# *Curriculum Vitae* of Luca Muccioli

## Current position

Since September 2019, I am working as associate professor of Physical Chemistry in the Department of Industrial Chemistry "Toso Montanari" at the University of Bologna and part of the the Spectroscopy and Computational Chemistry Group (SC2).

## Contacts


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## Research profile

### Techniques

My scientific activity focuses on the study of structural and electronic properties of soft matter through computer simulations (Molecular Dynamics, Metropolis and Kinetic Monte Carlo) methods and quantum chemistry calculations, with particular attention to the comparison with experiments and the quantitative accuracy of the results, achieved by: i) careful modeling and testing of intermolecular potentials; ii) adequate statistics provided by large system sizes and long simulations; iii) development of software tools for the calculation of observables directly or indirectly measurable with experimental techniques; iv) search for thermodynamic equilibrium by simulating self-assembling processes. The main topics and achievements are shortly listed below, divided for sake of simplicity in (overlapping) classes of materials.

### Liquid Crystals

The very first and still active subject of my research has been the study of phase organization and physical properties of liquid crystals, in their calamitic, discotic and biaxial variants. I have been particularly interested to the quantitative prediction of phase structures and transition temperatures, and in the qualitative effects of polymerization, nanoconfinement, molecular electrostatic potential, and flexibility on the phase diagrams of this fascinating class of compounds. To this end, I employ both simple, molecular level models (notably the Gay-Berne one) and of atomic-level ones. Indeed the internationally recognized world leadership of the group of Prof. Claudio Zannoni on atomistic simulations of liquid crystals originates from my PhD thesis work and has been established in the last 15 years of intense research, carried out with several other master and PhD students, and postdoc researches. While at the beginning we focused on bulk properties only, the most recent investigations are directed to understand the effect of inorganic and organic surface properties to the alignment of nematic liquid crystals.

### Organic Semiconductors

Immediately after my PhD, thanks also to a postdoctoral stay at the University of Mons in 2005 and to the involvement of the Bologna group in successful EU projects on the subject, I started interesting myself to organic electronics materials. This line of investigation has been stimulated by the growing interest in the field for the self-assembling properties typical of liquid crystals, and also by the urgency of a better comprehension of the morphology of molecules in devices and its influence on the electronic processes

which are at the basis of their functioning. The activity, consisting in the synergistic combination of atomistic simulations and electronic structure calculations, has naturally extended to bulk organic crystals, oligomers, polymers, for which in several instances we showed the intimate relationship between structural and energetic disorder, charge mobility and exciton diffusion. More recently this (collaborative) research has developed towards the study of interfaces and of the assembling of organic molecules on surfaces. More specifically, on one hand we are currently investigating the origin and the extent of the different energetic contributions which govern charge separation at the donor-acceptor interface in organic solar cells, with the help of classical microelectrostatic calculations. On the other, we are attempting to gain new insights on the mechanism of growth of organic crystals by simulating the vapor deposition process on organic surfaces. A recent success along this line is the award from SAMSUNG of a 2013 GRO SAIT research grant for the computational study of blue-emitting OLED materials, which triggered a new line of research on thermally activated delayed fluorescence materials.

### Other materials

Throughout the years, several side projects and collateral lines of research have emerged, mainly driven by suggestions from collaborators or simply by the desire of trying something different with respect to the two "mainstream" classes of compounds previously described. Despite the heterogeneity of these investigations, two main themes emerge. The first one is the measurement of chirality: we studied with the use of mathematical indexes both the solvation of chiral aldehydes and the secondary structure of peptides and proteins. The second, albeit linked one, is the solvent effect in complex systems: for instance we investigated the formation of perylene/melamine gels in water and the effect of organic solvents on azobenzene isomerization mechanism. Although rather scattered in terms of subject, many of these studies were successful in terms of citations, demonstrating that the usefulness of the methodologies I employ goes beyond liquid crystals and semiconductors, and my ease in tailoring them to the scientific problem under investigation.

## Dissemination

I presented my work with oral communications at about 30 national and international scientific conferences, schools, and workshops, and reported the research activity at several project meetings. In total I authored about

100 peer-reviewed publications, that at present received more than 4000 citations overall, for a Hirsch's index of 34.

## Education and professional experience

I studied Industrial Chemistry at the University of Bologna. Since my graduation in 1998 and until 2014, I carried out my scientific and academic activity at the department of Physical and Inorganic Chemistry thereby. I then moved to University of Bordeaux for two years, as Junior Chair (assistant professor) in "Theoretical modeling at the frontier between soft matter and organic electronics". In 2016 I came back to Bologna at the Department of Industrial Chemistry, serving as assistant professor (2016-2019), and then associate professor in Physical Chemistry (2019-now).

- *Habilitations:* I received the French *Habilitation à Diriger des Recherches* (Chimie-Physique, 2016) and the Italian *Abilitazione Scientifica Nazionale* (03/A2 MODELLI E METODOLOGIE PER LE SCIENZE CHIMICHE, ordinary professor, 2022-2031).
- *Education:* I received a PhD in Chemical Sciences (2003), and a Master Degree in Industrial Chemistry (1998).
- *Previous experience:* My research experience amounts to one year of predoctoral grant (1999), 3 years of PhD studies (2000-2002) and 10 years of postdoctoral contracts (2003-2013). I was assistant professor at the University of Bordeaux (2014-2016) and at the University of Bologna (2016-2019).
- *EU projects:* I have been local project leader in Claudio Zannoni's group for four EU projects dealing with organic electronics
- *Teaching:* I have been contract professor of "Nanotechnologies for materials - physical chemistry for nanotechnology" (2009, 2010, 2011), and contract tutor of "Aid to the study of Mathematics" (2002, 2003, 2005) at the university of Bologna. I have been professor of "Theoretical chemistry" at the university of Bordeaux (2016), and since 2016 I am teaching "Physical Chemistry" and "Mathemathics" (2017), at the university of Bologna.
- *Supervising:* I co-supervised 1 Bachelor thesis, 12 Master theses and 6 PhD theses. I am currently co-supervising 2 postdocs, 1 PhD student, and 2 Master students.

