Curriculum Vitae

EMILIO LORINI

Postdoc in Computational Chemistry

PERSONAL DETAILS

Full name:	Emilio Lorini
Date of birth:	13/05/1996
Place of birth	Borgo San Lorenzo, Florence, Italy
Nationality:	Italian
Work address:	Via Piero Gobetti, 85, 40129 Bologna BO Italy
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CURRENT POSITION

Postdoctoral Researcher — 01/2025 – ongoing

Department of Industrial Chemistry "Toso Montanari" – University of Bologna (IT)

Grant title: Organic Semiconductor Crystal Structure Prediction on Surfaces

Project: EXTended Model of Organic Semiconductors (EXTMOS)

Supervisor: Prof. Luca Muccioli

I investigate the factors underlying the molecular growth and electronic functioning of organic semiconductors in the thin film phase, with particular focus on the influence of the substrate. Specifically, I perform simulations of *physical vapor deposition*, *free energy calculations*, *surface crystal structure prediction*, and *charge transport* simulations in disordered films. Other research interests include *conformational analysis* of light-driven molecular rotors and *excited state calculations* for thermally activated delayed fluorescence molecules.

EDUCATION

PhD in Future Earth, Climate Change and Societal Challenges — 01/2022 – 12/2024

Department of Industrial Chemistry "Toso Montanari" – University of Bologna (IT)

Specialization: Physical and Theoretical Chemistry

Thesis: "*From crystalline growth to charge transport: simulations of organic semiconductor thin films for sustainable electronics*"

Supervisor: Prof. Luca Muccioli

Master's degree in Chemistry — 09/2019 – 10/2021

Department of Chemistry "Giacomo Ciamician"- University of Bologna (IT)

Specialization: Synthesis Methodologies and Bioorganic Chemistry.

Thesis: "*Testing the impact of MM description and sampling modes in QM/MM excited state calculations*"

Supervisors: Prof. Marco Garavelli ; Prof. Leticia González

Final grade: 110/110 cum laude

Bachelor's degree in Chemistry — 09/2015 – 04/2019
Department of Chemistry "Ugo Schiff" - University of Florence (IT)

Thesis: "*Metabolomics via ^{1}H-NMR of patients with polyposis and colon cancer*"

Supervisors: Prof. Claudio Luchinat ; Prof. Leonardo Tenori

Final grade: 107/110

Secondary School Diploma — 09/2010 – 07/2015
Liceo Scientifico "Giotto Ulivi" – Borgo San Lorenzo, Florence (IT)

RESEARCH PERIODS

Visiting Researcher (during PhD) — 05/2024
CNR-ICCOM – Pisa (IT)

Theme: Calculation of electronic couplings in disordered structures

Tutor: Dr. Samuele Giannini

Using the fast Analytic Overlap Method (AOM), I calculated transfer integrals in large-scale disordered molecular structures adsorbed on surfaces and evaluated the relative static and dynamic disorder of the distribution. These electronic parameters were used to simulate charge transport with a hopping model.

Visiting Researcher (during PhD) — 01 – 07/2023
Heliatek GmbH R&D – Dresden (DE)

Theme: Morphological study for organic solar cell applications

Tutor: Dr. Karsten Walzer

During my stay in Heliatek, producer and developer of organic solar cells (OSCs), I wrote a Python interface (MYTHOS) for the morphological search of prototype molecules for photovoltaic applications. The program performs MD calculations with NAMD software and evaluates the preferential crystalline arrangements of molecular aggregates grown on flat surfaces.
I also gained practical experience of PVD process for the construction of solar cells and subsequent optical absorption and efficiency measurements.

Erasmus+ Traineeship (during Master) — 03 – 07/2021
Institute for Theoretical Chemistry – University of Vienna (AT)

Theme: Excited states dynamics of solvated chromophores

Supervisor: Prof. Leticia González

Trajectory surface hopping (TSH) calculations within a QM/MM scheme for the description of the photochemical decay of solvated chromophores (guanine, fulvene). Evaluation of the excited state population dependence over the MM description, through the test of several water force fields, and over the starting geometries of the TSH dynamics, through the employment of three different generation methods.

Erasmus+ Traineeship (Post-Graduate) 05 – 08/2019
Faculty of Engineering – University of Porto (PT)

Theme: Sampling and analysis of environmental samples

Supervisor: Prof. Nuno Ratola

Environmental sampling campaigns in coastal areas for biological samples (soil and vegetation). Analytical methods for the extraction of semi-volatile organic compounds: sonication and gas chromatography-mass spectrometry (GC/MS).

University Internship (during Bachelor) 01 – 04/2019
CERM – University of Florence (IT)

Theme: Metabolomic analysis of biological samples

Supervisor: Prof. Claudio Luchinat

I analyzed the metabolomic fingerprint of many biological samples of patients affected by colorectal cancer. Metabolite detection was performed with ^{1}H-NMR technique and statistical analysis: multivariate (PCA and OPLS) and univariate. The R programming language was used for the analysis.

