STEFANÍ GAMBOA

Ph.D. in Computational Chemistry

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Skills

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

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

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

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).

- Benchmark of state-of-the-art computational methods to predict magnetic properties of copper dimers using single and multireference methods such as DFT, CASSF, DMRG and DDCI.
- Experimental and computational study of the magneto-structural correlation in dinuclear copper complexes.
- Design and implementation of a new theoretical reaction mechanism pathway of selective intramolecular O-atom transfer by bio-inspired copper complexes to design novel sustainable catalysts.
- Theoretical modelling of nickel and cobalt complexes' oxygen evolution reaction mechanism for artificial photosynthesis.

Researcher – *de novo* Design, Supramolecular Chemistry, Bioinspired Design

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 specialties.

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 **Cheminformatics Specialization** - *Neovarsity*

2023 **Advance Machine Learning for Drug Discovery** - *Neovarsity*

Publications

- **Stefani Gamboa-Ramirez**, Michel Giorgi, Sylvain Bertaina, A. Jalila Simaan, and Maylis Orio. ***"Magneto-structural correlation in polynuclear copper complexes: counterion effect"*** Manuscript in preparation.
- **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