- *High Performance Computing:* I successfully applied to several HPC projects, including two DEISA Extreme Computing Initiatives (2009, 2010).
- *Fund Raising and Awards:* I was awarded a SAMSUNG GRO grant 2013 for a project on blue OLED materials (100k US dollars shared with two colleagues). The junior chair of excellence in Bordeaux was granted with about 600k euros for salaries and functioning. The Bordeaux unit in the MODIGLIANI M.era-net project was funded for 120k euros. The Bologna unit in the PRIN 2017 project "HARVEST" is funded with 105k euros.
- *Languages:* I am able to write and speak in Italian (mother tongue), English and French.

# Annex: list of titles

This section contains detailed lists of all my professional activities.

## Previous employments

ix 9/2016-9/2019: I was hired as assistant professor (tenure track "RTDB") of Physical Chemistry at the Department of Industrial Chemistry "Toso Montanari" of the University of Bologna

viii 9/2014-9/2016: I served as Junior Chair (assistant professor) in "Theoretical modeling at the frontier between soft matter and organic electronics", at the Laboratoire de Chimie des Polymères Organiques (LCPO) of the University of Bordeaux (FR), with a personal project dealing with multiscale modeling of organic electronics materials and devices (Sept 2014 - Aug 2017), in the framework of the AMADEus cluster of excellence.

vii 6/2012–8/2014: Assegno di ricerca (post doctoral grant, University of Bologna) funded by the Italian PRIN project "Novel ordered systems for high response molecular devices", in in the group of Prof. Claudio Zannoni, department of Industrial Chemistry "Toso Montanari", Bologna (Italy).
Research theme: *"Computer simulations at molecular and atomistic detail of liquid crystal phases and their response to external fields"*

vi 12/2009–5/2012: Research contract (University of Bologna) funded by the EU project "Modelling of electronic processes at interfaces in organic-based electronic devices" (MINOTOR) CP-FP228424-2, in the group of Prof. Claudio Zannoni, Dipartimento di Chimica Fisica e Inorganica (DCFI), Bologna (Italy).
Research theme: *"Simulations of organic semiconductor/dielectric interfaces"*.

v 5/2008–11/2009: Research contract (funded by Consorzio Interuniversitario Nazionale per la Scienza e la Tecnologia dei Materiali, INSTM, www.instm.it) funded by EU project "Modelling Electro-active COnjugated materials at the Multiscale" (MODECOM) NMP3-CT-2006-016434 in the group of Prof. Claudio Zannoni, DCFI, Bologna (Italy).
Research theme: *"Simulation of pentacene-fullerene heterojunctions"*.

iv 8/2005–3/2008: Research contract (INSTM) funded by EU project "NAnoscale Integrated processing of self-organizing Multifunctional Organic materials" (NAIMO) NMP4-CT-2004-500355 in the group of Prof. Claudio Zannoni, DCFI, Bologna (Italy).
Research theme: *"Modeling and simulations of molecules for organic electronics"*.

iii 7/2003–7/2005: Assegno di ricerca (official Italian postdoctoral grant since 1997) in the group of Prof. Claudio Zannoni, DCFI, Bologna (Italy).
Research theme: *"Modeling and simulation of liquid crystalline systems"*.

ii 2003: 6 months postdoctoral grant funded by Italian Ministry of University and Research in the group of Prof. Claudio Zannoni, DCFI, Bologna (Italy).
Research theme: *"Modeling and simulation of liquid crystals"*

i 1999: Yearly research predoctoral grant (INSTM) in the group of Prof. Claudio Zannoni, DCFI, Bologna (Italy).
Research theme: *"Theoretical modeling of linear and non-linear optical properties of molecular systems"*

## Education

iii PhD in Chemical Sciences (XV Italian PhD cycle). University of Bologna (Italy), April 24, 2003. PhD thesis: *"Molecular modeling and atomistic simulations of mesophases"*.
Supervisor: Prof. Claudio Zannoni.

ii Degree in Industrial Chemistry (mark $110/110$). Faculty of Industrial Chemistry, University of Bologna (Italy), October 30, 1998.
Degree thesis: *"Theoretical study of structure and vibrational properties: compounds of transition elements of groups XI and XII"*.
Supervisor: Prof. Riccardo Tarroni, co-supervisor Prof. Paolo Palmieri.

i High school diploma specializing in scientific subjects and informatics (mark $58/60$). Liceo scientifico Gregorio Ricci Curbastro, Lugo (IT), year 1992.

## Teaching activity

**as tutor and teacher**

xiii Teacher of the "Physical Chemistry of Adhesion" module (1 ECTS), Master in Composite Materials - Faenza (MACOF), academic years 2020-2024, University of Bologna (IT).

xii Professor of "Mathematics" (module 2, 4 ECTS, code 74790), Bachelor degree course in "Chemistry and technologies for environment and for materials" academic years 2019-2025, University of Bologna (IT).

xi Professor of "Physical Chemistry of Materials for Energy and Environment" (module 1, 3 ECTS, code 88377, in English), Master degree course in "Low carbon technologies and sustainable chemistry" academic years 2018-2025, University of Bologna (IT).

x Professor of "Physical Chemistry" (6 ECTS, code 67035), Bachelor degree course in "Chemistry and technologies for environment and for materials" academic years 2016-2025, University of Bologna (IT).

ix Professor of "Chemical-Physical Methods for the characterization of materials" (4 ECTS, code 66956), Bachelor degree course in "Chemistry and technologies for environment and for materials" academic year 2023-2024, University of Bologna (IT).

viii Professor of "Mathematics" (module 3, 2 ECTS, code 74790), Bachelor degree course in "Chemistry and technologies for environment and for materials" academic year 2017-2018, University of Bologna (IT).

vii Professor of "Chimie Théorique" (3 ECTS, code D1CH821A), Master "Sciences, Technologies, Santé", Chemistry curriculum, options "Chemistry" and "Physical Chemistry of Materials", academic year 2015-2016, University of Bordeaux (FR).

vi Annual contract professor of: "Nanotechnologies for materials - physical chemistry for nanotechnology" (3 ECTS, code 257, in English), Master degree course "Materials and Sensor Engineering For Environmental Sustainability" (code 8490), academic year 2011-2012, Faculty of Engineering, University of Bologna (IT).

v Annual contract professor of: "Nanotechnologies for materials - physical chemistry for nanotechnology" (3 ECTS, code 35775-30692, in English), Master degree course "Materials and Sensors Systems for Environmental Technologies" (code 0934), academic year 2010-2011, Faculty of Engineering, University of Bologna (IT).

iv Annual contract professor of: "Nanotechnologies for materials - physical chemistry for nanotechnology" (3 ECTS, code 30689-30692, official language: English), Master degree course "Materials and Sensors Systems for Environmental Technologies" (code 0944), academic year 2009-2010, Faculty of Engineering, University of Bologna (IT).

