Curriculum Vitae

EMILIO LORINI

Postdoc in Computational Chemistry

PERSONAL INFORMATION

Full name: Emilio Lorini
Date of birth: 13/05/1996
Place of birth Borgo San Lorenzo, Florence (IT)
Nationality: Italian
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CURRENT POSITION

Postdoctoral Researcher — 01/2025 – ongoing
Industrial Chemistry Department – University of Bologna (IT)

Title: Organic Semiconductor Crystal Structure Prediction on Surfaces

Supervisor: Prof. Luca Muccioli

Funds: MARGINE_EXTMOS

I perform Molecular Dynamics (MD) calculations to investigate the factors underlying the growth and functioning of organic semiconductors in thin film phase. Some examples are simulations of physical vapor deposition (PVD), free energy calculations of surfaces, analysis of the growth mechanism, crystal structure prediction and charge transport simulations in deposited structures.

EDUCATION

PhD in Future Earth, Climate Change and Societal Challenges — 01/2022 – 12/2024
Industrial Chemistry Department – University of Bologna (IT)

Specialization: **Physical and Theoretical Chemistry**

Theme: Simulations of structure and physical properties of organic semiconductors films for green applications

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

Supervisor: Prof. Luca Muccioli

Funds: ESF+ (REACT-EU)

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 EXPERIENCE

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

Theme: Calculation of electronic couplings in grain boundaries

Tutor: Dr. Samuele Giannini

I performed Quantum Mechanical (QM) calculations to evaluate the electronic parameters necessary to simulate charge transport and optical properties in organic semiconductor deposited structures characterized by the presence of grain boundaries.

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 computational code in Python3 for the morphological search of new prototype molecules for photovoltaic applications. The program interfaces MD calculations, performed with NAMD software, with subsequent analysis of the preferential crystalline arrangement of molecular aggregates growing 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

I performed calculations of trajectory surface hopping (TSH) method within the QM/MM scheme for the description of the photochemical decay of solvated reference chromophores. I evaluated the dependence over the MM description, through the test of many water Force Fields (FF), and over the starting geometries of the TSH dynamics, through the employment of 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

Participation in environmental sampling campaigns in coastal areas and for other biological samples (soil and vegetation) and use of sampling techniques for biogas. Training in analytical methodologies for the extraction of semi-volatile organic compounds (VOCs): sonication, Quechers and gas chromatography coupled to 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 mentioned analysis.

TEACHING EXPERIENCE

Teaching Tutor for Physical Chemistry Laboratory 2022 – 2024
Rimini Campus - University of Bologna

I worked as an assistant in Physical Chemistry Laboratory of bachelor's degree in "Chemistry and Technologies for the Environment and Materials". Lessons are held in October / November, and I assisted for three academic years.

University Orientation Day 2024
Faenza Campus - University of Bologna

I assisted in the organization of a university orientation day on computational chemistry for high school students.

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

LANGUAGES

Italian: Native
English: Advanced (C1)

DIGITAL SKILLS

Operating systems: Linux, Windows

Programming languages:

Very good knowledge of Python and Bash. Basic knowledge of Fortran

Software:

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

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

Graphical tools: gnuplot, matplotlib, Office

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 2024**, 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

List of Publications

1. D. Avagliano,* E. Lorini, L. Gonzàlez*
   Sampling Effects in QM/MM Trajectory Surface Hopping Nonadiabatic Dynamics
   Phil. Trans. R. Soc. A, **380** (2223), 20200381 (2022), 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., ***6*** (7), 2300080 (2023), 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., [under review] (2024), 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
   JCIM, [submitted] (2025)

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
   JACS, [submitted] (2025)

6. E. Lorini, S. Giannini, G. D'Avino, L. Muccioli
   Simulation of charge transport through grain boundaries
   [in preparation]

7. E. Lorini, L. Muccioli
   Diindenoperylene growth on silica through vapor deposition simulations
   [in preparation]