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 and Organic • 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 • RDKit • PaDEL

Work Experience

Ph.D. Researcher – Computational Chemistry, Data Analysis, 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.
- Researched and created a dataset of molecules with experimental exchange coupling constants. I applied techniques to curate, analyze and visualize the data, calculate molecular fingerprints to extract information from the molecular structures, compare different machine learning algorithms and finally refine the predictive model.
- Designed and implemented a 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*

2023 **Exploratory Data Analysis for Machine Learning** - *IBM*

2023 – to date **Google Data Analytics Professional Certificate** – *Google*

Publications

- **Stefani Gamboa-Ramirez**, Bruno Faure, Marius Réglier, A. Jalila Simaan, and Maylis Orio. ***"Computational Insights of Selective Intramolecular O-atom Transfer Mediated by Bioinspired Copper Complexes"*** *Chem. Eur. J.* **2022**, e202202206.
- Agnideep Das, Hannah Jobelius, Jules Schleinitz, **Stefani Gamboa-Ramirez**, Geordie Creste, Gwendal Kervern, Jesus Raya, Nolwenn Le Breton, Aurélie Guénet, Zahia Boubegtiten-Fezoua, Laurence Grimaud, Maylis Orio, Guillaume Rogez, Petra Hellwig, Sylvie Choua, Sylvie Ferlay and Marine Desage-El Murr. ***"A hybrid bioinspired catechol-alloxazine triangular nickel complex stabilizing protons and electrons"*** *Inorg. Chem. Front.*, **2021**, 8, 5286.
- Ana C. García-Álvarez, **Stefani Gamboa-Ramírez**, Diego Martínez-Otero, Maylis Orio and Ivan Castillo. ***"Self-assembled nickel cubanes as oxygen evolution catalysts"*** *Chem. Commun.*, **2021**, 57, 8608.
- Gurjot Singh, **Stefani Gamboa**, Maylis Orio, Dimitrios A. Pantazis and Michael Roemelt. ***"Magnetic exchange coupling in Cu dimers studied with modern multireference methods and broken-symmetry coupled-cluster theory"*** *Theoretical Chemistry Accounts*, **2021**, 140:139.

Languages

Spanish | Native language

English | Full professional proficiency

French | Intermediate/Low