**Co-supervisor of master and bachelor thesis projects**

1 *"Modeling and simulation of banana-shaped mesogens"*
Andrea Maestrello, Master thesis in Industrial Chemistry
Supervisors: C. Zannoni, R. Berardi, L. Muccioli.
Faculty of Industrial Chemistry, University of Bologna (IT), March 2002.

2 *"Computer simulations of crystallization and dissolution models"*
Alberto Costantini, Master thesis in Industrial Chemistry
Supervisors: C. Zannoni, R. Berardi, S. Orlandi, L. Muccioli.
Faculty of Industrial Chemistry, University of Bologna (IT), October 2002.

3 *"Molecular Dynamics study of the photoisomerization of an azobenzene derivative in a nematic liquid crystal"*
Giustiniano Tiberio, Master thesis in Industrial Chemistry
Supervisors: C. Zannoni, A. Arcioni, R. Berardi, L. Muccioli.
Faculty of Industrial Chemistry, University of Bologna (IT), July 2003.

4 *"Atomistic simulation of a hexarepeat avian prion protein fragment in aqueous solution"*
Adriana Pietropaolo, Diploma thesis of master degree in Chemistry and school of superior studies
Supervisors: E. Rizzarelli, C. Zannoni, L. Muccioli.
Faculty of Science, University of Catania (IT), June 2005.

5 *"Computer simulations of orienting effects of nematic solvents on solutes"*
Maria Beatrice Di Cicco, Master thesis in Industrial Chemistry
Supervisor: C. Zannoni, R. Berardi, L. Muccioli, G. Tiberio.
Faculty of Industrial Chemistry, University of Bologna (IT), March 2006.

6 *"Study of liquid crystalline phases of 4-n-octyl-4' cyanobiphenyl via computer simulations"*
Mattia Felice Palermo, Bachelor thesis in Industrial Chemistry (code 0882)
Supervisors: C. Zannoni, L. Muccioli, A. Pizzirusso.
Faculty of Industrial Chemistry, University of Bologna (IT), October 2009.

7 *"Atomistic simulations of bulk and free standing film smectics"*
Mattia Felice Palermo, Master thesis in Industrial Chemistry (code 0884)
Supervisors: C. Zannoni, L. Muccioli, A. Pizzirusso.
Faculty of Industrial Chemistry, University of Bologna (IT), October 2011.

8 *"Polymer-liquid crystal interface: a molecular dynamics study"*
Federico Bazzanini, Master thesis in Industrial Chemistry (class LM-71)
Supervisors: C. Zannoni, L. Muccioli, M. F. Palermo.
Faculty of Industrial Chemistry, University of Bologna (IT), July 2013.

9 *"Self-assembling and structure of fluorescent organic nanoparticles in pure water and in a water/THF mixture by molecular dynamics simulations"*
Laurie Lescos, Master thesis in Physical Chemistry
Supervisor: L. Muccioli.

Physical Chemistry & Chemical Physics International master program University of Bordeaux (FR), July 2018.

10 *"A study of the trans-cis photoisomerization mechanism of azobenzene in liquid crystals"* Lorenzo Soprani, Master thesis in Industrial Chemistry (class LM-71), Supervisors: C. Zannoni, L. Muccioli, L. Querciagrossa.
Department of Industrial Chemistry, University of Bologna (IT), October 2018.

11 *"Excited State Energy Surfaces of Flexible Emitters for Thermally Activated Delayed Fluorescence"* Panukorn Sombut, Master thesis in Advanced Spectroscopy in Chemistry (class LM-71)
Supervisors: L. Muccioli, R. Berardi, S. Orlandi, A. Arcioni, L. Soprani.
Department of Industrial Chemistry, University of Bologna (IT), July 2019.

12 *"Simulating the aggregation of DNA oligonucleotides"* Silvia Cristofaro, Master thesis in Industrial Chemistry (class LM-71)
Supervisors: S. Orlandi, R. Berardi, L. Muccioli, A. Arcioni, C. Zannoni, L. Querciagrossa.
Department of Industrial Chemistry, University of Bologna (IT), October 2019.

13 *"Computational characterization of carbazole- benzonitrile derivatives for applications in Organic Light Emitting Diodes"* Francesco Rizzo, Master thesis in Industrial Chemistry (class LM-71)
Supervisors: L. Muccioli, S. Orlandi, A. Arcioni.
Department of Industrial Chemistry, University of Bologna (IT), July 2020.

14 *"Simulazioni di dinamica molecolare dell'autoassemblaggio di oligomeri di DNA"* Dario Mazzacurati, Bachelor thesis in Industrial Chemistry (class LM-71)
Supervisors: S. Orlandi, L. Muccioli, S. Cristofaro.
Department of Industrial Chemistry, University of Bologna (IT), Oct 2022.

15 *"Parametrizzazione e validazione di campi di forza polarizzabili per l'acetonitrile"* Carlo Marco Carabini, Master thesis in Industrial Chemistry (class LM-71)
Supervisors: S. Orlandi, L. Muccioli, L. Soprani.
Department of Industrial Chemistry, University of Bologna (IT), Oct 2022.

16 *"Understanding metal oxides as battery materials via theory and experiments: from simple systems to high entropy oxides"* Lucas Francisco Rodríguez Almeida, Master thesis in Advanced Spectroscopy in Chemistry
Supervisors: L. Muccioli, F. Segatta, M. Giorgetti
Department of Industrial Chemistry, University of Bologna (IT), Oct 2023.

**Co-supervisor of PhD theses**

1 *"Molecular Dynamics simulations of liquid crystals and photoresponsive systems"*
Giustiniano Tiberio, PhD thesis in Chemical Sciences
Supervisor: C. Zannoni. Co-supervisors: A. Arcioni, R. Berardi, L. Muccioli.
University of Bologna (IT), 2006 (XIX Italian PhD cycle).

2 *"Structure determination of proteins and peptides in solution: simulation, chirality and NMR studies"*
Adriana Pietropaolo, PhD thesis in Chemical Sciences

Supervisor: C. Zannoni. Co-supervisor: L. Muccioli.
University of Bologna (IT), 2007 (XX Italian PhD cycle).

