

Daniele Padula

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Personal Information

- **Date of Birth:** 01 March 1985.
- **Place of Birth:** Pisa, Italy.
- **Gender:** Male.
- **Citizenship:** Italian.

Languages

- **Italian:** native speaker.
- **English:** fluent.
- **Spanish:** fluent.

Education

- **Università di Pisa** Pisa, IT
Ph.D., Chemical Sciences *January 2010–January 2013*
Dissertation: "Structure and Properties of Simple and Aggregate Systems by Circular Dichroism Spectroscopy".
- **ICCOM–CNR** Pisa, IT
Visiting Ph.D. Student *February 2011–December 2012*
- **Università di Pisa** Pisa, IT
Master's Degree, Organic Chemistry *September 2007–September 2009*
- **Scuola Normale Superiore** Pisa, IT
Diploma, Chemistry *October 2007–September 2009*
Excellence Studies parallel to Master's at Università di Pisa.
- **Università della Basilicata** Potenza, IT
Bachelor's Degree, Chemistry *September 2003–June 2007*

Appointments

- **Associate Professor** Siena, IT
Università di Siena *Feb 2024–*
- **Tenure Track Position** Siena, IT
Università di Siena *Feb 2021–Jan 2024*
Project on "Designing New Organic Molecules for Energy Applications with Stochastic Optimisation and Machine Learning".
- **Lecturer** Siena, IT
Computational Photochemistry and Photobiology group, Università di Siena *Jan 2020–Jan 2021*
Project on "Development and application of software for spectroscopy and photochemistry of chromophores embedded in protein environment".

- **Research Scientist** **Dübendorf, CH**
Laboratory for Functional Polymers, EMPA *March 2019–December 2019*
 Project on the Computational Exploration of Near-Infrared Absorbing Polymethine Dyes.
- **Postdoctoral Research Associate** **Liverpool, U.K.**
Prof. Alessandro Troisi's group, University of Liverpool *August 2017–February 2019*
 Participation in the ERC funded project ESTYMA (Grant No. 615834), concerning Exciton Dynamics in Photosynthetic Antennae and Organic Materials.
- **Postdoctoral Research Associate** **Coventry, U.K.**
Prof. Alessandro Troisi's group, University of Warwick *April 2016–July 2017*
 Participation in the ERC funded project ESTYMA (Grant No. 615834), concerning Exciton Dynamics in Photosynthetic Antennae.
- **Postdoctoral Researcher** **Pisa, IT**
Prof. Benedetta Mennucci's group, Università di Pisa *April 2015–March 2016*
 Participation in the ERC funded project EnLight (Grant No. 277755), concerning the Simulation of Excitonic Optical Properties of Biopolymers
- **Postdoctoral Fellow** **Prague, CZ**
Computational Spectroscopy group, IOCB *March 2013–March 2015*
 Postdoctoral Fellowship concerning a Combined Spectroscopic/Computational Study of Magnetic Optical Properties of Lanthanide Complexes and Biological Chromophores.

Grants & Fellowships

Total competitive funding > 800k € and > 400k GPU/CPU hours as PI/Co-PI.

- **F-NF Grant** **Siena, IT**
Università di Siena *December 2024–November 2026*
 PI. Project: "Coarse-graining the chiral aggregation of conjugated polymers". 20k€.
- **HPC, Big Data, Quantum Computing Open Call Grant**
Italian National Research Council *October 2024–November 2025*
 Co-PI. Project: "Rethinking Organic Materials: from Design to Efficient Optoelectronics". ≈ 290k€.
- **PRIN Grant**
Italian Ministry of University and Research *October 2023–September 2025*
 PI. Project: "Enhancing Circularly Polarised Emitters Quantum Efficiency Exploiting Singlet-Triplet Inversion". ≈ 235k€.
- **F-Cur Grant** **Siena, IT**
Università di Siena *February 2022–June 2023*
 PI. Project: "Triplet Transport in Thermally Activated Delayed Fluorescent Aggregates". ≈ 25k€.
- **Young Researchers "Rita Levi Montalcini" Grant**
Italian Ministry of University and Research *February 2021–January 2024*
 PI. Project: "Designing New Organic Molecules for Energy Applications with Stochastic Optimisation and Machine Learning". ≈ 260k€.
- **ISCRA C Grant** **Bologna, IT**
CINECA
 PI of several ISCRA C projects granting access to CINECA HPC facilities. ≈ 400k GPU/CPU hours.

