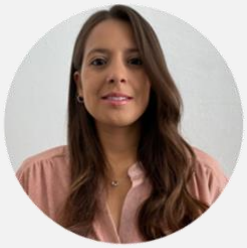

STEFANÍ GAMBOA

Ph.D. in Computational and Bio-inorganic Chemistry

Keywords: Quantum Chemistry, Coordination Chemistry, Transition Metal Complexes, Spectroscopy, Magneto-Structural Correlation, Reactivity, Redox Chemistry, Machine Learning, Cheminformatics

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Education

2019 – 2023 **Ph.D.** Computational and Bio-Inorganic Chemistry. *Aix-Marseille Université* - Marseille

2016 – 2018 **M.Sc.** Molecular Chemistry. *Université Paris Descartes - Paris*

2008 – 2014 **PharmD** Pharmaceutical Chemistry. *Universidad de la República – Montevideo*

Work Experience

Ph.D. Researcher – Structure-function relationship in polynuclear bio-inspired copper complexes: Combined experimental and computational studies

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).

- Benchmarked advanced computational methods (BS-DFT, CASSF, DMRG, DDCI) for magnetic properties prediction in copper dimers (https://doi.org/10.1007/s00214-021-02830-0).
- Synthesized and characterized polynuclear copper complexes (NMR, EPR, MS, XRD) and measured the magnetic properties (*J* values using SQUID) to study their magneto-structural correlation.
- Designed a theoretical predictive tool for the exchange coupling constant of the previous complexes using BS-DFT and *J* Recomposition Method (Manuscript in preparation).
- Investigated reaction mechanisms of bioinspired copper complexes for C-H bond activation and hydroxylation using DFT calculations (https://doi.org/10.1002/chem.202202206)
- Modelled oxygen evolution reaction mechanisms in nickel and cobalt complexes for artificial photosynthesis applications (https://doi.org/10.1039/d1cc03227e).
- Elucidated the electronic structure and calculated the magnetic properties of a trinuclear Ni-complex (https://doi.org/10.1039/d1qi01131f).

Research Chemist – Supramolecular Chemistry and 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 α-peptides.

Research Chemist – 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 Avibactam analogues, contributing to a library for β-lactamase inhibitors.
- Designed a synthetic route for isotopically labelled S-adenosyl methionine, enabling selective *in-cell* NMR detection of tRNA methylation.

Assistant of Technical Direction – Regulatory Affairs

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

- Managed regulatory dossiers for pharmaceutical product authorization, focusing on compliance with health authority standards.

Analytical Chemist – Pharmaceutical Quality Control

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

- Performed physical-chemical analyses of pharmaceutical products, ensuring quality control and regulatory adherence.

Skills

Theoretical Methods| •Quantum Chemistry (DFT and wavefunction-based methods): Orca, Gaussian, HPC •Molecular Dynamics and Docking: Gromacs, AutoDock, MGLTools •Machine Learning: Python, Scikit-Learn, TensorFlow •Cheminformatics: RDKit •Molecular Visualization and Analysis: Chemcraft, Pymol

Organic-Inorganic Chemistry| •Heterocyclic and nucleoside synthesis •Peptide synthesis •Multistep synthesis •Polynuclear transition metal complexes synthesis •Schlenk technique •Crystallization methods

Analytical Chemistry| •Chromatography: HPLC, UPLC, GC •Spectroscopy: UV, NMR, FTIR, GC-MS, EPR •Magnetometer: SQUID •Peptide synthesizer and microwave

Certifications

2023

- **Machine Learning Specialization** – *DeepLearning.AI and Stanford University Online*
- **Exploratory Data Analysis for Machine Learning** – *IBM*
- **Cheminformatics Specialization** – *Neovarsity*
- **Advance Machine Learning for Drug Discovery** - *Neovarsity*

Languages

• **Spanish** | Native language • **English** | Full professional proficiency • **French** | Intermediate/Low

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.