3 *"Computer simulations of ordering and dynamics in liquid crystals in the bulk and close to the surface"*
Antonio Pizzirusso, PhD thesis in Chemical Sciences
Supervisor: C. Zannoni.
Co-supervisors: R. Berardi, L. Muccioli, M. Ricci.
University of Bologna (IT), 2008 (XXI Italian PhD cycle).

4 *"Complex liquid crystalline systems: a computer simulation and ESR study"*
Isabella Miglioli, PhD thesis in Chemical Sciences
Supervisor: C. Zannoni. Co-supervisors: A. Arcioni, C. Bacchiocchi, L. Muccioli.
University of Bologna (IT), 2009 (XXII Italian PhD cycle).

5 *"Atomistic simulations of liquid crystals in the bulk and at their interfaces"*
Mattia Felice Palermo, PhD thesis in Physical Chemistry
Supervisor: C. Zannoni. Co-supervisor: L. Muccioli.
University of Bologna (IT), 2015 (XXVII Italian PhD cycle).

6 *"Theoretical modeling of advanced polymeric materials for organic electronics"*
Sai Manoj Gali, PhD thesis in Physical Chemistry.
Supervisors: L. Muccioli and F. Castet.
University of Bordeaux (FR), 2014-2017.

7 *"Computing the structural and vibrational properties of polymorphic organic molecular crystals through van der Waals corrected density functional theory and the electronic properties of organic thin films through microelectrostatic calculations."*
Andrea Giunchi, PhD thesis in Physical Chemistry.
Supervisor: R. G. Della Valle; Co-supervisors: E. Venuti, L. Muccioli.
University of Bologna (IT), 2021 (XXXIII Italian PhD cycle).

8 *"Molecular modelling of organic functional materials"*
Lorenzo Soprani, PhD thesis in Physical Chemistry.
Supervisor: L. Muccioli; Co-supervisors: R. Berardi
University of Bologna (IT), 2022 (XXXIV Italian PhD cycle).

9 *"Computer simulations of polymeric functional materials"*
Silvia Cristofaro, PhD thesis in PhD thesis in Physical Chemistry.
Supervisor: S. Orlandi; Co-supervisors: L. Muccioli
University of Bologna (IT), 2024 (XXXVI Italian PhD cycle).

## Publications in peer-reviewed journals

1 R. Berardi, L. Muccioli, C. Zannoni *Can nematic transitions be predicted by atomistic simulations? A computational study of the odd–even effect*
ChemPhysChem **5**, 104-111 (2004)

2 R. Berardi, L. Muccioli, S. Orlandi, M. Ricci, C. Zannoni *Mimicking electrostatic interactions with a set of effective charges. A genetic algorithm*
Chem. Phys. Lett. **389**, 373-378 (2004)

3 R. Berardi, D. Micheletti, L. Muccioli, M. Ricci, C. Zannoni *A computer simulation study of the influence of a liquid crystal medium on polymerization*
J. Chem. Phys. **121**, 123–9130 (2004)

4 R. Berardi, G. Cainelli, P. Galletti, D. Giacomini, A. Gualandi, L. Muccioli, C. Zannoni *Can the $\pi$–facial selectivity of solvation be predicted by atomistic simulation?*
J. Am. Chem. Soc. **127**, 10699-10706 (2005)

5 D. Micheletti, L. Muccioli, R. Berardi, M. Ricci, C. Zannoni *Effect of nanoconfinement on liquid crystal polymer chains*
J. Chem. Phys. **123** 224705 (2005)

6 L. Muccioli, C. Zannoni *A Deformable Gay-Berne Model for the simulation of Liquid Crystals and Soft Materials*
Chem. Phys. Lett. **423**, 1-6 (2006)

7 R. Berardi, A. Costantini, L. Muccioli, S. Orlandi, C. Zannoni *A computer simulation study of the formation of liquid crystal nanodroplets from a homogeneous solution*
J. Chem. Phys. **126**, 044905 (2007)

8 L. Muccioli, R. Berardi, S. Orlandi, M. Ricci, C. Zannoni *Molecular properties and stacking of 1-substituted hexa-alkoxy-triphenylenes*
Theor. Chem. Acc. **117**, 1085-1092 (2007)

9 I. Miglioli, L. Muccioli, S. Orlandi, M. Ricci, R. Berardi, C. Zannoni *A computer simulation of model discotic dimers*
Theor. Chem. Acc. **118**, 203-210 (2007)

10 S. Orlandi, L. Muccioli, M. Ricci, R. Berardi, C. Zannoni *Core charge distribution and self assembly of columnar phases: the case of triphenylenes and azatriphenylenes*
Chem. Cent. J. **1**, 15 (2007)

11 A. Pietropaolo, L. Raiola, L. Muccioli, G. Tiberio, C. Zannoni, R. Fattorusso, C. Isernia, D. La Mendola, G. Pappalardo, E. Rizzarelli *An NMR and Molecular Dynamics investigation of the avian prion hexarepeat conformational features in solution*
Chem. Phys. Lett. **442**, 110-118 (2007)

12 A. Pietropaolo, L. Muccioli, R. Berardi, C. Zannoni *A chirality index for investigating protein secondary structures and their time evolution*
Proteins: Structure, Function, and Bioinformatics **70**, 667-677 (2008)

13 R. Berardi, L. Muccioli, C. Zannoni *Field Response and Switching Times in Biaxial Nematics*
J. Chem. Phys. **128**, 024905 (2008)

14 C. Bacchiocchi, E. Hennebicq, S. Orlandi, L. Muccioli, D. Beljonne, C. Zannoni *A reduced distributed monopole model for the efficient prediction of energy transfer in condensed phases*
J. Phys. Chem. B **112**, 1752-1760 (2008)

15 A. Pietropaolo, L. Muccioli, C. Zannoni, D. La Mendola, G. Maccarone, G. Pappalardo, E. Rizzarelli *Unveiling the role of histidine and tyrosine residues on the conformation of the avian prion hexarepeat domain*
J. Phys. Chem. B **112**, 5182-5188 (2008)

16 R. Berardi, L. Muccioli, S. Orlandi, M. Ricci, C. Zannoni *Computer simulations of biaxial nematics*
J. Phys: Condens. Matter **20**, 463101 (2008)

