Pol Benítez Colominas

FI PhD candidate at UPC and Visiting Researcher at UTokyo
Tokyo, Japan

Profile

I am a PhD Candidate in Computational Physics at the Polytechnic University of Catalonia (UPC) and Visiting Researcher at The University of Tokyo, working under the supervision of Prof. Claudio Cazorla. My research lies in Computational Materials, where I employ first-principles atomistic modeling methods and machine learning approaches, such as Density Functional Theory, Machine Learning Interatomic Potentials, and Graph Neural Networks, to investigate condensed matter systems. By studying materials in silico, from their structural to their optoelectronic properties, we can help to advance the understanding and design of materials for next-generation energy and optoelectronic technologies.

Contact Information

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Research Interests

First-principles computational modeling of materials for energy and optoelectronic applications.

Investigation of thermal effects and electron-phonon coupling in perovskite systems using first-principles and machine learning approaches.

Crystal structure prediction and phase transitions discovery assisted by machine learning interatomic potentials (MLIPs).

Application of graph neural networks (GNNs) and MLIPs for materials property prediction and accelerated materials discovery.

Education

Universitat Politècnica de Catalunya – PhD in Computational and Applied Physics (2023 - Present)

Universitat Politècnica de Catalunya – Master's degree in Engineering Physics (2022 - 2023)

Universitat de Barcelona – Bachelor's degree in Physics, Mention in Fundamental Physics (2016 - 2022)

Research Experience

The University of Tokyo, Tokyo, Japan
Visiting Researcher, Oct 2025 – Present

Visiting PhD student in Professor Teruyasu Mizoguchi's group (Nano-Materials Design Laboratory, NMDL), focusing on the application of artificial intelligence in materials science.

Universitat Politècnica de Catalunya, Barcelona, Spain
Predoctoral Researcher, Sep 2023 – Present

PhD Candidate under the supervision of Professor Claudio Cazorla and co-supervision of Professor Edgardo Saucedo. Research involves the use of first-principles techniques and machine learning methods, such as density functional theory (DFT), graph neural networks (GNNs), and machine learning interatomic potentials (MLIPs), for computational materials science. Projects range from the discovery of new polymorphs and phase transitions in novel materials to the study of the optoelectronic properties of distorted perovskite semiconductors.

University of Cambridge, Cambridge, United Kingdom
Visiting Researcher, Sep 2024 – Nov 2024

Visiting PhD student in Professor Bartomeu Monserrat's group (Monserrat Lab). Investigated the role of electron–phonon coupling in the optoelectronic properties of anharmonic perovskite semiconductors and the behavior of excitons in two-dimensional anharmonic materials. This collaboration resulted in two first-author publications.

Universitat Politècnica de Catalunya, Barcelona, Spain
Graduate Researcher, Jan 2023 – Aug 2023

Conducted research under the supervision of Professors Claudio Cazorla and Edgardo Saucedo. Focused on modeling the structural and optoelectronic properties of novel semiconductor materials for photovoltaic applications using first-principles methods.

Universitat de Barcelona, Barcelona, Spain
Undergraduate Researcher, Feb 2021 – May 2022

Conducted undergraduate research under the supervision of Professor Aurora Hernández-Machado. The work focused on theoretical studies of the dynamics of non-Newtonian fluids in microfluidic systems and the application of machine learning methods to predict hematological diseases based on the fluidic properties of blood.

Publications

List of peer-reviewed publications (as of October 21, 2025):

1. **P. Benítez**, et al. "Band-Gap Tunability in Anharmonic Perovskite-like Semiconductors Driven by Polar Electron-Phonon Coupling." *J. Am. Chem. Soc.*, 147, 41, 37506-37520 (2025).

2. I. Caño, A. Navarro-Güell, E. Maggi, A. Gon Medaille, D. Rovira, A. Jiménez-Aguijo, A. Torrens, M. Jiménez, C. López, **P. Benítez**, et al. "Ribbons of Light: Emerging (Sb,Bi)(S,Se)(Br,I) Van der Waals Chalcohalides for Next-Generation Energy Applications." *Small*, 21, e05430 (2025).

