Daniele Padula

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Personal Information

- **Date of Birth:** 01 March 1985.
- **Place of Birth:** Pisa, Italy.
- **Sex:** 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

- ***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€.

- **ISCRA C Grant** — **Bologna, IT**
  CINECA — *May 2023–February 2024*
  PI. Project: "Effect of anharmonicity on charge transport in organic materials through classical molecular dynamics and differentiable machine learning models". ≈100K CPU hours.

- **ISCRA C Grant** — **Bologna, IT**
  CINECA — *November 2022–August 2023*
  PI. Project: "Polymer/non-fullerene acceptors Organic Photovoltaics: from Morphology to Efficiency". ≈100K CPU hours.

- ***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€.
- **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–*
- **15^{th} Symposium on Computing π–Conjugated Compounds** **Siena, Italy**
  Co–organiser *February 2025*
- **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.
- **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).

- **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.
  - 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

  48 hrs course on Spectroscopic Characterisation and Identification of Organic Compounds to 3^{rd} year Chemistry students.
  - October 2023–November 2023 (Syllabus).
  - October 2022–November 2022 (Syllabus).
  - November 2021–January 2022 (Syllabus).

- **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.
  - 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 2^{nd} 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 1^{st} year Biotechnology students.
  - November 2024–January 2025 (Syllabus).

- **Physical Chemistry** — **Coventry, U.K.**
  University of Warwick — *May 2017*

  10 hrs tutoring on Spectroscopy to 1^{st} year Chemistry students.

- **Computational Chemistry** — **Pisa, IT**
  Università di Pisa — *December 2015–January 2016*

  10 hrs tutoring on Classical Molecular Dynamics to 5^{th} year Biology students.

- **Organic Chemistry** — **Pisa, IT**
  Università di Pisa — *April 2010–May 2010*

  10 hrs tutoring to 1^{st} year Biology students.

- **Supervision of PhD projects**
  - Simone Veglianti (Università di Siena, November 2024–)

- **Supervision of MSc projects**
  - Simone Veglianti (Università di Siena, October 2023–October 2024)
- **Supervision of BSc projects**
  - Riccardo Carpini (Università di Siena, February 2025–)
  - Febe Lilla Ferraro (Università di Siena, September 2024–February 2025)
  - Mehmed Dzeljo (Università di Siena, April 2024–October 2024)
  - Alessandro Michieletti (Università di Siena, October 2023–July 2024)
  - Noemi Romagnoli (Università di Siena, September 2023–April 2024)
  - Tommaso Cinaglia (Università di Siena, October 2022–June 2023)
- **Supervision of short projects**
  - Leonardo Rotondi (150 hours, Università di Siena, November 2023–December 2023)
  - Robin Hany (remote summer project, Universität Zürich, June 2022–September 2022)
- **Co-supervision of PhD projects**
  - Kirsten Claridge (University of Warwick and University of Liverpool, April 2016–March 2019)
- **Co-supervision of MSc projects**
  - Razan Daoud (Università di Siena, October 2020–October 2021)
  - Ömer H. Omar (University of Liverpool, October 2018–March 2019)
  - Jack D. Simpson (University of Liverpool, October 2017–March 2018)
- **Co-supervision of BSc projects**
  - Giacomo Agostini (Università di Siena, October 2023–July 2024)
  - Lucy Grant (University of Liverpool, October 2017–March 2018)
  - Alina Kuzmich (University of Warwick, June 2016–September 2016)

Bibliometric Parameters

- **Scopus:** 62 papers, ≈ 1500 citations, h-index $= 23$ (February 2025, ID 24463809800).
- **Google Scholar:** ≈ 1800 citations, h-index $= 26$ (February 2025, link to profile).

Current 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.
- **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
  Crown St
  L69 7ZD, Liverpool, UK
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- **Prof. Frank Nüesch**
  Laboratory for Functional Polymers
  Swiss Federal Laboratories for Materials Science and Technology
  Überlandstrasse 129
  8600, Dübendorf, Switzerland
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- **Prof. Massimo Olivucci**
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