internship was the study and use of a Machine Learning program called "PROTEUS," developed by Professor Rivalta's research group. To use this program, which is capable of proposing molecules presenting the best possible value for a selected property, I had to deepen my knowledge of Python programming and learn to use the quantum-chemical software ORCA 6.1.0 and the software Multiwfn, useful to analyse molecular excitations.

In November 2025, I began my **PhD in Theoretical and Computational Chemistry**, which led me to further deepen my knowledge of the **Gaussian16** quantum-chemical

software. With this software, I performed **geometry optimizations (both ground and excited states), frequency calculations, TDDFT calculations, and rigid or relaxed potential energy surface (PES) scans** (the latter including a geometry optimization at each scan step).

The first project I focused on involved investigating a library of organic photosensitizers capable of promoting photocatalysis via energy transfer from their first triplet state T_1 (obtained through intersystem crossing after initial excitation to a singlet state from the ground state S_0) in the model reaction of isomerization of fumarate to maleate, which occurs in the T_1 state through rotation around the central C=C double bond. The molecules investigated included six acridone derivatives, benzophenone, 2-acetonaphthone, xanthone, and thioxanthone. These were studied by optimizing their ground state, their first triplet excited state and by analyzing the latter's wavefunction obtained via TDDFT calculations. The PES scan of fumarate isomerization (with respect to the dihedral angle formed by the four central carbon atoms during rotation) was also performed in both the ground state S_0 and the T_1 state to obtain a comprehensive picture of the system's energetics.

Other skills and competences

- Competitive tennis player (with participation to the national championships of Albarella in the single and team competitions).
- Competitive chess player (CERG provincial champion under 12 in 2013).
- Participation to the mathematics olympics during the five years of high school, with qualification to the provincial phase in my second and third year.
- Participation to the Italian language (grammar) olympics during the second year of high school.
- Participation to the science olympics during the fourth year of high school.
- Participation to the "Creative Writing Club" of the École normale supérieure of Parigi during my period abroad in the academic year 2024/2025.

Experiences abroad

- **Erasmus+ Traineeship Mobility Grant** awarded to carry out my Master's internship and thesis over a six-month period at the *Laboratoire de Chimie Théorique (LCT)* of the Sorbonne Université of Paris under the supervision of Professor Eleonora Luppi during the second semester of the 2025/2026 academic year. Project title: *"Investigation of the Coupled Nuclear and Electronic Motion: The Role of Non-Adiabatic Coupling."*
- **International Mobility Grant** from the Collegio Superiore of Bologna for an exchange at the École Normale Supérieure de Paris – PSL, undertaken concurrently with the Erasmus+ traineeship during the second semester of the 2025/2026 academic year. Project title: *"Microscopic–Macroscopic Connection for High-Harmonic Generation: Applications to Organic and Biological Molecules."*

Publications

- E. Sala, V. Galli, P. Mondelli, A. D. Scaccabarozzi, E. Gutiérrez-Fernández, D. Bondi, F. Negri, D. Fazzi, S. Pecorario, B. Sun, R.R. Tykwinski, P. Marabotti, S. Melesi, C. S. Casari, M. Caironi, "Charge Transport in tetraphenyl[5]cumulene: From Solution to Thin-Film and Organic Field Effect Transistors" **in preparation.**

Recognitions and prizes

- **Admission to the International PhD College** of the Collegio Superiore of Bologna as a PhD student in *Chemistry*: ranked 5th in the scientific area in the 2025 selection.
- **Thematic PhD Scholarship** "Computational Strategies for Luminescent Molecular Materials," 41st cycle, within the PhD Program in "Chemistry" at the University of Bologna.