- **IOCB Postdoctoral Fellowship** **Prague, CZ**
Institute of Organic Chemistry and Biochemistry *March 2013–March 2015*
- **Graduate School “G. Galiei” Ph.D. Fellowship** **Pisa, IT**
Università di Pisa *January 2010–December 2012*
- **Scuola Normale Undergraduate Fellowship** **Pisa, IT**
Scuola Normale Superiore *October 2007–September 2009*

Additional Qualifications

- **Computing π -Conjugated Compounds Society**
Member of the Scientific Committee *February 2025–*
- **15th Symposium on Computing π -Conjugated Compounds** **Siena, Italy**
Co-organiser *February 2025*
- **Abilitazione Scientifica Nazionale (Full Professor)** **Italy**
Class 03/C1
 - *Class 03/C1: Organic Chemistry (March 2025–March 2037)*
- **Abilitazione Scientifica Nazionale (Associate Professor)** **Italy**
Class 03/C1, 03/B2, 03/A2
 - *Class 03/A2: Models and Methodologies in Chemical Sciences (January 2022–January 2031)*
 - *Class 03/B2: Chemical Foundations of Technologies (April 2021–April 2030)*
 - *Class 03/C1: Organic Chemistry (July 2020–July 2029)*
- **Habilitation à Maître de Conférences (Associate Professor)** **France**
Class 31 and 32 *February 2018–February 2022*
 - *Class 31: Theoretical, Physical, and Analytical Chemistry.*
 - *Class 32: Organic, Industrial, and Mineral Chemistry.*
- **Editor**
Theoretical Chemistry Accounts, Springer *March 2025–*
 Member of the Editorial Board for the journal *TCA* published by Springer.
- **Associate Editor**
Science and Technology of Advanced Materials: Methods, Taylor&Francis *January 2021–*
 Open access journal STAM: Methods published by Taylor&Francis.
- **Subject Editor**
Science and Technology of Advanced Materials, Taylor&Francis *January 2020–March 2024*
 Subject: Materials Informatics for the Open access journal STAM published by Taylor&Francis.
- **Topic Editor**
Molecules, MDPI *September 2020–*
 Topic Editor for the Open access journal *Molecules* published by MDPI.
- **Reviewer**
ACS, Elsevier, Wiley, MDPI journals, Grant Panels

- ACS: *J. Am. Chem. Soc.*, *Acc. Chem. Res.*, *J. Chem. Theory Comput.*, *J. Phys. Chem.*, *J. Chem. Inf. Model.*, *ACS Omega*
- Wiley: *Adv. Funct. Mater.*, *ChemPhotoChem*, *Energy Technol.*, *Chirality*
- Elsevier: *Org. Electron.*, *Sol. Energy*, *J. Mol. Struct.*, *Artificial Intelligence Chemistry*
- MDPI: *Energies*, *Molecules*
- ERC Starting Grant, ADMIRE COFUND MSCA Postdoctoral Fellowship