17 G. Tiberio, L. Muccioli, R. Berardi, C. Zannoni *Towards in silico liquid crystals. Realistic transition temperatures and physical properties for n-cyanobiphenyls via molecular dynamics simulations*
ChemPhysChem **10**, 125-136 (2009)

18 A. Pietropaolo, L. Muccioli, C. Zannoni, E. Rizzarelli *Conformational preferences of the full avian prion protein in solution and its differences with respect to mammals*
ChemPhysChem **10**, 1500-1510 (2009)

19 O. Francescangeli, V. Stanic, S. I. Torgova, A. Strigazzi, N. Scaramuzza, C. Ferrero, I. Dolbnya, T. M. Weiss, R. Berardi, L. Muccioli, S. Orlandi, C. Zannoni *Ferroelectric response and induced biaxiality in the nematic phase of bent-core mesogens*
Adv. Funct. Mater. **19**, 2592-2600 (2009)

20 N. G. Martinelli, M. Savini, L. Muccioli, Y. Olivier, F. Castet, C. Zannoni, D. Beljonne, J. Cornil *Modeling polymer dielectrics/pentacene interfaces: on the role of electrostatic energy disorder on charge carrier mobility*
Adv. Funct. Mater. **19**, 3254-3261 (2009)

21 S. Orlandi, L. Muccioli, M. Ricci, C. Zannoni *Self assembled fullerene walls in di-mesogenic-C60 materials*
Soft Matter **5**, 4484-4491 (2009)

22 Y. Olivier, L. Muccioli, V. Lemaur, Y. H. Geerts, C. Zannoni, J. Cornil *Theoretical Characterization of the Structural and Hole Transport Dynamics in Liquid-Crystalline Phthalocyanine Stacks*
J. Phys. Chem B **113**, 14102-14111 (2009)

23 G. Tiberio, L. Muccioli, R. Berardi, C. Zannoni *How does the $trans \rightarrow cis$ photo–isomerization of azobenzene take place in organic solvents?*
ChemPhysChem **11**, 1018-1028 (2010)

24 A. Pizzirusso, M. Savini, L. Muccioli*, C. Zannoni *An atomistic simulation of the liquid–crystalline phases of sexithiophene*
J. Mater. Chem. **21**, 125-133 (2011)

25 D. Beljonne, J. Cornil, L. Muccioli, C. Zannoni, J.-L. Brédas, F. Castet *Electronic Processes at Organic-Organic Interfaces: Insight from Modeling and Implications for Opto-Electronic Devices*
Chem. Mater. **23**, 591-609 (2011)

26 M. Gonidec, R. Biagi, V. Corradini, F. Moro, V. De Renzi, U. del Pennino, D. Summa, L. Muccioli, C. Zannoni, D. B. Amabilino, J. Veciana *Surface supramolecular organization of a terbium (III) double-decker complex on graphite and its single molecule magnet behavior as studied by XMCD*
J. Am. Chem. Soc. **133**, 6603-6612 (2011)

27 T. A. Papadopoulos, L. Muccioli*, S. Athanasopoulos, A. B. Walker, C. Zannoni, D. Beljonne *Does supramolecular ordering influence exciton transport in conjugated systems? Insight from atomistic simulations*
Chem. Sci. **2**, 1025-1032 (2011) [inside cover]

28 L. Muccioli*, G. D'Avino, C. Zannoni *Simulation of vapor-phase deposition and growth of a pentacene thin film on $C_{60}$ (001)*
Adv. Mater. **23**, 4532-4536 (2011) [frontispiece]

29 P. Sukul, D. Asthana, P. Mukhopadhyay, D. Summa, L. Muccioli, C. Zannoni, D. Beljonne, A. Rowan, S. Malik *Assemblies of Perylene Diimide Derivatives with Melamine into Luminescent Hydrogels*
Chem. Commun. **47**, 11858-11860 (2011)

30 A. Pizzirusso, R. Berardi, L. Muccioli, M. Ricci, C. Zannoni *Predicting surface anchoring: molecular organization across a thin film of 5CB liquid crystal on silicon*
Chem. Sci. **3**, 573-579 (2012)

31 M. Lamarra, L. Muccioli*, S. Orlandi, C. Zannoni *Temperature dependence of charge mobility in model discotic liquid crystals*
PhysChemChemPhys **14**, 5368-5375 (2012) [front cover]

32 A. Pizzirusso, M. B. Di Cicco, G. Tiberio, L. Muccioli, R. Berardi, C. Zannoni *Alignment of small organic solutes in a nematic solvent: the effect of electrostatic interactions*
J. Phys. Chem. B **116**, 3760-3771 (2012)

33 A. C. J. Weber, A. Pizzirusso, L. Muccioli, C. Zannoni, W. L. Meerts, C. A. de Lange , E. E. Burnell *Efficient analysis of highly complex Nuclear Magnetic Resonance spectra of flexible solutes in ordered liquids by using Molecular Dynamics*
J. Chem. Phys. **136**, 174506 (2012)

34 J. Cornil, S. Verlaak, N. G. Martinelli, A. Mityashin, Y. Olivier, T. Van Regemorter, G. D'Avino, L. Muccioli, C. Zannoni, F. Castet, D. Beljonne, P. Heremans *Exploring the Energy Landscape of the Charge Transport Levels in Organic Semiconductors at the Molecular Scale*
Acc. Chem. Res. **46**, 434-443 (2013)

35 M. F. Palermo, A. Pizzirusso, L. Muccioli, C. Zannoni *An atomistic description of the nematic and smectic phases of 4-n-octyl-4′cyanobiphenyl (8CB)*
J. Chem. Phys. **138**, 204901 (2013) [front cover]

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*NOTE: My name underlined indicates my role as first author or first author of the group. An asterisk * indicates my role as corresponding author.*

## Other publications

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## Scientometric data

*Current data from Web of Science, Jun 26, 2024:*

| | |
|---|---|
| Results found | 104 |
| Hirsch index | 35 |
| Total citations | 4402 |
| Citing articles | 3147 |

*Current data from Google Scholar, Jun 26, 2024:*

| | |
|---|---|
| Hirsch index | 38 |
| i10-index | 87 |
| Total citations | 5580 |

