Davide ACCOMASSO's Curriculum Vitae

PERSONAL DATA

FIRST NAME:	Davide
LAST NAME:	Accomasso
PLACE AND DATE OF BIRTH:	Asti, Italy | April 8, 1992
PERSONAL ADDRESS:	Viale Pilone 21, 14100 Asti, Italy
ACADEMIC ADDRESS:	Università di Bologna, Dipartimento di Chimica Industriale "Toso Montanari", via Piero Gobetti 85, Bologna (Italy)
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GOOGLE SCHOLAR:	Davide Accomasso
ORCID:	0000-0002-4100-4679

POSTDOCTORAL EXPERIENCE

October 1, 2024 - present
Postdoctoral Research Fellowship (assegno di ricerca),
University of Bologna, Department of Industrial Chemistry "Toso Montanari", Bologna (Italy)
Project title: "Development of a protocol for simulating transient XANES spectroscopy based on multi- reference electronic structure methods for investigating ultrafast internal conversion in transition metal complexes"
Supervisor: Prof. Artur Nenov

October 1, 2023 - September 30, 2024
POLONEZ BIS Marie Skłodowska-Curie Postdoctoral Fellowship,
Faculty of Chemistry, University of Warsaw (Poland)
Project title: "Unravelling and optimizing the photoisomerization dynamics of light-driven molecular rotary motors"
Role: Principal Investigator of the project
Mentor: Dr. Joanna Jankowska
Budget: 820 976,00 PLN (co-funded by the National Science Centre and the European Union's Horizon 2020 research and innovation program under the Marie Skłodowska-Curie grant agreement No. 945339)
Project website: polonezbis-lightdynamo

September 1, 2021 -
Postdoctoral Research Fellowship (assegno di ricerca),

August 31, 2023 — University of Pisa, Department of Chemistry and Industrial Chemistry, Pisa (Italy)
Project title: "Development of multiscale methods for the study of photochemical and photophysical processes in photoresponsive proteins"
Supervisors: Prof. Benedetta Mennucci, Dr. Lorenzo Cupellini

January 1 - July 31, 2021 — **Research Fellowship** (borsa di ricerca), University of Pisa, Department of Chemistry and Industrial Chemistry, Pisa (Italy)
Project title: "Computational Simulation of Singlet Fission in Novel Organic Chromophores"
Supervisors: Prof. Maurizio Persico, Prof. Giovanni Granucci

EDUCATION

2017-2021 — **PhD in Chemistry and Material Science**, University of Pisa (Italy)
Thesis title: "Singlet Fission in Molecular Crystals and Covalent Dimers: from Chromophore Design to Nonadiabatic Dynamics Simulation"
Supervisors: Prof. Maurizio Persico, Prof. Giovanni Granucci
Final Mark: Optimum cum Laude
Graduation date: May 6, 2021

2014-2017 — **Master in Chemistry**, University of Pisa (Italy)
Thesis title: "Computational study of 2,3-diamino-1,4-benzoquinone as a proposed chromophore for singlet fission"
Supervisors: Prof. Maurizio Persico (University of Pisa), Prof. Giovanni Granucci (University of Pisa), Prof. Remco W.A. Havenith (University of Groningen), Prof. Ria Broer (University of Groningen)
Grade Point Average: 28.96/30
Final Mark: 110/110 summa cum laude
Graduation date: July 13, 2017

2015-2017 — **European Master** in "Theoretical Chemistry and Computational Modelling" (TCCM), University of Pisa
Graduation date: July 13, 2017

March 1 - May 31, 2016 — **Erasmus Traineeship** at "Zernike Institute for Advanced Materials and Stratingh Institute for Chemistry", University of Groningen, Groningen (The Netherlands)
Supervisors: Prof. Remco W.A. Havenith, Prof. Ria Broer

2011-2014 — **Bachelor in Chemistry**, University of Eastern Piedmont

"Amedeo Avogadro", Alessandria (Italy)
Thesis title: "Ab initio calculation of absorption and emission spectra of the N719 dye in solution"
Supervisor: Prof. Maurizio Cossi
Grade Point Average: 29.61/30
Final Mark: 110/110 summa cum laude
Graduation date: October 28, 2014

2006-2011 **High School**, Liceo Scientifico "F. Vercelli", Asti (Italy)
Final Grade: 80/100

2003-2006 **Secondary School**, Scuola Media "O. e L. Jona", Asti (Italy)

