Daniele Padula

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Personal Information

- **Date of Birth:** 01 Mar 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 — *Jan 2010–Jan 2013*
  Dissertation: *Structure and Properties of Simple and Aggregate Systems by Circular Dichroism Spectroscopy*.
- **ICCOM–CNR** — **Pisa, IT**
  Visiting Ph.D. Student — *Feb 2011–Dec 2012*
- **Università di Pisa** — **Pisa, IT**
  Master's Degree, Organic Chemistry — *Sep 2007–Sep 2009*
- **Scuola Normale Superiore** — **Pisa, IT**
  Diploma, Chemistry — *Oct 2007–Sep 2009*
  Excellence Studies parallel to Master's at Università di Pisa.
- **Università della Basilicata** — **Potenza, IT**
  Bachelor's Degree, Chemistry — *Sep 2003–Jun 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 — *Mar 2019–Dec 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 — *Aug 2017–Feb 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 — *Apr 2016–Jul 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 — *Apr 2015–Mar 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 — *Mar 2013–Mar 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 — *Dec 2024–Nov 2026*
  PI. Project: "Coarse–graining the chiral aggregation of conjugated polymers". 20k€.

- **HPC, Big Data, Quantum Computing Open Call Grant**
  Italian National Research Council — *Oct 2024–Nov 2025*
  Co–PI. Project: "Rethinking Organic Materials: from Design to Efficient Optoelectronics". ≈ 290k€.

- **PRIN Grant**
  Italian Ministry of University and Research — *Oct 2023–Sep 2025*
  PI. Project: "Enhancing Circularly Polarised Emitters Quantum Efficiency Exploiting Singlet-Triplet Inversion". ≈ 235k€.

- **F-Cur Grant** — **Siena, IT**
  Università di Siena — *Feb 2022–Jun 2023*
  PI. Project: "Triplet Transport in Thermally Activated Delayed Fluorescent Aggregates". ≈ 25k€.

- **Young Researchers "Rita Levi Montalcini" Grant**
  Italian Ministry of University and Research — *Feb 2021–Jan 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 — *Mar 2013–Mar 2015*

- **Graduate School "G. Galilei" Ph.D. Fellowship** — **Pisa, IT**
  Università di Pisa — *Jan 2010–Dec 2012*
- **Scuola Normale Undergraduate Fellowship** — **Pisa, IT**
  Scuola Normale Superiore — *Oct 2007–Sep 2009*

Additional Qualifications

- **Computing π–Conjugated Compounds Society**
  Member of the Scientific Committee — *Feb 2025–*
- **15^{th} Symposium on Computing π–Conjugated Compounds** — **Siena, Italy**
  Co–organiser — *Feb 2025*
- **Abilitazione Scientifica Nazionale (Full Professor)** — **Italy**
  Class 03/C1
  - *Class 03/C1*: Organic Chemistry (Mar 2025–Mar 2037)
- **Abilitazione Scientifica Nazionale (Associate Professor)** — **Italy**
  Class 03/C1, 03/B2, 03/A2
  - *Class 03/A2*: Models and Methodologies in Chemical Sciences (Jan 2022–Jan 2031)
  - *Class 03/B2*: Chemical Foundations of Technologies (Apr 2021–Apr 2030)
  - *Class 03/C1*: Organic Chemistry (Jul 2020–Jul 2029)
- **Habilitation à Maître de Conférences (Associate Professor)** — **France**
  Class 31 and 32 — *Feb 2018–Feb 2022*
  - *Class 31*: Theoretical, Physical, and Analytical Chemistry.
  - *Class 32*: Organic, Industrial, and Mineral Chemistry.
- **Editor**
  Theoretical Chemistry Accounts, Springer — *Mar 2025–*
  Member of the Editorial Board for the journal *TCA* published by Springer.
- **Associate Editor**
  Science and Technology of Advanced Materials: Methods, Taylor&Francis — *Jan 2021–*
  Open access journal STAM: Methods published by Taylor&Francis.
- **Subject Editor**
  Science and Technology of Advanced Materials, Taylor&Francis — *Jan 2020–Mar 2024*
  Subject: Materials Informatics for the Open access journal STAM published by Taylor&Francis.
- **Topic Editor**
  Molecules, MDPI — *Sep 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 *Jul 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 4^{th} year Chemistry students.
  - Apr 2027–Jun 2027 (Syllabus and Material).
  - Apr 2026–Jun 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 4^{th} year Chemistry students.
  - Apr 2025–May 2025 (Syllabus and Material).
  - Mar 2024–May 2024 (Syllabus and Material).
  - Mar 2023–May 2023 (Syllabus and Material).
  - Mar 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 3^{rd} year Chemistry students.
  - Oct 2026–Nov 2026 (Syllabus and Material).
  - Oct 2023–Nov 2023 (Syllabus, only 48 hrs Lab).
  - Oct 2022–Nov 2022 (Syllabus, only 48 hrs Lab).
  - Nov 2021–Jan 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 2^{nd} year Pharmacy students.
  - Mar 2026–Jun 2026 (Syllabus and Material).
  - Mar 2025–Jun 2025 (Syllabus and Material).
  - Mar 2024–Jun 2024 (Syllabus and Material).
- **Organic Chemistry Laboratory** **Siena, IT**
  Università di Siena
  48 hrs course on basic Organic Chemistry Laboratory techniques and syntheses to 2^{nd} year Chemistry students.
  - Mar 2021–Apr 2021 (Syllabus).
  - Mar 2020–Apr 2020 (Syllabus).
- **Organic Chemistry** **Siena, IT**
  Università di Siena
  48 hrs course on basic Organic Chemistry to 1^{st} year Biotechnology students.
  - Dec 2026 (at the Siena College of Future Biotechnology, Nantong University, course in English).
  - Oct 2026–Dec 2026 (Syllabus, course in Italian).
  - Mar 2026–Jun 2026 (Syllabus, course in English).
  - Nov 2025–Jan 2026 (Syllabus, course in Italian).
  - Nov 2024–Jan 2025 (Syllabus, course in Italian).
- **Supervision of Postdocs**
  - Marco Campetella (Università di Siena, Dec 2024–Nov 2025)
  - Stefano Vaghi (Università di Siena, Dec 2024–Nov 2025)

- **Supervision of PhD projects**
  - Simone Veglianti (Università di Siena, Nov 2024–Oct 2027)
- **Supervision of 3 MSc projects, 7 BSc projects, and 4 Internships**

Bibliometric Parameters

- **Scopus:** 74 papers, ≈ 2100 citations, h-index $= 25$ (Jul 2026, ID 24463809800).
- **Google Scholar:** ≈ 2600 citations, h-index $= 29$ (Jul 2025, link to profile).

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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  University of Liverpool
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- **Prof. Massimo Olivucci**
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