## Oral communications at national and international congresses

1 *"MD simulation of the odd-even effect in liquid crystals"*
International School of Liquid Crystals, 6th course
Erice (IT), 25–28/10 2001

2 *"Study of liquid crystalline properties of imino cinnamates"*
Workshop "La Nuova Convenzione CINECA/INSTM"
CINECA, Casalecchio di Reno (IT), 6/9 2002

3 *"Simulation of the diastereofacial solvation of (R)-phenyl-propanal in alkanes"*
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Siena (IT), 18–19/12 2003

4 *"Simulation study of the mesogenic properties of triphenylenes"*
VI meeting nazionale della Società Italiana Cristalli Liquidi (SICL)
Ischia (IT), 2–5/6 2004

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6 *"Self-assembling semiconductors: structural and charge transport properties of columnar phthalocyanines"*
CERC3 Young Chemists Workshop "Modeling of complex systems"
Perugia (IT), 1–4/5 2008 [invited]

7 *"Physical properties of n-cyano biphenyls from Molecular Dynamics simulations"*
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Erice (IT), 27/10–1/11 2008

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$23^{rd}$ International Liquid Crystal Conference
Kraków (PL), 11-16/7 2010 [invited]

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Pisa (IT), 22-23/2 2012

15 *"Simulating self-assembling materials with molecular and atomistic models"*
6th WINTERSCHOOL ON ORGANIC ELECTRONICS - Self-Assembly and Hybrid Devices
Planneralm (AT) 4-9/3 2012 [invited]

16 *"Growth of pentacene thin films on SiO2 by simulating organic vapor deposition"*
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17 *"Atomistic molecular dynamics simulations of cyanobiphenyls: a test bench for liquid crystal theories"*
Workshop "Analytical and Computational Paths from Molecular Foundations to Continuum Descriptions" Isaac Newton Institute for Mathematical Sciences, Cambridge (UK), 18-22/3 2013 [invited]

18 *"Microscopic origin of efficient charge separation in organic P3HT:PCBM solar cells"*
XLI Congresso Nazionale di Chimica Fisica, Alessandria (IT), 23-27/6 2013

19 *"Surface anchoring of liquid crystals from atomistic simulations"* 5th European Symposium on Computing II-Conjugated Compounds
Linköping (SE), 5-7/2 2014

20 *"Charge separation in organic solar cells: strategies to counter Coulomb interaction"* Winter Modeling 2014, Modena (IT), 13-14/3 2014

21 *"Modelling organic/organic interfaces: structure and energy levels"* ICOE satellite meeting "Predictive Modelling and Computational Methods for Organic Electronics"
Modena (IT), Jun 10/6, 2014 [invited]

22 *"Charge dissociation at interfaces between discotic liquid crystals: the surprising role of column mismatch"* $25^{th}$ International Liquid Crystal Conference Dublin (EI), 29/6-4/7 2014

23 *"Microscopic modelling of interfaces for plastic electronics: from morphology to electronic properties"* International workshop on organic and graphene electronics and spintronic (Elecspin 2015)
Barcelona (ES), 12-13/3 2015 [invited]

24 *"Interfaces between organic semiconductors: from structure to charge separation"* Collaborative Science & Technology Workshop: "Beyond the Standard: DFT Approaches for the Simulation of Next-Generation Electronics" London (UK), 13-14/4 2015

25 *"Molecular simulations as a tool for predicting the physical properties of organic materials"* First Workshop of Physical-Chemistry and Chemical-Physics International Master, Talence (FR), 22-23/6 2017 [invited]

26 *"Modeling the electromechanical response of rubrene single crystals"* CECAM Workshop "Multiscale modelling of organic semiconductors: from elementary processes to devices" Grenoble (FR), 12-15/9 2017

27 *"Modeling the electromechanical response of rubrene single crystals"* ERC AdG – Barone – DREAMS: final meeting "Advances in computational modelling: from isolated molecules to soft matter" Pisa (IT), 29/11-2/12 2017

28 *"Atomistic simulations of thin films of organic molecules (liquid crystals on surfaces)"* IUPAC MODSIM workshop 2018 "Modelling and simulation of large molecules: can we disentangle time- and length-scales?" Milano (IT), 20/2/2018 [invited]

29 *"Modeling the electromechanical response of rubrene single crystals"* e-MRS Spring Meeting 2018 Strasbourg (FR), 18-22/6/2018

30 *"Interfacial effects from simulations of materials for organic electronics"* ITN "Spins in Efficient Photovoltaic devices based on Organic Molecules" school Mons (BE), 10/4/2019 [invited]

31 *"Atomistic simulations of organic crystal growth from vapor"* CECAM Workshop "Fabrication processes and molecular organization in organic thin films: theory and simulation meet experiments" Lecco (IT), 17-20/7 2019 [invited]

32 *"Dynamic fluctuations of nonlinear optical response of organic molecules"* XLVIII National Congress of Physical Chemistry Genova (IT), 6/7 2022

## Oral communications at research projects meetings

1 *"Solvent effects in the trans→cis isomerization mechanism of azobenzene"*
RTN Functional Liquid-Crystalline Elastomers Meeting
Strasbourg (FR), 23–25/9 2004

2 *"Interaction potentials for discotics and oligofluorenes"*
NAIMO [1] 6month Meeting
Bruxelles (BE), 13–15/10 2004

3 *"Interaction potentials for triphenylenes, oligofluorenes and phthalocyanines"*
NAIMO 12month Meeting
Cambridge (UK), 4–6/4 2005

4 *"Phase behaviour of model discotic mesogens"*
NAIMO 18month Meeting
Manchester (UK), 12–14/10 2005

5 *"Nanoconfined radical polymerization of a liquid crystalline monomer"*
NAIMO 24month Meeting
Mons (BE), 12–14/4 2006

6 *"Progress on simulations of potential liquid crystalline semiconductors"*
NAIMO 30month Meeting
Eindhoven (NL), 11–13/11 2006

7 *"Overview of the simulation studies within Naimo"*
NAIMO 36month Meeting
Napoli, 2–4/4 2007

8 *"A reduced distributed monopole model for energy transfer"*
MODECOM [2] midyear meeting
Bath (UK), 14–15/5 2007

9 *"Molecular Dynamics simulations for molecular electronics"*
MODECOM annual review meeting
Metz (FR), 4/9 2007