1998-2003 **Primary School**, Scuola Elementare "F. Baracca", Asti (Italy)

LANGUAGES

ITALIAN: Mother Tongue

ENGLISH:
- Erasmus+ Language Assessment in English (May, 2016):
  Reading Comprehension B2,
  Listening Comprehension C2,
  Grammar B2,
  Vocabulary B2,
  Key Communicative Phrases C2,
  Overall Level C1
- First Certificate in English (FCE), Level B2 (March, 2010)
- Preliminary English Test (PET), Level B1 (March, 2009)

FRENCH: Basic Knowledge

COMPUTER SKILLS

Scripting Languages:	Tcsh and Bash Unix shells
Programming Languages:	Fortran;[a] Foo (object oriented Fortran);[b] Python (basic knowledge)
Computational Chemistry Packages:	MOPAC-PI;[c] Gaussian;[d] (Open)Molcas;[e] Molpro;[f] Tinker;[g] Crystal;[h] Cost Package (Toulouse);[i] TeraChem;[j] Newton-X;[k] GAMESS-US;[l] ORCA[m]
Chemistry Visualization Software:	Molden, GaussView, VMD, Moldraw
Other Software:	LaTeX, Gnuplot, Matplotlib, OpenOffice, LibreOffice, Jupyter Notebook

[a] Developer and maintainer of the MOPAC-PI semiempirical program (https://gitlab.com/granucci/mopacpi).
[b] Implementation of a new model to calculate molecular electronic states based on geminals in the Tonto package (https://github.com/dylan-jayatilaka/tonto/tree/Nice-branch).
[c] Single point calculations, geometry optimizations with the semiempirical FOMO-CI method, simulations of nonadiabatic excited state dynamics using the Surface Hopping technique, and QM/MM simulations.
[d] Single point calculations and geometry optimizations at the DFT and TD-DFT levels.
[e] Single point calculations and geometry optimizations at the CASSCF, MC-PDFT, and CASPT2 levels.
[f] Single point calculations using the CASSCF and NEVPT2 methods.
[g] Geometry optimizations and classical molecular dynamics.
[h] Single point calculations and geometry optimizations of periodic crystal structures at the DFT level.
[i] Single point calculations at the CASSCF and MR-CI level, using the Casdi and Casdiloc techniques.
[j] Single point calculations and geometry optimizations at the CASSCF and FOMO-CASCI levels.
[k] Surface hopping nonadiabatic dynamics with a semiempirical Frenkel exciton model.
[l] Single point calculations, minimum-energy and conical intersection geometry optimizations using the Mixed-Reference Spin-Flip (MRSF) TDDFT method.
[m] Single point calculations using the CASSCF and NEVPT2 methods, and geometry optimizations at the CASSCF level.

SOFTWARE DEVELOPMENTS

- Developer and maintainer of the MOPAC-PI program (https://gitlab.com/granucci/mopacpi).
- Development and implementation of a diabatization procedure for multi-chromophoric systems based on the localization of molecular orbitals in the MOPAC-PI program (*ChemPhotoChem.*, **2019**, 3, 933-944.).
- Implementation of a new model to calculate molecular electronic states based on geminals in the Tonto package (https://github.com/dylan-jayatilaka/tonto/tree/Nice-branch) under the supervision of Dr. Patrick Cassam-Chenaï at Université Nice Sophia Antipolis (*J. Chem. Phys.*, **2023**, 158, 074106.).

RESEARCH SKILLS AND EXPERTISE

- Computational photochemistry
  - Theory of photochemical processes (e.g. photoisomerizations, photoinduced energy transfer, multi-exciton generation)
  - Characterization of potential energy surfaces (PESs)
  - Investigation of (non)adiabatic excited state dynamics
- Electronic structure calculations
  - Single-reference methods based on the density functional theory ((TD)DFT)
  - Ab initio multi-configurational methods (CASSCF, FOMO-CI)
  - Ab initio multi-reference methods (CASPT2, NEVPT2, MRCI)
  - Semiempirical multi-configurational methods (semiempirical FOMO-CI)
  - Construction of (quasi-)diabatic electronic states
- Nonadiabatic dynamics simulations
  - Mixed quantum-classical trajectory surface hopping method
  - Ab initio multiple spawning method
- Molecular and multiscale modeling
  - Molecular mechanics techniques
  - Quantum mechanics/molecular mechanics (QM/MM) schemes
  - Excitonic models for multi-chromophoric systems
- Singlet fission process
- Computational design of photoactive organic materials
- Excited state dynamics of carotenoids
- Photochemistry and photophysics of photoresponsive and light-harvesting proteins
- Excited state dynamics of light-driven molecular rotary motors