Teaching

- **Introduction to Chiroptical Spectroscopy** Siena, IT
Università di Siena July 2021
 12 hrs course to Chemical and Pharmaceutical Sciences PhD students ([Syllabus](#)).
- **Applied Computational Chemistry** Siena, IT
Università di Siena
 32 hrs course on Computational Modelling of Photophysical Processes to 4th year Chemistry students.
 - April 2027–June 2027 ([Syllabus](#) and [Material](#)).
 - April 2026–June 2026 ([Syllabus](#) and [Material](#)).
- **Quantum Chemistry Applied to Thermal and Photochemical Reactions** Siena, IT
Università di Siena
 32 hrs course on Computational Modelling of Ground and Excited state reactivity of Organic Molecules to 4th year Chemistry students.
 - April 2025–May 2025 ([Syllabus](#) and [Material](#)).
 - April 2024–May 2024 ([Syllabus](#) and [Material](#)).
 - March 2023–May 2023 ([Syllabus](#) and [Material](#)).
 - March 2022–May 2022 ([Syllabus](#) and [Material](#)).
- **Organic Analysis Laboratory** Siena, IT
Università di Siena
 24 hrs class + 48 hrs Lab course on Spectroscopic Characterisation and Identification of Organic Compounds to 3rd year Chemistry students.
 - October 2026–November 2026 ([Syllabus](#) and [Material](#)).
 - October 2023–November 2023 ([Syllabus](#), only 48 hrs Lab).
 - October 2022–November 2022 ([Syllabus](#), only 48 hrs Lab).
 - November 2021–January 2022 ([Syllabus](#), only 48 hrs Lab).
- **Chemistry of Heterocyclic Compounds** Siena, IT
Università di Siena
 48 hrs course on properties and reactivity of heterocyclic molecules to 2nd year Pharmacy students.
 - March 2026–June 2026 ([Syllabus](#) and [Material](#)).
 - March 2025–June 2025 ([Syllabus](#) and [Material](#)).
 - March 2024–June 2024 ([Syllabus](#) and [Material](#)).
- **Organic Chemistry Laboratory** Siena, IT
Università di Siena
 48 hrs course on basic Organic Chemistry Laboratory techniques and syntheses to 2nd year Chemistry students.
 - March 2021–April 2021 ([Syllabus](#)).
 - March 2020–April 2020 ([Syllabus](#)).
- **Organic Chemistry** Siena, IT
Università di Siena

48 hrs course on basic Organic Chemistry to 1st year Biotechnology students.

- December 2026 (at the [Siena College of Future Biotechnology, Nantong University](#), course in English).
- October 2026–December 2026 ([Syllabus](#), course in Italian).
- March 2026–June 2026 ([Syllabus](#), course in English).
- November 2025–January 2026 ([Syllabus](#), course in Italian).
- November 2024–January 2025 ([Syllabus](#), course in Italian).

○ **Supervision of Postdocs**

- Marco Campetella (Università di Siena, December 2024–November 2025)
- Stefano Vaghi (Università di Siena, December 2024–November 2025)

○ **Supervision of PhD projects**

- Simone Veglianti (Università di Siena, November 2024–October 2027)

○ **Supervision of 3 MSc projects, 7 BSc projects, and 4 Internships**

Key International Collaborations

- **Prof. Alessandro Troisi** (University of Liverpool, UK): high-throughput screening of organic materials for energy applications (organic photovoltaics, singlet fission, emitters).
- **Prof. Frank Nüesch, Dr. Roland Hany** (Empa, Dübendorf, Switzerland): dynamics of electron traps in OLEDs.
- **Prof. Marco Fusè** (Università di Brescia, Italy) and **Prof. Cristiano Zonta** (Università di Padova, Italy): development of inverted singlet–triplet chiral emitters and photocatalysts.
- **Dr. Giacomo Prampolini** (ICCOM–CNR, Pisa, Italy): effect of alkyl side chains on electronic properties of organic semiconductors, structural properties of aggregates through MD.
- **Dr. Alessandro Landi** (Università di Salerno, Italy): charge and exciton transport in organic photovoltaics, light emitting diodes, and organic field-effect transistors.

References

- **Prof. Alessandro Troisi**
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- **Prof. Gennaro Pescitelli**
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- **Prof. Massimo Olivucci**
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