



Sergi Ortiz Roperó

Nationality: Spanish **Date of birth:** 14 May 2002

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ABOUT ME

Sergi Ortiz is a junior researcher and a prospective master's student with special interest in Theoretical Chemistry and Computational Modeling. Honored with an excellence award, the two BScs in Physics and Chemistry have allowed him to pursue research in atomistic modeling, including the study of enzymatic systems at UAB and the study of the physical adequacy of Machine Learning Interatomic Potentials at ICMA3. With a published paper at JACS, he is now focusing on learning Japanese before venturing out further in his scientific career.

EDUCATION AND TRAINING

BSc in Physics

Autonomous University of Barcelona [Sep 2020 – Jul 2025]

City: Barcelona | Country: Spain | Website: <https://www.uab.cat/web/estudiar/ehea-degrees/general-information/physics-1216708259085.html?param1=1345944833018> | Field(s) of study: Natural sciences, mathematics and statistics: • Physics | Final grade: 8.79 / 10.00 | Type of credits: ECTS | Number of credits: 240 | Thesis: Study of the physical adequacy of Machine Learning Potentials

BSc in Chemistry

Autonomous University of Barcelona [Sep 2020 – Jul 2025]

City: Barcelona | Country: Spain | Website: <https://www.uab.cat/web/estudiar/l1istat-de-graus/informacio-general/quimica-1216708251447.html?param1=1263194083206> | Field(s) of study: Natural sciences, mathematics and statistics: • Chemistry | Final grade: 9.28 / 10.00 | Type of credits: ECTS | Number of credits: 240 | Thesis: Resolving inflammation: computational study on the positional regioselectivity of 5-HETE and 5-HpETE in human ALOX15

Erasmus exchange program

Uppsala University [Sep 2024 – Jan 2025]

City: Uppsala | Country: Sweden | Website: <https://www.uu.se/en/study/programme/masters-programme-chemistry-theoretical-and-computational-chemistry> | Field(s) of study: Natural sciences, mathematics and statistics: • Physics • Chemistry | Type of credits: ECTS | Number of credits: 20

Courses taken: Applied Deep Learning in Physics and Engineering, Scientific Programming in Python with Applications in Physics, Chemical Bonding and Computational Chemistry.

Computational Modelling: from Molecules to Materials

IQTC-UB [12 Feb 2024 – 16 Feb 2024]

City: Barcelona | Country: Spain

Short training course at IQTC-UB covering a wide range of theories and software readily used in computational modeling, including Quantum Chemistry methods via Gaussian and GaussView, Material simulation via ASE Python package, Excited States, Machine Learning for chemical systems, Statistical Mechanics, Quantum Dynamics and VR software for biomolecular visualization.

WORK EXPERIENCE

🏢 **Barcelona Supercomputing Center** – Barcelona, Spain

Summer Internship

Summer Internship at EAPM group under the supervision of Martin Floor and Víctor Guàllar, with the objective of developing new analysis tools in Python for Free Energy Perturbation (FEP) alchemical simulations for the in-house simulation software PELE. Scientific skills involved include the use of BASH and Python scripting languages for scientific programming, data analysis of FEP/PELE simulations, a fundamental understanding of atomistic modeling techniques (FEP, Docking calculations and MD/Monte Carlo simulations) and biochemical visualization software (UCSF Chimera, Schrodinger Maestro). Transversal skills include project management, oral communication, critical thinking and reasoning.

SKILLS

Programming Software

Scientific programming / Python / Data analysis / BASH / SLURM / Git

Computational Modeling Techniques

MD / Steered MD / QM/MM / Monte Carlo simulations / Molecular Docking / Machine Learning Interatomic Potentials / FEP / DFT / Hartree-Fock / post HF methods

Computational Modeling Software

ASE / GOLD Docking / GROMACS / AMBER / ChemShell / GaussView / Gaussian / UCSF Chimera / VMD / PyMOL

Transversal skills

Project mangament / Critical thinking

LANGUAGE SKILLS

Mother tongue(s): Spanish | Catalan

Other language(s):

English

LISTENING C2 **READING** C2 **WRITING** C2

SPOKEN PRODUCTION C2 **SPOKEN INTERACTION** C2

Japanese

LISTENING B1 **READING** B1 **WRITING** B1

SPOKEN PRODUCTION B1 **SPOKEN INTERACTION** B1

Levels: A1 and A2: Basic user; B1 and B2: Independent user; C1 and C2: Proficient user

HONOURS AND AWARDS

[Dec 2023] Autonomous University of Barcelona

Best academic record in Chemistry and Physics after completing the first three years of studies Honored with an excellence award for the best academic record in my Bachelor's Degrees in Physics and Chemistry after completing the first three years (180 credits ECTS).

[Dec 2025] Autonomous University of Barcelona

Best academic record in Chemistry and Physics Honored with an excellence award for the best academic record in my BScs in Physics and Chemistry (2020-2025)

PUBLICATIONS

[2025]

Rare-Earth Silicates as High-Temperature Surfactants for the Controlled Synthesis of ϵ -Fe₂O₃ Nanoparticles

Authors: Naureen Khanam, Zheng Ma, Sergi Ortiz Roperro, Nico Dix, Ana Vila Costa, Judit Oró-Solé, José Luis García-Muñoz, Jordi Faraudo, Martí Gich | **Journal Name:** Journal of the American Chemical Society | **Volume, Issue and Pages:** Vol. 147, Issue 37, 33403–33412 | **Publisher:** American Chemical Society

Naureen Khanam, Zheng Ma, Sergi Ortiz Roperro, Nico Dix, Ana Vila Costa, Judit Oró-Solé, José Luis García-Muñoz, Jordi Faraudo, and Martí Gich Journal of the American Chemical Society 2025 147 (37), 33403-33412 DOI: 10.1021/jacs.5c05058