PEER-REVIEWED PUBLICATIONS

14 publications (9 first/main author, 4 corresponding author): 13 articles, 1 book chapter

14. E. Sangiogo Gil*, A. Giustini, D. Accomasso*, and G. Granucci*. **Excitonic Approach for Nonadiabatic Dynamics: Extending Beyond the Frenkel Exciton Model.** *J. Chem. Theory Comput.*, **2024**, XXXX, XXX, XXX-XXX. URL
    * Corresponding authors.

13. D. Accomasso*, G. Londi, L. Cupellini, and B. Mennucci*. **The nature of carotenoid S^* state and its role in the nonphotochemical quenching of plants** *Nat. Commun.*, **2024**, 15, 847. URL
    * Corresponding authors.

12. L. M. Pedraza González†, D. Accomasso†, L. Cupellini, G. Granucci, and B. Mennucci. **Ultrafast Excited-State Dynamics of Luteins in the major light-harvesting complex LHCII.** *Photochem. Photobiol. Sci.*, **2024**, 23, 303-314. URL
    † These authors contributed equally to this work.

11. G. Salvadori, P. Mazzeo, D. Accomasso, L. Cupellini, and B. Mennucci. **Deciphering Photoreceptors Through Atomistic Modeling from Light Absorption to Conformational Response.** *J. Mol. Biol.*, **2024**, 436(5), 168358. URL

10. M. Persico, G. Granucci, and D. Accomasso. **The Quantum Decoherence Problem in Nonadiabatic Trajectory Methods.** Book chapter in *Comprehensive Computational Chemistry, Elsevier Inc.*, **2024** (Vol. 4, pages 273-292). URL

9. A. Arcidiacono, D. Accomasso, L. Cupellini, and B. Mennucci. **How orange carotenoid protein controls the excited state dynamics of canthaxanthin** *Chem. Sci.*, **2023**, 14(40), 11158-11169. URL

8. D. Accomasso*, N. Ben Amor, M. Persico, and G. Granucci. **Computational design of covalently bound dimers for singlet fission.** *J. Photochem. Photobiol. A: Chem.*, **2023**, 443, 114836. URL
    * Corresponding author.

7. P. Cassam-Chenaï, T. Perez, and D. Accomasso. **2D-block geminals: A non 1-orthogonal and non 0-seniority model with reduced computational complexity.** *J. Chem. Phys.*, **2023**, 158, 074106. URL.

6. D. Accomasso†, S. Arslancan†, L. Cupellini, G. Granucci, and B. Mennucci. **Ultrafast excited state dynamics of carotenoids and the role of the S_X state.** *J. Phys. Chem. Lett.*, **2022**, 13(29), 6762-6769. URL
    † These authors contributed equally to this work.

5. D. Accomasso*, M. Persico, and G. Granucci. **Computational design of singlet fission biradicaloid chromophores.** *J. Photochem. Photobiol. A: Chem.*, **2022**, 427, 113807. URL
    * Corresponding author.

4. D. Accomasso, G. Granucci, and M. Persico. **Singlet fission in covalent dimers of methylene-locked 1,3-diphenyl-isobenzofuran: Semiclassical simulations of nonadiabatic dynamics.** *J. Mater. Chem. A*, **2021**, 9(38), 21897-21909. URL

3. D. Accomasso, G. Granucci, M. Wibowo, and M. Persico. **Delocalization effects in singlet fission: Comparing models with two and three interacting molecules.** *J. Chem. Phys.*, **2020**, 152, 244125. URL

2. D. Accomasso, M. Persico, and G. Granucci. **Diabatization by localization in the framework of configuration interaction based on floating occupation molecular orbitals (FOMO-CI).** *ChemPhotoChem.*, **2019**, 3, 933-944. URL

1. D. Accomasso, G. Granucci, R.W.A. Havenith, and M. Persico. **Testing new chromophores for singlet fission: A computational protocol applied to 2,3-diamino-1,4-benzoquinone.** *Chem. Phys.*, **2018**, 515, 635-642. URL

PREPRINT PAPERS

1. D. Accomasso, and J. Jankowska. **Quantum-classical simulations reveal the photoisomerization dynamics of a prototypical first-generation rotary motor.** *ChemRxiv*, 2024. URL

PAPERS IN PREPARATION

2. G. Granucci, M. Persico, D. Accomasso, E. Sangiogo Gil et al. **MOPAC-PI: a program for excited state dynamics simulations based on nonadiabatic trajectories and semiempirical electronic structure calculations**.