10 *"Insights on the microscopic organization of liquid crystalline semiconductors"*
NAIMO 42month Meeting
Barcelona (ES), 3–5/10 2007

11 *"Computational studies of NAIMO materials and processes (WP3, WP4)"*
NAIMO 48month Meeting
Leuven (BE), 3–5/3 2008

[1] NAIMO: EU FP6 Integrated Project "NAnoscale Integrated processing of self-organizing Multifunctional Organic materials" IP 500355 (2004-2008)

[2] MODECOM: EU FP6 STREP "Modelling Electro-active Conjugated Materials at the Multiscale" NMP3-CT-2006-016434 (2006-2010)

12 *"Organic semiconductor interfaces"*
MODECOM midyear meeting
Strasbourg (FR), 10/4 2008

13 *"A nanoscale view of organic semiconductors"*
MODECOM annual review EU-US meeting
Atlanta (US), 18/7 2008

14 *"Phase organization of model Acceptor-Donor-Acceptor mesogens"*
OneP [3] 6month review meeting
Mons (BE), 1–2/7 2009

15 *"Molecular organization of indenofluorene oligomers"*
MODECOM final review meeting
Copenhagen (DK), 8/9 2009

16 *"Atomistic simulation of pentacene vapor growth on $C_{60}$"*
MINOTOR [4] 6month meeting
Ludwigshafen (DE), 18/11 2009

17 *"Liquid crystalline phases of sexithiophene"*
MINOTOR 12month meeting
Linköping (SE), 20/5 2010

18 *"Simulation of the sexi-3-hexyl-thiophene / C60 interface"*
ONEP 18month meeting
Leuven (BE), 28-30/6 2010

19 *"First simulations of F4-TCNQ crystals"*
MINOTOR 18month meeting
Leuven (BE), 18/11 2010

20 *"Modeling Self-Assembled-Monolayers on silica"*
MINOTOR 24month meeting
Bologna (IT), 26/5 2011

21 *"Deposition of pentacene on silica"*
MINOTOR 30month meeting
Enschede (NL), 17/11 2011

22 *"Theoretical modeling at the frontier between soft matter and organic electronics"*
Journées scientifiques AMADEus[5]
Bordeaux (FR), 11-12/12 2014

23 *"From molecules to organic electronics devices: a bottom-up computational approach"*
AMADEus international advisory panel meeting
Bordeaux (FR), 19/1 2015

24 *"Methodological advances in modeling materials for all-organic LEDs"*
Journée scientifique AMADEus
Bordeaux (FR), 24/6 2015

25 *"Activity report TRC1 organic electronics WP4 theory"*
Journées scientifiques AMADEus
Bordeaux (FR), 19-20/1 2016

26 *"About charge delocalization in fullerene derivatives"*
Journées scientifiques AMADEus
Bordeaux (FR), 23-24/6 2016

[3] OneP: EU FP7 Integrated Project "Organic nanomaterials for Electronics and Photonics" IP 212311 (2009-2011)

[4] MINOTOR: EU FP7 small or medium scale focused research project "Modelling of electronic processes at interfaces in organic-based electronic devices" CP-FP228424-2 (2009-2012)

[5] AMADEus: Cluster of excellence "Advanced Materials by Design", French national grant ANR-10-LABX-0042-AMADEus

## Seminars at research institutes

1 *"Molecular models for liquid crystals simulations"*
Laboratory for Chemistry of Novel Materials
Mons (BE), 3/2/2005

2 *"Local chirality of proteins: a new tool for structural bioinformatics"*
Laboratory for Chemistry of Novel Materials
Mons (BE), 7/11/2007

3 *"Investigating soft-matter self-assembly with computer simulations"*
Institut des Sciences Moléculaires
Bordeaux (FR), 27/9/2011

4 *"Molecular dynamics simulations for organic electronics: realism as a key to electronic properties"*
Cavendish Laboratory, OptoElectronics group
Cambridge (UK), 19/3/2013

5 *"Computational Chemists: Who we are and what we do"*
Departamento de Quimica Fisica
Alicante (ES), 26/11/2013

6 *"Simulating organic materials at technologically-relevant interfaces: morphology and electronic properties"*
Unité de Formation et de Recherche (UFR) de Chimie
Bordeaux (FR), 17/12/2013

7 *"Charge separation in organic solar cells: strategies to counter Coulomb interaction"*
Centre Interdisciplinaire de Nanoscience de Marseille
Marseille (FR), 18/4/2014

8 *"Microscopic modelling of interfaces for plastic electronics: from morphology to electronic properties"* Laboratoire de Chimie des Polymères Organiques (LCPO)
Bordeaux (FR), 1/4/2015

9 *"Simulating organic crystals: from structure to electronic properties"* Laboratory for Chemistry of Novel Materials
Mons (BE), 21/10/2015

10 *"Multi-dimensional charge transport in helical foldamers"* Laboratory for Chemistry of Novel Materials
Mons (BE), 11/9/2018

11 *"Dynamic fluctuations of nonlinear optical response of organic molecule"* Laboratory for Chemistry of Novel Materials
Mons (BE), 7/6/2022

12 *Series of lectures "Everything You Always Wanted to Know About Molecular Dynamics"*
Invited FNRS professor, University of Mons, 2022

13 *"Atomistic modelling of materials for organic electronics"* Scuola di Dottorato in Scienze Chimiche
Università di Bologna, 26/5/2023

14 *"Atomistic modelling of materials for organic electronics"* Dipartimento di Scienze Chimiche, della Vita e della Sostenibilità Ambientale
Università di Parma (IT), 23/7/2023

15 *"Atomistic modelling of materials for organic electronics"* Doctoral School in Chemistry
Universidad de Malaga (ES), 19/2/2024

## Seminars for High School Students

1 *"La chimica dei materiali fuori dal laboratorio: progettare al computer materiali che ancora non esistono"*
online seminar, 29/3/2021, 24/2/2022

2 *"La chimica dei materiali fuori dal laboratorio: progettare materiali che ancora non esistono. Modellazione al computer di nuovi materiali."*
Introductory lecture with practical computer examples, Faenza, 30/5/2022; 14/11/2023; 8/2/2023; 20/11/2023; 1/2/2024

## Successful projects

1 ISCRA: Several Italian SuperComputing Resource Allocation projects (http://hpc-iscra.cineca.it/) (2010, 2011, 2012)

2 DEISA Extreme Computing Initiative 2008-2009 (DECI): "Phase Transitions in discotic semiconductors"
(∼800K core hours, www.deisa.eu/science/deci)

3 DECI 2009-2010: "Azobenzene photoisomerization in liquid crystal mesophases" (∼1M core hours)

4 SAMSUNG GRO 2013: I was awarded a shared 100K $ grant as co-investigator for the project "Bottom-up computational design of efficient blue emitting materials for OLEDs", alongside my colleagues Juan-Carlos Sancho-García (University of Alicante) and Yoann Olivier (University of Mons).

