

PERSONAL INFORMATION

Family Name, First name: **Agostini, Federica** federica.agostini@university-paris-saclay.fr
Date of birth: May 27th, 1982 Website: <https://federicaagostini.wordpress.com>
Nationality: Italian Twitter: @FedericaAgosti9

ACADEMIC POSITIONS

- **September 2016 - present**
Maître de Conférences – Institut de Chimie Physique (ICP) at the University Paris-Saclay, Orsay (France).
- **November 2010 - August 2016**
Postdoctoral researcher – Max Planck Institute of Microstructure Physics, Halle (Germany).
- **November 2009 - October 2010**
Postdoctoral researcher – Ecole Normale Supérieure, Paris (France).

EDUCATION

- **2006 - 2009 PhD in Physics** – Theoretical Physics, Molecular Dynamics.
Universities Pierre et Marie Curie, Paris (France) and Sapienza, Rome (Italy) [Dual PhD program].
PhD Advisors: Prof. G. Ciccotti, Prof. R. Vuilleumier. Defence date: February 12th, 2010.
- **2004 - 2006 Master Program in Physics** – Theoretical Physics, Molecular Dynamics.
University Sapienza, Rome (Italy). Advisors: Prof. G. Ciccotti, Prof. S. Caprara. Grade: 110/110 cum laude.
- **2001 - 2004 B. Sc. Program in Physics** – Theoretical Physics.
University Sapienza, Rome (Italy) Advisors: Prof. V. Ferrari. Grade: 110/110 cum laude.

AWARDS

- **2022 Young Researcher Prize** awarded by the Division de Chimie Physique of the Société Chimique de France.
- **2019 Young Researcher Prize** awarded by the Fédération de Chimie Physique of the University Paris-Saclay.

RESEARCH GRANTS

- **2022-2024 LabEx PALM:** Project LIGHT-UP “Strong light-matter coupling to control ultrafast processes in molecules” coordinated by Dr. Federica Agostini.
- **2021-2024 ANR JCJC:** Project Q-DeLight “Quantum decoherence in light-induced charge transfer phenomena” coordinated by Dr. Federica Agostini.
- **2020-2024 ANR PRC:** Project HyTRAJ “Hybrid quantum-classical trajectory method for reaction dynamics of complex systems” coordinated by Dr. Yohann Scribano (University of Montpellier).
- **2018-2022 ANR PRC:** Project Dichroprobe “Vibrational circular dichroism as a probe of non-covalent interactions” coordinated by Dr. Anne Zehnacker (University Paris-Saclay/CNRS).
- **2020-2021 CNRS:** Reduction of 50% of teaching duties upon approval of a research proposal.
- **2019-2021 CNRS:** International Emerging Actions. Project “On the Dynamics through conical intersections” coordinated by Dr. Federica Agostini in collaboration with Prof. Basile Curchod.
- **2018-2021 LabEx-PALM:** Project Dyn-OC2H4 “Collision of O(³P) with ethylene: A dynamical study of intersystem crossings” coordinated by Dr. Federica Agostini.

BIBLIOMETRICS

I have authored 44 papers and 2 book chapters.

- **Google Scholar** 1531 citations, h-index = 22 (based on 43 publications)
- **Scopus** 1109 citations, h-index = 19 (based on 42 publications)

LIST OF 5 RECENT PUBLICATIONS

1. *A photochemical reaction in different theoretical representations.*
L. M. Ibele, B. F. E. Curchod, and F. Agostini, *J. Phys. Chem. A* **126** (2022) 1263.
2. *Nonadiabatic dynamics with coupled trajectories.*
C. Pieroni, and F. Agostini, *J. Chem. Theory Comput.* **11** (2021) 5969.

3. *Spin-orbit interactions in ultrafast molecular processes.*
F. Talotta, S. Morisset, N. Rougeau, D. Lauvergnat, and F. Agostini, *Phys. Rev. Lett.* **124** (2020) 033001.
4. *On the dynamics through a conical intersection.*
B. F. E. Curchod, and F. Agostini, *J. Phys. Chem. Lett.* **8** (2017) 831.
5. *Different flavors of nonadiabatic molecular dynamics.*
F. Agostini, and B. F. E. Curchod, *WIREs Comput. Mol. Sci.* **9** (2019) e1417.

SELECTED INVITED PRESENTATIONS

I have been invited to give more than 40 oral presentations at workshops and conferences as well as more than 20 seminars/webinars at universities and research institutes (in Europe and overseas). Selected items are:

- **Excited state dynamics symposium** at Pacificchem 2021, December 2021, Honolulu, Hawaii, USA – online format.
- **Nonequilibrium phenomena, nonadiabatic dynamics and spectroscopy**, July 2021, Telluride, Colorado (USA) – hybrid format.
- **Modeling dynamics in dense manifolds of electronic states** at the Spring 2019 American Chemical Society National Meeting, April 2019, Orlando, Florida, USA.
- **Anharmonicity in medium-sized molecules and clusters (AMOC)**, April 2018, Budapest, Hungary.
- **Nonadiabatica**, March 2018, Jerusalem, Israel.
- **7th Time-dependent density-functional theory: Prospects and applications**, September 2016, Benasque, Spain.
- **Computation of quantum systems in cold-matter physics and chemistry**, February 2016, Toronto, Canada.
- **18th Workshop on computational physics and materials science: Total energy and force methods**, January 2016, Luxembourg, Luxembourg.
- **Conference on computational physics 2015**, December 2015, Guwahati, India.

INSTITUTIONAL RESPONSIBILITIES

- **2021 - present** Departmental board of the Chemistry Department of the University Paris-Saclay.
- **2019 - 2020** Council of the Institut de Chimie Physique.
- **2019 - present** Scientific advisory board of LabEX PALM, section “Ultrafast dynamics”.
- **2020 - present** Scientific advisory board of the GDR ThÉMS.

EDITORIAL ACTIVITIES

- **2022** Together with Prof. Basile Curchod invited editor for a topical issue of the Philosophical Transactions of the Royal Society A on “Chemistry without the Born-Oppenheimer approximation”.

REFEREEING ACTIVITIES

- **Peer-reviewed journals:** Science, Accounts of Chemical Research, Journal of Physical Chemistry Letters, Journal of Chemical Theory and Computation, Journal of Physical Chemistry, The Journal of Chemical Physics, European Physical Journal B, ChemPhysChem, International Journal of Quantum Chemistry, Theoretical Chemistry Accounts, Physical Review A, Physical Review Research, Physical Review Letters, Scientific Reports.
- **Research proposal:** European Research Council (Starting grant); Marie Skłodowska Curie COFUND Fellowships (FCFP) at the Freiburg Institute for Advanced Studies (FRIAS); Agence Nationale de la Recherche (ANR); Austrian Science Fund (FWF); Deutsche Forschung Gemeinschaft (DFG); The Catholic University of Leuven; LabEX PALM of the University Paris-Saclay.

ORGANIZATION OF WORKSHOPS, SCHOOLS, CONFERENCES AND WEBINARS

- **Institut Pascal of the University Paris-Saclay:** in 2022 in Saclay (France).
- **Les Houches Physics School:** in 2019 in Les Houches (France).
- **CECAM Workshops:** in 2015 in Lausanne (Switzerland), in 2017 in Saclay (France), in 2023 in Lausanne (Switzerland).
- **E-CAM Extended Software Development Workshops:** in 2018 in Saclay (France), in 2019 in Durham (UK).
- **Lorentz Workshop:** in 2021 which took place online.
- **VISTA seminars:** since 2020 taking place bi-weekly online (<https://quantum-dynamics-hub.github.io/VISTA/>).