1. D. Accomasso, D. Frassi, and G. Granucci. **Ultrafast singlet fission in newly designed covalent dimers**.

DISSEMINATION ARTICLES

1. D. Accomasso. **La fissione di singoletto studiata al computer.** La Chimica & L'Industria, Anno VII, N° 1, Gennaio/Febbraio 2023. http://dx.medra.org/10.17374/CI.2023.105.1.68

ORAL PRESENTATIONS

10. D. Accomasso, G. Londi, L. Cupellini, and B. Mennucci. **The nature of carotenoid S^* state and its role in the nonphotochemical quenching of plants.** SCI 2024 - XXVIII National Congress, Allianz MiCo Congress Center, Milano (Italy), August 26-30, 2024. Link to conference webpage

9. D. Accomasso, and J. Jankowska. **In silico investigation of the photoisomerization dynamics of a first-generation rotary motor.** IMAMPC'2024 conference, The University of Warsaw Biological and Chemical Research Centre, Warsaw (Poland), July 9-12, 2024. Link to conference webpage

8. D. Accomasso. **Excited-state dynamics of carotenoids: the case of Lutein.** Flash presentation at the CECAM workshop "Standardizing nonadiabatic dynamics: towards common benchmarks", Paris-Saclay (France), May 21 - 24, 2024. Link to workshop webpage

7. D. Accomasso. **Excited-state dynamics of carotenoids in photoresponsive and light-harvesting proteins.** Invited seminar at the Centre of New Technologies (CeNT), University of Warsaw, Warsaw (Poland), April 26, 2024. Abstract available at:
https://cent.uw.edu.pl/pl/blog/seminar-davide-accomasso-phd-faculty-of-chemistry-university-of-warsaw/

6. D. Accomasso, G. Londi, L. Cupellini, and B. Mennucci. **Uncovering a carotenoid quencher state in the CP29 light-harvesting complex of plants.** Workshop on "Principles of Light Induced Charge Transfer for Optogenetics (CT4OPTO)", Modena (Italy), CNR Nano Modena, July 3 - 5, 2023. Link to conference webpage

5. D. Accomasso, G. Granucci, and M. Persico. **Singlet fission dynamics in molecular crystals and covalent dimers.** 7^{th} Congress of the Theoretical and Computational Chemistry Division of the Italian Chemical Society, Modena (Italy), University of Modena and Reggio Emilia, September 21 - 23, 2022.

4. D. Accomasso, S. Arslancan, L. Cupellini, G. Granucci, and B. Mennucci. **Shedding light on the ultrafast photochemistry of carotenoids: Surface hopping simulations of lutein in condensed phase.** DCTC 2022 - Workshop organized by the Division of Computational and Theoretical Chemistry (DCTC) of the Italian Chemical Society (SCI), Firenze, Aula Magna del Rettorato, April 8, 2022.

3. D. Accomasso, G. Granucci, M. Wibowo, and M. Persico. **Delocalization Effects in Singlet Fission: Comparing Models with Two and Three Interacting Molecules.** VCTC 2020 - Virtual Conference on Theoretical Chemistry 2020, July 27 - 29, 2020. Lightning Talk available on YouTube at:
https://www.youtube.com/watch?v=2wp2Xi49xkM&feature=youtu.be.

2. D. Accomasso, G. Granucci, and M. Persico. **A diabatization procedure for molecular dimers applied to singlet fission.** TUMA 2018 - XXXVI Convegno Interregionale delle sezioni Toscana - Umbria - Marche - Abruzzo della Società Chimica Italiana (Interregional Congress of the Italian Chemical Society), Pisa, Centro Congressi "Le Benedettine", October 4 - 5, 2018.

1. D. Accomasso, G. Granucci, M. B. Stella, and M. Persico. **Attempting to maximize singlet fission by tuning the interchromophore coupling.** TCCM 2018 - Theoretical Chemistry and Computational Modelling, Final Workshop, Pisa, Department of Chemistry and Industrial Chemistry, University of Pisa, July 23 - 25, 2018.

