Curriculum Vitae Maria Letizia Merlini

Education

2016 – 2022: **PhD in Science (Computational Chemistry and Biochemistry)**
École Polytechnique Fédérale de Lausanne (EPFL) - Lausanne, Switzerland
Advisor: Prof. Ursula Röthlisberger
"Computational Studies of the Proton-Coupled Metal Ion Transport in the SLC11/NRAMP Family of Transporters"

2013 – 2016: **Master's degree in chemical science, LM-54**
Università degli Studi di Perugia - Perugia, Italy
Grade: 110/110 cum Laude
Advisor: Prof. Paola Belanzoni
"Theoretical study of a Bio-Inspired Mn(II) Complex with Catalase-like Antioxidant Activity"

2006 – 2013: **Bachelor Degree in Chemistry, L-27**
Università degli Studi di Perugia – Perugia, Italy
Grade: 110/110
Advisor: Prof. Paola Belanzoni
"Theoretical study of an Iridium-based EDTA Catalyst for Water Oxidation"

Participation and Contributions to Schools and Conferences

- Poster communication at the **"Frontiers and Challenges of Computing Metals for Biochemical, Medical and Technological Applications" CECAM Workshop**, July 11-13 2018, CECAM-FR-MOSER, Paris (FR). Poster title: "Computational study of the coupled H^+/Mn^{2+} transport mechanism in the SLC11/NRAMPs family of transporters";

- Participation to the **"Physiological role of ions in the brain: towards a comprehensive view by molecular simulation" CECAM Workshop**, May 21-23 2018, Scuola Normale Superiore, Pisa (IT);

- Participation to the **"Hybrid Quantum Mechanics/Molecular Mechanics (QM/MM) Approaches to Biochemistry and Beyond" CECAM School**, May 15-19 2017, CECAM-HQ-EPFL, Lausanne (CH);

- Participation to the **MolSim 2017 CECAM School**, January 9 – 20 2017, CECAM-NL, Amsterdam (NL).

Research Interest

My research interest is mainly focused on the computational simulation of inorganic as well as biological systems containing transition metals and on their characterization. These transition metal complexes are widely used in catalysis, renewable energies and to mimick enzymes. Metal complexes are also present in biological systems where they play a crucial role in most physiological reactions as cofactors of enzymes. These complexes have been investigated by me both through static (DFT) and dynamical (Born-Oppenheimer and Car-Parrinello AIMD) computational methodologies. I also focused on the hybrid QM/MM simulation of metallic ions transport through protein channels in biological membranes.

Teaching Experience

- **Spring 2019:** Tutor for the "Mathematics 1a for Mise à Niveau" course at EPFL **(62 hrs)** (english language);

- **Spring 2018:** Tutor for the "Mathematics 1b for Mise à Niveau" course at EPFL **(80 hrs)** (english language);

- **Fall 2017:** Tutor for the "Biooriented Chemical Chemistry" course at EPFL (**40 hrs)** (english language);

- **Fall 2017:** Tutor for the "Molecular and Cellular Biophysics 1" course at EPFL **(45 hrs)** (english language);

- **Spring 2017:** Tutor for the "Coordination Chemistry" course at EPFL **(72 hrs)** (english language);

- **Spring 2017:** Tutor for the "Projects of Computational Chemistry" course at EPFL **(42 hrs)** (english language).

Publications

"Understanding the Catalase-Like Activity of a Bioinspired Manganese (II) Complex with a Pentadentate NSNSN Ligand Framework. A Computational Insight into the Mechanism"
Merlini M. L., Britovsek G. J. P., Swart M., Belanzoni P., *ACS Catalysis*, **8**, 2944-2958, **2018.**

Other Certifications

- **Cambridge English B1 Preliminary (PET)** certification;

- **English level B2 Certificate: BI Level B2 Certificate in ESOL International (B2 CEFR)** achieved at the British Institutes Examination Board;

- Achievement of the **24 ECTS (European Credit Transfer System)** in the anthropo-psycho-pedagogical and teaching methodologies areas required for teaching **(D.M. 616/2017)**;

- **Advanced training course** on the **CLIL teaching methodology (ENGLISH LANGUAGE)** obtained at Giustino Fortunato University;

- **Two-years advanced training course** on **"I Nuovi Processi di Potenziamento delle Conoscenze: dalla Progettazione delle Competenze alla Cultura Sistemica"** achieved at Giustino Fortunato University;

- **IT Certifications:**

  1. **"Le nuove tecnologie dell'informazione didattica - Utilizzo della LAVAGNA INTERATTIVA MULTIMEDIALE (LIM)"**
  2. **"CORSO DIGITALE SULL'UTILIZZO DEL MONITOR TOUCH"**
  3. **"USO DIDATTICO DEL TABLET - LE NUOVE TECNOLOGIE DELL'INFORMAZIONE" 4. "CODING E PENSIERO COMPUTAZIONALE"**

obtained at “Scuola Alta Formazione”.

Computer Skills

- Operating systems: Windows, Mac OS, Linux;
- File editing softwares: Office package, LATEX, Biorender;
- Programming languages: Python, Bash, Fortran;
- Computational chemistry softwares: Gromacs, Amber, CPMD, Gaussian, ADF, Quantum Espresso;
- Molecular and crystal structure visualization softwares: Molden, VMD, PyMOL, Rasmol, Avogadro, Chimera.

Language skills

Italian (mother tongue)

English (fluent)

French (basic)