Alexandre Pinto



Postdoctoral Researcher

Faculty of Sciences, University of Porto (FCUP)

alexandre.pinto@fc.up.pt · Porto, Portugal

ORCID · ResearcherID · Google Scholar · GitHub · LinkedIn

About Me

Computational chemist with experience in leveraging quantum and classical computational methods to uncover enzyme mechanisms and explore the properties of materials at the nanoscale. Highly skilled in atomistic molecular dynamics and quantum chemistry methods, with proficiency in hybrid QM/MM or QM/MM MD approaches. Contributed to multiple HPC projects, executing large-scale parallel calculations on prominent European HPC infrastructures (MeluXina, JURECA, MareNostrum 4, Snellius, VEGA).

Experience

2026 – 2027 — **ENCORE Project**
Research Fellow · LAQV@REQUIMTE/FCUP
"Enzymatic Nylon Conversion for Recycling" - NNF24OC0090669

2026 – 2027 — **FCT Advanced Computing Projects**
Principal Investigator · FCUP
"Molecular Dynamics Screening of Engineered Plastic-Degrading Enzymes" - 2026.07067.CPCA.A2
"Atomistic Models of Nylon Surfaces: Development and Validation" - 2026.05885.CPCA.A1

2026 — **Invited Assistant Professor**
Universidade do Porto · FCUP
Courses Lectured: Bioinformatics

2026 — **FEBS Short-Term Fellowship**
Principal Investigator · Universitat de Girona
"Deep Learning Approaches for Enzyme Design at Polymer Surfaces" - ST-2026-047

2025 – 2026 — **En'Zync Project**
Research Fellow · FCUP
"Enzymatic Deconstruction of Thermoset Plastics" - 0072891

2021 — **HPC-Europa3 Project**
Principal Investigator · University of Groningen
"The Human Synovial secreted PLA2 enzyme: an insight on the reaction mechanism of sPLA2s" - HPC17H98I1

Publications (Selected)

2026 — Clausen, K.S.R. *et al.* "Enhancing the k_{cat} of *Is*MHETase through a single active site mutation", *Chem Circularity*, doi:10.1016/j.checir.2026.100117

2025 — Castro-Amorim, J. *et al.* "Beyond Fang's fury: a computational study of the enzyme-membrane interaction and catalytic pathway of the snake venom phospholipase A2 toxin", *Chemical Science*, doi:10.1039/d4sc06511e

2024 — Pinto, A.V. *et al.* "Revisiting the reaction pathways for phospholipid hydrolysis catalyzed by phospholipase A2 with QM/MM methods", *Chemical Science*, doi:10.1039/d4sc02315c

2023 — Pinto, A.V. *et al.* "Development of nanoscale graphene oxide models for the adsorption of biological molecules", *The Journal of Physical Chemistry B*, doi:10.1021/acs.jpcb.2c06037

2021 — Pinto, A.V. *et al.* "Reaction mechanism of MHETase, a pet degrading enzyme", *ACS Catalysis*, doi:10.1021/acscatal.1c02444

Skills

Computational Software & Packages
GROMACS, AMBER, Gaussian, CP2K, VMD, ChimeraX

Programming Languages
Bash and Python scripting for workflow automation

High-Performance Computing
Parallel programming (MPI, OpenMP) within SLURM

Simulation Methods
cMD, DFT, DFTB, QM/MM, QM/MM MD

Protein Modelling and Design
RFdiffusion, ProteinMPNN, AlphaFold, MODELLER, FoldX, FuncLib, PROSS

Data Analysis and Machine Learning
Linear and multiple regressions, LOOCV; cluster analysis and principal component analysis

Languages

Portuguese — Native

English — C1

Spanish — B2

Awards

Best Oral Communication
IJUP 2019 - 12th Meeting of Young Researchers of University of Porto

Review Activity

ACS Omega · ACS, 2023
RSC Advances · RSC, 2025
ChemBioChem · Wiley, 2025

Organisation & Outreach

Organising Committee, TheoBio 2026 (FCUP)