POSTER PRESENTATIONS

12. D. Accomasso, K. Szychta, J. Jankowska. **Unravelling the photoisomerization reactions of light-driven molecular rotary motors by nonadiabatic dynamics simulations.** 29^{th} PhotoIUPAC conference, Valencia (Spain), July 14 - 19, 2024.

11. A. Arcidiacono[‡], D. Accomasso, L. Cupellini, and B. Mennucci. **The photochemical mechanism of the activation of Orange Carotenoid Protein.** Chemistry for the Future, Pisa (Italy), Department of Chemistry and Industrial Chemistry, University of Pisa, June 28 - 30, 2023.
    [‡] This author prepared and presented the poster.

10. D. Accomasso, S. Arslancan, L. Cupellini, G. Granucci, and B. Mennucci. **The ultrafast photodynamics of carotenoids.** 28^{th} PhotoIUPAC conference, Amsterdam (The Netherlands), July 17 - 22, 2022.

9. D. Accomasso, A. Arcidiacono, L. Cupellini, B. Mennucci. **The simulation of excited state dynamics of cantaxanthin in the Orange Carotenoid Protein.** Chemistry for the Future, Pisa (Italy), Department of Chemistry and Industrial Chemistry, University of Pisa, June 28 - July 1, 2022.

8. D. Accomasso, G. Granucci, M. Wibowo, and M. Persico. **Delocalization Effects in Singlet Fission: Comparing Models with Two and Three Interacting Molecules.** VCTC2020 - Virtual Conference on Theoretical Chemistry 2020, July 27 - 29, 2020.

7. D. Accomasso, G. Granucci, and M. Persico. **Diabatization by localization as a tool for studying multi-chromophoric systems.** European Summer School in Quantum Chemistry, Altavilla Milicia (Palermo, Italy), Hotel Villaggio Torre Normanna, September 8 - 21, 2019.

6. D. Accomasso, G. Granucci, and M. Persico. **Construction of Diabatic Electronic States of Configuration Interaction type by Localization of Molecular Orbitals with Floating Occupations.** 10^{th} Congress of the International Society of Theoretical Chemical Physics, Tromsø (Norway), Clarion Hotel The Edge, July 11 - 17, 2019.

5. D. Accomasso, M. Wibowo, G. Granucci, and M. Persico. **Beyond the dimer-based model of singlet fission: nonadiabatic dynamics simulation of three 2,5-bis(fluorene-9-ylidene)-2,5-dihydrothiophene molecules embedded in their crystal environment.** Chemistry for the Future, Pisa (Italy), Department of Chemistry and Industrial Chemistry, University of Pisa, July 3 - 5, 2019.

4. D. Accomasso, G. Granucci, and M. Persico. **A diabatization procedure for molecular dimers applied to singlet fission.** DCTC 2018 - Quinto Congresso della Divisione di Chimica Teorica e Computazionale della Società Chimica Italiana (5^{th} Congress of the Theoretical and Computational Chemistry Division of the Italian Chemical Society), Trieste (Italy), Department of Chemical and Pharmaceutical Sciences, University of Trieste, September 19 - 21, 2018.

3. D. Accomasso, G. Granucci, M. B. Stella, and M. Persico. **A computational strategy to test newly proposed chromophores for singlet fission.** Chemistry for the Future, Pisa, Department of Chemistry and Industrial Chemistry, University of Pisa, July 4 - 6, 2018.

2. D. Accomasso, G. Granucci, M. B. Stella, and M. Persico. **A computational protocol to test new chromophores for singlet fission.** PPES 2018 - Photoinduced Processes in Embedded Systems, Pisa (Italy), University of Pisa, Aula Magna di Scienze, area Pontecorvo, June 24 - 27, 2018.

1. D. Accomasso, M. B. Stella, G. Granucci, and M. Persico. **Covalent dimers for singlet fission: design strategy and suitability test.** Jerusalem Nonadiabatica 2018, Jerusalem (Israel), Israel Institute of Advanced Studies, the Hebrew University of Jerusalem in Israel, March 12 - 15, 2018.

PARTICIPATION IN RESEARCH GROUPS

- **Theoretical chemistry subgroup** of Dr. J. Jankowska
  Institution: Faculty of Chemistry, University of Warsaw (Poland).
  Period: October 1, 2023 - September 30, 2024.
  Research activity: The work focused on investigating, by means of computational simulations, the cis-trans photoisomerization reactions of Feringa's light-driven molecular rotary motors.

