STEFANÍ GAMBOA

Ph.D. in Computational Chemistry

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Skills

Simulation methods | DFT • *ab-initio* • Molecular dynamics • High-performance cluster computing

Computational chemistry | Bio-inorganic • Bioinspired catalyst design • Solid and liquid state • Polynuclear metal complexes • Molecular magnetism • Reactivity • Spectroscopy

Computational tools | Chemcraft • Pymol • Gromacs • Orca and Gaussian *ab initio*, DFT and semiempirical SCF-MO package • Python • Scikit-Learn • Tensorflow

Work Experience

Ph.D. Researcher – Computational Chemistry, Molecular Magnetism, Catalyst Design, Bioinspired Architecture, Artificial Photosynthesis

Institut des Sciences Moléculaire de Marseille, Marseille | Oct 2019 – Feb 2023

Supervisors: Dr. M. Orio (maylis.orio@univ-amu.fr) and Dr. J. Simaan (jalila.simaan@univ-amu.fr).

- Led a state-of-the-art computational assessment to predict magnetic properties using DFT and *ab-initio* methods to develop new magnetic materials. This resulted in one publication collaborating with the Max Planck Institute in Germany.
- Designed and implemented new theoretical reaction mechanism pathway of selective intramolecular O-atom transfer by bio-inspired copper complexes to design novel sustainable catalysts, resulting in one publication and one international talk.
- Designed and implemented theoretical modelling of nickel and cobalt complexes' oxygen evolution reaction mechanism for artificial photosynthesis application in collaboration with Universidad Autónoma de México. This resulted in one publication, and one international talk.

Researcher – Supramolecular Chemistry, Bioinspired Design, Structural Biology

Institut Européen de Chimie et Biologie de Bordeaux, Bordeaux | Oct 2018 – Aug 2019

- Led a *de novo* synthesis of enzyme-like architectures using supramolecular assemblies of water-soluble peptide-oligourea chimera, mimicking a-peptides.

Research Intern – Organic Synthesis, Drug Design, Molecular Docking

Laboratoire de Chimie et Biochimie Pharmacologiques et Toxicologiques, Paris | Feb 2017 – Aug 2017 and Jan 2018 – Aug 2018

- Performed multi-step synthesis of a non-β-lactam β-lactamase inhibitor (Avibactam) analogues to provide structural diversity and generate a library.
- Designed a synthetic route of isotopically labelled S-adenosyl methionine to follow the methylation of specific modified sites of the tRNA for selective detection *in-cell* NMR.

Assistant of Technical Direction – Pharmaceutical Industry, Regulatory Affairs

GlaxoSmithKline Uruguay S.A, Montevideo | Apr 2015 – Jul 2016

- Analyzed, designed and prepared the regulatory dossiers for marketing authorization, amendments and renewals of pharmaceutical products to the Health Authority.
- Updated security information on pharmaceutical products.

Analytical Chemist – Pharmaceutical Industry, Analytical Chemistry, Regulatory

Eurofarma Uruguay S.A, Montevideo | Jul 2014 – Mar 2015

- Performed physical-chemical analysis of raw material, process and finished products.
- Implemented a regulatory procedure for the analytical analysis of pharmaceutical specialities.

Education

2019 – 2023 **PhD**: Computational and Bio-Inorganic Chemistry. *Aix-Marseille Université* - Marseille

2016 – 2018 **Master of Science**: Molecular Chemistry. *Université Paris Descartes - Paris*

2008 – 2014 **Pharmaceutical Sciences**: Chemistry and Pharmaceutical Chemistry. *Universidad de la República - Montevideo*

Certifications

2023 **Machine Learning Specialization** – *DeepLearning.AI and Stanford University Online*

Languages

Spanish | Native language

English | Full professional proficiency

French | Intermediate/Low