Interview on AI for plastic-degrading enzymes, *Jornal de Notícias* (2026)

Education

2021 – 2025 **Ph.D. in Chemistry** · FCUP
Thesis: "Computational study of MHETase for PET plastic biodegradation"

2017 – 2019 **M.S. in Biochemistry** · FCUP
Dissertation: "Computational Modelling of Carbon Nanotubes as Drug Carriers"

2014 – 2017 **B.S. in Biochemistry** · FCUP
Project Report: "Aspartate-semialdehyde Dehydrogenase (ASADH): A QM/MM Model Preparation"

Funding & Grants (Selected)

2026 – 2027 **Research Scholarship**
Novo Nordisk Fonden
"ENCORE - Enzymatic Nylon Conversion for Recycling"

2026 – 2027 **Awarded Computing Projects**
Fundação para a Ciência e a Tecnologia
"Molecular Dynamics Screening of Engineered Plastic-Degrading Enzymes"
"Atomistic Models of Nylon Surfaces: Development and Validation"

2026 **Awarded Project**
FEBS
"Deep Learning Approaches for Enzyme Design at Polymer Surfaces"

2025 – 2026 **Research Scholarship**
FCUP
"En'Zync - Center for enzymatic deconstruction of thermoset plastics for a sustainable society"

2022 – 2024 **PhD Scholarship**
Fundação para a Ciência e a Tecnologia
"Computational study of MHETase for PET plastic biodegradation"

2021 **Awarded Project**
Horizon 2020
"The Human Synovial secreted PLA2 enzyme: an insight on the reaction mechanism of sPLA2s"

Conference Presentations

2026 **Poster Presentation**
European RosettaCon

2026 **Poster Presentation**
10th Theoretical Biophysics Symposium, TheoBio

2023 **Poster Presentation**
EuChemS CompChem
"Unraveling the Catalysis of GIIA sPLA2 through Classical and QM/MM Approaches"

2023 **Oral Presentation**
15º Encontro Nacional de Química Física
"Nanoscale Graphene Oxide Models for the Adsorption of Biological Molecules"

2019 **Poster Presentation**
XXVI Encontro Nacional da Sociedade Química Portuguesa
"A DFT on SWCNT End-Functionalization: Intramolecular Hydrogen Bonds as a Molecular Gate"

2019 **Oral Communication**
12th Meeting of Young Researchers of University of Porto, IJUP
"A Theoretical study on SWCNT End-Functionalization: Intramolecular Hydrogen Bonds as a Molecular Gate"

Workshops & Courses

Python Programming
FCUP · 2025

ACS Reviewer Lab
American Chemical Society · 2023

Introduction to Supercomputing at JSC: Theory & Practice
Jülich Supercomputing Centre · 2022

Advanced GROMACS Workshop
CSC IT Center for Science · 2022

BioExcel/PerMedCoE PATC course on Introduction to HPC for Life scientists
PRACE Advanced Training Center · 2022

FEBS Advanced Course: Computational Approaches to Understanding and Engineering Enzyme Catalysis
Federation of European Biochemical Societies · 2021

GROMACS Workshop: A Collaboration Between Bioexcel And the Portuguese National EuroHPC Competence Center
BioExcel & BioData.pt · 2020

Virtual Workshop on Best Practices in QM/MM Simulation of Biomolecular Systems
BioExcel · 2020

Mentoring Experience

Mentored a Master's degree student performing MD simulations of graphene oxide (2021)

Mentored a Doctoral student performing MD and QM/MM MD simulations of *Bothrops Asper* sPLA2 (2024-2025)

Co-supervised a Master's student from the Universitat de Barcelona in simulations of the CutC:CutD complex (2026)

Scientific Journal Covers

Front Cover, *ACS Catalysis*, Volume 11, Issue 16 (2021)

Front Cover, *Nature Reviews Chemistry*, Volume 6, Issue 7 (2022)

Front Cover, *The Journal of Physical Chemistry B*, Volume 127, Issue 2 (2023)