- **Molecolab group** of Prof. B. Mennucci
  Institution: Department of Chemistry and Industrial Chemistry, University of Pisa (Italy).
  Period: September 1, 2021 - August 31, 2023.
  Research activity: The research work was focused on the simulation of the light-induced dynamics in carotenoid pigments embedded in different protein environment. This work allowed to identify the molecular nature of debated spectroscopic states of carotenoids, such as the so-called S_X and S^* states, and to associate them with specific roles in the photosynthetic function of carotenoids.

- **Theoretical photochemistry group** of Prof. M. Persico and Prof. G. Granucci
  Institution: Department of Chemistry and Industrial Chemistry, University of Pisa (Italy).
  Period: February 1, 2016 - July 31, 2021.
  Research activity: The work aimed at investigating the singlet fission process in two different kinds of materials, namely molecular crystals and covalently bound dimers. This research activity allowed to identify novel candidate chromophores and materials for singlet fission, as well as to contribute to the fundamental understanding of the singlet fission phenomenon. Moreover, during this research work, novel computational protocols and methodologies were developed.

ORGANISATION AND DIRECTION OF RESEARCH ACTIVITIES

- **POLONEZ BIS MSCA project group**
  I have directed and coordinated the research group working on the POLONEZ BIS MSCA project entitled "Unravelling and optimizing the photoisomerization dynamics of light-driven molecular rotary motors" for which I was the Principal Investigator. The group working on this project comprised two Master students (Dominika Makoś and Kamil Szychta) and the project Mentor, Dr. Joanna Jankowska.
  Period: October 1, 2023 - September 30, 2024.
  Research activity: The work aims at investigating the cis-trans photoisomerization reactions of the light-driven molecular rotary motors developed by the Nobel laureate Feringa. This research activity allowed to uncover the photoisomerization mechanisms in a number of investigated rotary motors and to contribute to the development of general rules connecting the molecular structure of the motor with its photochemical behaviour.
  Publications: One manuscript is under review (preprint available at https://doi.org/10.26434/chemrxiv-2024-4t9hj) and two additional papers are in preparation.
  Project website: polonezbis-lightdynamo

- **Additional proposed research activities**
  I am the main proposer of the following research activities:

  - Development and implementation of a diabatization procedure for multi-chromophoric systems based on the localization of molecular orbitals in the MOPAC-PI program (Published paper available at *ChemPhotoChem.*, **2019**, 3, 933-944.).
  - Computational design of novel biradicaloid chromophores for singlet fission (Published paper available at *J. Photochem. Photobiol. A: Chem.*, **2022**, 427, 113807.).
  - Singlet fission dynamics simulations in covalently bound dimers, by means of GPU-accelerated ab initio electronic structure calculations and the Ab Initio Multiple Spawning (AIMS) technique. The computational resources for this research activity (130 000.00 CPU hours) were granted by the HPC-Europa3 Transnational Access programme (https://hpc-europa.cineca.it/).

SHORT RESEARCH VISITING PERIODS ABROAD

April 26 - June 27, 2021
HPC-Europa3 virtual visit
Durham University, Department of Chemistry, Durham, United Kingdom
Supervisor: Dr. Basile Curchod
Research activity: Singlet fission dynamics simulations in covalently bound dimers.

November 24 - December 22, 2019
Université Paul Sabatier, Laboratoire de Chimie et Physique Quantiques, Toulouse, France
Supervisor: Dr. Nadia Ben Amor
Research activity: Ab-initio calculation of diabatic state energies and couplings in promising covalent dimers for singlet fission.

September 30 - October 26, 2019; October 28 - December 1, 2018
Université Nice Sophia Antipolis, Laboratoire J. A. Dieudonné, Parc Valrose, Nice, France
Supervisor: Dr. Patrick Cassam-Chenaï
Research activity: Implementation of a quantum chemistry model to compute molecular electronic states built as antisymmetrized products of bielectronic wavefunctions, i.e. "geminals".

TEACHING ACTIVITY

- Lecturer in the course "Photochemistry: theoretical aspects" (Fotochimica: aspetti teorici) of Prof. G. Granucci for the Master program in Chemistry at the University of Pisa, for a total of 3 teaching hours (1 hours on May 3, 2018 + 2 hours on May 8, 2024). Topic: Theory of photoinduced energy transfer processes in molecular systems.