5 In April 2014, I was awarded a French LABEX Junior chair (∼ 600K €) for developing my three years research project Mol2Dev "From molecules to organic electronics devices: a bottom-up computational approach" at the University of Bordeaux.

6 In November 2014, our proposal for an UCL French Embassy workshops 2014-15 on "Beyond the Standard: DFT Approaches for the Simulation of Next-Generation Electronics" was accepted and financed with ∼ 5K € (with D. R. Bowler, F. Castet, C. O'Rourke, L. Truflandier, A. Fritsch)

7 In April 2015, the project "Mise en ordre de nanodomaines à base de copolymères à blocs: une approche guidée image de la guérison des défauts" was financed for 40K € (with K. Aïssou, C. Dobrzynski, P. Ramet, G. Vignoles)

8 In May 2015, the M-ERA.NET project "Modelling Photoswitchable Organic-Graphene Hybrids" was accepted for funding, financed with ∼ 120K € for the Bordeaux unit.
(myself, F. Castet, and L. Truflandier). International partners are D. Beljonne (University of Mons), W. Wenzel (Karlsruhe Institute of Technology), P. Samorì (ISIS Strasbourg).

9 In January 2017, the PRC Royaume-Uni CNRS-Royal Society project "Simulation of optical properties of polymers using linear-scaling DFT approaches" was funded with 5K € (with D. R. Bowler, F. Castet, L. Truflandier)

10 In December 2018, our PRIN project "From natural to artificial light-harvesting systems: unveiling fundamental processes towards a bio-inspired materials design" (HARVEST) was financed by the Italian Ministry of Research (MIUR). The Bologna unit

was awarded of about 105K €. Italian partners are G. Cerullo (Politecnico Milano, coordinator), Benedetta Mennucci (University of Pisa), Tullio Scopigno (University La Sapienza, Rome), Luca Dall'Osto (University of Verona), Deborah Prezzi (National Research Council, Modena).

11 In March 2023 the project "Getting the MOST out of the sun" was selected for funding by the International Foundation Big Data and Artificial Intelligence for Human Development (IFAB) with 100K €. Partnership with the company E4 Engineering.

## Periods spent in foreign laboratories

- 20/1-9/4 2005; 5-9/11 2007, 22/6-2/7 2009, 15-17/11 2010, 1-8/2 2012, 28/5-1/6 2012, 23-26/9 2013, 23-25/6 2014, 19-23/10 2015, 6-9/6 2017, 10-12/9 2018, 7-10/7 2022 "Laboratory for Chemistry of Novel Materials", Mons (BE)
- 25-28/11 2013 "Departamento de Quimica Fisica", Alicante (ES)
- 29/11-8/12 2016, 10-18/1 2017, 7/3-6/4 2017, 9-13/10 2017, 25/4-4/5 2018, 12-19/12/2018, 25-29/3 2019, 25-29/10 2021 "Institut des Sciences Moléculaires", Talence (FR)

## Services to the scientific community

- "A Scientific Journey in the World of Liquid Crystals and Beyond" (International School of Liquid Crystals, XXV course)
  Erice (IT), 7-10/10 2018; organizing committee.
- "XLVI Congresso Nazionale della Divisione di Chimica Fisica della Società Chimica Italiana"
  Bologna (IT), 25-28/6 2018; organizing committee.
- Series of symposia "Computing II-Conjugated Compounds":
  board member, and organizer of the 2016 symposium, Bordeaux (FR), 12-13/2/2016 (https://sites.google.com/site/cpic2016/).
- OneP Spring School "Organic nanomaterials for Electronics and Photonics" (International School of Liquid Crystals, XVII course)
  Erice (IT), 13-20/4 2010; organizing committee.
- workshop "Transport and Molecular Organisation in Organic and Bioorganic Electronics"
  Bologna, 14/1 2009; organizing committee.
- Regular or casual referee for several international journals ( ACS Appl. Mater. Interfaces, ACS Appl. Nanomater., Adv. Interf. Mater., Adv. Theor. Simul., App. Surf. Sci., Braz. J. Phys., Chem. Mater., Chem. Papers, Chem. Phys., Chem. Phys. Lett., ChemPhysChem, Comput. Mater. Sci., Cryst. Growth Des., Dyes Pigm., Front. Chem., J. Chem. Phys., J. Chem. Theory Comput., J. Mater. Chem. C, J. Mol. Struct., J. Photochem. Photobio. A, J. Phys. Cond. Matter, J. Phys. Chem., J. Phys. Chem. Lett., Langmuir, Liq. Cryst., New J. Chem., Mater. Chem. Phys., Mol. Cryst. Liq. Cryst., Nanoscale, Nanoscale Res. Lett., Org. Electron., PhysChemChemPhys, Phys. Scr., Phys. Rev. Appl., Phys. Rev. B, Phys. Rev. E, Phys. Rev. Mater., Phys. Rev. X, RSC Adv., Theor. Chem. Acc. ).

See also https://www.webofscience.com/wos/author/record/615239 .

- Member of jury for the obtainment of the degree of Doctor of Philosophy:

  2015 Gabin Fabre, PhD in Pharmacy, University of Limoges (FR)

  2019 Cristian D'Urso, PhD in Chemistry, University of Calabria (IT)

  2021 Manuel Reche Tamayo, PhD in Chemistry, University of Mons (BE) / Sorbonne University (FR)

  2021 Mila Miletic, PhD in Physics, Humboldt University Berlin (DE)

  2021 Sebastien Hoyas, PhD in Chemistry, University of Mons (BE)

  2021 Laurie Lescos, PhD in Chemistry, University of Bordeaux (FR)

  2023 Francesca Miglioli, Dang Khoa Andrea Phan Huu, Marianna Potenza, PhD in Chemistry, University of Parma (IT)