- Awarding of the "Bando di tutorato didattico per i corsi di studio del Dipartimento di Chimica "Giacomo Ciamician" per l'a.a. 2025/2026, II ciclo ed estensivi" for the laboratory component of the course ''Molecular Materials: Properties and Modelling'' in the Master's degree in "Photochemistry and Molecular Materials", taught by Professor Fabrizia Negri.
- Admission to the PhD Program in "Chemical Sciences" at Sapienza University of Rome: ranked 7th in the 41st cycle selection.
- **Erasmus+ Traineeship Mobility Grant** to carry out my Master's internship and thesis at the Sorbonne Université of Paris.
- **International Mobility Grant** from the Collegio Superiore of Bologna for an exchange at the École Normale Supérieure de Paris – PSL.
- Merit-Based Scholarship awarded to students enrolled in degree programs in disciplines of particular national interest for the academic year 2021/2022.
- **Admission to the Collegio Superiore of Bologna** as a student in "Chemistry and Chemistry of Materials": ranked 2nd in the 2020 selection.
- Admission to the Scuola Normale Superiore of Pisa: ranked 12th in the 2020 selection.
- Inclusion in the Albo Nazionale delle Eccellenze – INDIRE following the achievement of a high school diploma with a final grade of 100/100 cum laude.
- Scholarship for outstanding academic achievement awarded upon obtaining the scientific high school diploma with a final grade of 100/100 with honors.
- Barbieri–Tarozzi Scholarship (2014/2015**)** awarded upon obtaining the lower secondary school diploma with a final grade of 10/10 cum laude.
- Third place in the "Coppa Ruffini" mathematical competition in 2014/2015.

Membership in groups / associations

- Collegio Superiore di Bologna (Università degli Studi di Bologna).
- I-PhD College of the Collegio Superiore of Bologna.

Participation to congresses, schools or missions

- Participation in the conference day "NextGenCHEM – New Frontiers in Chemistry: PhD Research"**,** with a poster entitled *"*Energy Transfer Catalysts for Fumarate to Maleate Isomerization: a Computational Investigation", which I presented during both poster sessions of the event.
- Participation in the workshop "Transformative Research – Nanotechnology Innovation by Creative Thinking", organized by the Department of Chemistry "Giacomo Ciamician" of the University of Bologna, featuring lectures by Professors Nathan Gianneschi, Maurizio Prato, Stefania Rapino, Francesco Zerbetto, Marco Garavelli, Paola Ceroni, Fabio Biscarini, Marco Montalti, Luca Prodi, and Marcella Bonchio (7 hours).
- Participation in the ORCA 6.0.1 tutorial sessions of the "Workshop on Computational Chemistry and Machine Learning for Chemical Physics" of the CY Cergy Paris Université (Neuville) on June 12–13 2025, held by Professor Chamil Sameera Wickramarachchi Millawalage (7 hours).
- Participation in the "7th edition of the mini-school on mathematics for theoretical chemistry and physics", organized by GDR NBODY in Paris in the May 19–21 2025 period. The mini-school focused on machine learning and was structured into two 12-hour courses: "(Un)supervised learning with applications to molecular dynamics" held by Professor Gabriel Stoltz (École des Ponts ParisTech); "From machine-learned wavefunctions to interatomic potentials" held by Professor Geneviève Dusson (CNRS and Université Franche-Comté) (24 hours total).
- Two-day university mission to Professor Morgane Vacher's laboratory at the University of Nantes aimed at learning surface hopping based simulation techniques.

Courses

- 14 hours course about the AutoCAD software.
- 8 hours online safety course held by Professor Fausto Costi (school year 2016/2017).

- Corso sulla sicurezza in Laboratorio Chimico: Modulo 1 – Formazione generale.
- Corso sulla sicurezza in Laboratorio Chimico: Modulo 2 – Formazione specifica rischio basso.
- Corso sulla sicurezza in Laboratorio Chimico: Modulo 3 – Formazione specifica rischio medio.
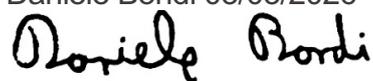
Certifications
- Language certification: First Certificate for the English language (C1).

Personal data   I authorize the treatment of my personal data in accordance with the Decreto Legislativo 30 giugno 2003, n. 196 "Codice in materia di protezione dei dati personali".

Daniele Bondi 03/03/2026