TUTORING AND SUPERVISION OF RESEARCH ACTIVITY

4. Dominika Makoś (Master student)
   Student scholarship under the POLONEZ BIS project LightDynaMo
   University of Warsaw, Faculty of Chemistry
   Research activity: Quantum chemical calculations and nonadiabatic dynamics simulations for a push-pull first-generation photomolecular rotary motor
   Supervisor: Dr. Davide Accomasso
   Year: 2024

3. Kamil Szychta (Master student)
   Student scholarship under the POLONEZ BIS project LightDynaMo
   University of Warsaw, Faculty of Chemistry

Research activity: Quantum chemical calculations and nonadiabatic dynamics simulations for a second-generation photomolecular rotary motor
Supervisors: Dr. Davide Accomasso and Dr. Joanna Jankowska
Year: 2024

2. Amanda Arcidiacono (Master student)
Master thesis in Chemistry
University of Pisa, Department of Chemistry and Industrial Chemistry
Thesis title: "The simulation of excited state dynamics of Canthaxanthin in the Orange Carotenoid Protein"
Supervisor: Prof. Benedetta Mennucci
Year: 2022-2023

1. Maria Bruna Stella (Bachelor student)
Bachelor thesis in Chemistry
University of Pisa, Department of Chemistry and Industrial Chemistry
Thesis title: "Investigation of the interaction between chromophores of 1,3-diphenylisobenzofuran for the singlet fission process"
Supervisor: Prof. Maurizio Persico
Year: 2018

PEER-REVIEW ACTIVITY

2. Review for *Dyes and Pigments* (2024).

1. Review for *Journal of Materials Chemistry C* (2022).

ORGANIZATION OF CONFERENCES

2. Co-organizer of the conference "Chemistry for the Future 2019", Pisa (Italy), Department of Chemistry and Industrial Chemistry, University of Pisa, July 3 - 5, 2019.

1. Co-organizer of the workshop "TCCM 2018" (Theoretical Chemistry and Computational Modelling, Final Workshop), Pisa, Department of Chemistry and Industrial Chemistry, University of Pisa, July 23 - 25, 2018.

RESEARCH GRANTS

2. POLONEZ BIS Marie Skłodowska-Curie Fellowship, National Science Centre, Poland, 2023. Project budget: 820 976.00 PLN ($\sim$ 191 500.00 EUR).

1. Ulam NAWA Scholarship, Polish National Agency for Academic Exchange, Poland, 2023. Project budget: 252 000.00 PLN ($\sim$ 58 500.00 EUR). Not accepted, due to incompatibility with POLONEZ BIS Fellowship.

COMPUTING GRANTS

3. ICM-HPC, Poland (https://kdm.icm.edu.pl/)
   Title: Simulations of photoisomerization reactions in light-driven molecular rotary motors
   Computation time: 1 000 000.00 CPU hours
   Period: February 5, 2024 - February 4, 2025

2. PLGrid Infrastructure, Poland (https://www.plgrid.pl/)
   Title: Quantum-chemical calculations on light-driven molecular rotary motors
   Computation time: 500 000.00 CPU hours
   Period: October 13, 2023 - October 12, 2024

1. HPC-Europa3 Transnational Access programme (https://hpc-europa.cineca.it/)
   EPCC supercomputing centre of the University of Edinburgh
   Title: Singlet fission dynamics simulations in covalently bound dimers
   Computation time: 130 000.00 CPU hours
   Period: April 26, 2021 - June 25, 2021

AWARDS AND PRIZES

5. POLONEZ BIS Marie Skłodowska-Curie Fellowship, National Science Centre, Poland, 2023.

4. Ulam NAWA Scholarship, Polish National Agency for Academic Exchange, Poland, 2023 (not accepted, due to incompatibility with POLONEZ BIS Fellowship).

3. "Colombaria 2022" prize for the best PhD thesis in Chemistry by the Italian institute "Accademia La Colombaria" (Firenze, Italy).

2. "Giuseppe Del Re" prize for the best PhD thesis of 2021 in the Theoretical Chemistry field by the Italian Chemical Society (SCI, "Società Chimica Italiana").

1. "Pier Luigi Nordio" prize for the best Master thesis of 2017 in the Theoretical Chemistry field by the Italian Chemical Society (SCI, "Società Chimica Italiana").

Date: Signature:

October 1, 2024

(Davide Accomasso)