RESEARCH EXPERTISE

Molecular Dynamics for Crystalline Growth on Surfaces

- Growth mechanism evaluation and morphological analysis
- Free energy profiles and surfaces (ABF method)
- Surface energy through contact angle simulations

Surface Crystal Structure Prediction

- Developer of a new predictive tool for molecular crystals: MYTHOS
- MD and systematic generation of surface aggregates
- Layer-sequential polymorph evaluation

Charge/Exciton Transport in Molecular Thin Films

- Electronic and excitonic couplings
- Site energies and polarization effects:
  - Microelectrostatics
  - Substrate polarization modelled through FF and periodic DFT
- Kinetic Monte Carlo for single or multiple carriers

Light-Driven Molecular Rotors

- DFT calculations of potential energy surfaces and energetic barriers
- TD-DFT excited state optimizations

Thermally Activated Delayed Fluorescence in Liquid Crystals

- Excited state characterization (LE / CT) of columnar aggregates

Trajectory Surface Hopping for Excited State Dynamics

COMPUTER SKILLS

Operating systems: Linux, Windows

Programming languages: Python, Bash, Fortran

Software:

Computational Chemistry: NAMD, Gaussian, ORCA, Q. ESPRESSO, GULP

Molecular Visualization: VMD, Molden, Mercury, GaussView, Avogadro

Graphical tools: gnuplot, matplotlib, Office

LANGUAGES

Italian: Mother tongue

English: Advanced C1 (assessed through Erasmus+ program)

Spanish: Basic A1 (assessed through Erasmus+ program)

TUTORING & SUPERVISION

Teaching Tutor 2022 –
Rimini Campus - University of Bologna

Laboratory assistant in Physical Chemistry Laboratory of Chemistry bachelor's degree during three academic years.

Student Supervision 2024 –
Department of Industrial Chemistry – University of Bologna

3. Irene Mondadori Monesi (Master student)
   Conformational characterization of photoactivated molecular rotors

2. Dario Mazzacurati (Master student)
   Simulation of thermally activated delayed fluorescence in liquid crystals
   Thesis co-supervisor

1. Mariano Migliozzi (Visiting master student)
   Simulation of dopant insertion in adsorbed semiconducting polymers

University Orientation Day 2024-
Faenza Campus - University of Bologna

Co-organizer of university orientation lectures on computational chemistry for high school students.

Private Lessons of General Chemistry 2013 – 2020
For high school and university students.

CONFERENCES & SEMINARS

1. Oral presentation – Gonzaléz Research Group, University of Vienna (AT) 2021
   QM/MM in excited state dynamics. Is it waterproof?

2. Poster presentation – **12th CπC Symposium**, Grenoble (FR) 2022
   Testing the impact of sampling modes in excited state QM/MM calculations

3. Oral presentation – Laboratory for Chemistry of Novel Materials, University of Mons (BE) 2022
   Simulating homogeneous and heterogeneous vapor depositions of pentacene and perfluoropentacene on graphite: analysis of their crystal growth

4. Oral presentation – **13th CπC Symposium**, Madrid (ES) 2023
   Simulation of pentacene, perfluoropentacene, and their 1:1 blend deposited on graphite: analysis of their crystal growth

5. Oral presentation – **14th CπC Symposium**, San Sebastián (ES) 2024
   MYTHOS: Morphological surveY for THin-films of Organic Semiconductors

6. Oral presentation – **CHITEL**, Namur (BE) 2024
   Simulation of pentacene, perfluoropentacene, and their 1:1 blend deposited on graphite: analysis of their crystal growth

7. Oral presentation – **15th CπC Symposium**, Siena (IT) 2025
   Simulating hole transfer through pentacene grain boundaries
   Prize for **Best Oral Presentation** awarded by InSiliBio

8. Poster presentation – **WATOC**, Oslo (NO) 2025
   Simulating hole transfer through pentacene grain boundaries

List of Publications

† First author(s), * corresponding author(s)

1. D. Avagliano,†* E. Lorini, L. Gonzàlez*
   Sampling Effects in QM/MM Trajectory Surface Hopping Nonadiabatic Dynamics
   Phil. Trans. R. Soc. A, **2022**, 380 (2223), 20200381, https://doi.org/10.1098/rsta.2020.0381

2. E. Lorini,† L. Soprani, L. Muccioli*
   Cocrystal Growth in Organic Semiconductor Thin Films: Simulation of Pentacene, Perfluoropentacene, and Their 1:1 Blend Deposited On Graphite
   Adv. Th. Sim., **2023**, 6 (7), 2300080, https://doi.org/10.1002/adts.202300080

3. F. Nicoli,† C. Taticchi,† E. Lorini, S. Borghi, F. Aleotti, S. Silvi, A. Credi, M. Garavelli, L. Muccioli,* M. Baroncini,* M. Curcio*
   Wavelength-Steered Unidirectional Rotation In An Autonomous Light-Driven Molecular Motor
   Nat. Chem., **2024**, [under review], https://doi.org/10.26434/chemrxiv-2024-03sk0

4. E. Lorini,†* K. Walzer, M. Pfeiffer, L. Muccioli
   MYTHOS: A Python Interface for Surface Crystal Structure Prediction of Organic Semiconductors
   J. Chem. Inf. Model., **2025**, [published online], https://doi.org/10.1021/acs.jcim.5c00669

5. M. Bouajhine,† E. Lorini,† S. Giannini,†* S. Frederix, K. Walzer, M. Levichkova, G. Mattersteig, M. Pfeiffer, E. Bittrich, P. Uhlmann, V. Lemaur, K. Vandewal, P. Brocorens, L. Muccioli, D. Beljonne*
   On the Design of Steep Optical Absorbers for Vacuum-Processed Organic Solar Cells: One Isopropyl Group Makes the Difference
   Adv. Funct. Mater., **2025**, [under review]

6. E. Lorini, S. Giannini, G. D'Avino, L. Muccioli
   Simulating Accurate Hole Transport in Disordered Pentacene Films Near the Surface Interface
   [in preparation]

7. C. Albonetti, E. Lorini, L. Muccioli
   Surface Energy–Dependent Climbing Barriers of α-Sexithiophene on Silica: Insights from Vapor Depositions and Molecular Simulations
   [in preparation]

8. E. Lorini, L. Muccioli
   Diindenoperylene Growth Mechanisms on Silica: Molecular Dynamics Insights into Morphology and Orientation
   [in preparation]

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