3. C. López, S. R. Kavanagh, **P. Benítez**, et al. "Chalcogen Vacancies Rule Charge Recombination in Pnictogen Chalcohalide Solar-Cell Absorbers." *ACS Energy Lett.*, 10, 7, 3562-3569 (2025).

4. **P. Benítez**, et al. "Giant Thermally Induced Band-Gap Renormalization in Anharmonic Silver Chalcohalide Antiperovskites." *J. Mater. Chem. C*, 13, 10399 (2025).

5. **P. Benítez**, et al. "Crystal Structure Prediction and Phase Stability in Highly Anharmonic Silver-Based Chalcohalide Antiperovskites." *PRX Energy*, 4, 023002 (2025).

6. C. López, I. Caño, D. Rovira, **P. Benítez**, et al. "Machine-Learning Aided First-Principles Prediction of Earth-Abundant Pnictogen Chalcohalide Solid Solutions for Solar-Cell Devices." *Adv. Funct. Mater.*, 34, 2406678 (2024)

7. I. Caño, J. Turnley, **P. Benítez**, et al. “Novel Synthesis of Semiconductor Chalcohalide Anti-Perovskites by Low-Temperature Molecular Precursor Ink Deposition Methodologies.” *J. Mater. Chem. C*, 12, 3154 (2024)

Conference Presentations

Oral presentation, “MLIPs for Crystal Structure Prediction and Thermodynamic Phase Diagrams,” From molecules to materials: 2nd workshop on benchmarking solid state properties, Bologna, Italy, September 2025.

Invited oral presentation, “Exploring the Use of MLIPs and GNNs to Accelerate Materials Calculations,” 10th IDMRCS, Barcelona, Spain, July 2025.

Oral presentation, “Thermal Effects on Optoelectronics: A Graph Neural Network Approach,” AI4X 2025, Singapore, Singapore, July 2025.

Oral presentation, “Thermal Effects on Anharmonic Semiconductor Optoelectronics via Graph Neural Networks,” ICMAT 2025, Singapore, Singapore, June 2025.

Oral presentation, “Phonon-Driven Band Gap Engineering in Chalcohalide Anti-Perovskites,” ICMAT 2025, Singapore, Singapore, June 2025.

Oral presentation, “Electron-Phonon Coupling Induces Giant Band Gap Reduction in Optoelectronic Materials,” NEXTGEN 2024, Palma de Mallorca, Spain, September 2024.

Oral presentation, “Predicting Thermal Effects on Optoelectronic Properties of Solid Solutions using Graph Neural Networks,” Artificial Intelligence for Advanced Materials 2024, Barcelona, Spain, July 2024.

Oral presentation, “Giant Thermal Effects in the Optoelectronic Properties of Chalcohalide Anti-Perovskite Materials,” EMRS Spring Meeting 2024, Strasbourg, France, May 2024.

Oral presentation, “Theoretical and Experimental Characterization of Highly Anharmonic Chalcohalide Anti-Perovskites for Energy Applications,” 2024 MRS Spring Meeting, Seattle, USA, April 2024.

Oral presentation, “Fast and Reliable Crystal Structure Prediction Using Random Search Algorithms and Machine Learning Interatomic Potentials,” Machine Learning Conference for X-Ray and Neutron-Based Experiments, Munich, Germany, April 2024.

Oral presentation, “Novel Phases and Optoelectronic Properties of Antiperovskite Chalcohalides from First-Principles Simulations,” 13th European Kesterite+ Workshop, Barcelona, Spain, July 2023.

Tutorial session (instructor), “Introduction to Machine Learning for Materials Science,” 13th European Kesterite+ Workshop, Barcelona, Spain, July 2023.

Awards and Fellowships

Fellowship, Joan Oró FI 2024, Predoctoral Research Fellowship awarded by AGAUR (the Agency for Management of University and Research Grants of the Government of Catalonia), May 2024 – May 2027, approximately 73,000€.

Award, Best Predoctoral Research Awards (1st edition) of the Department of Physics of UPC, February 2024, 617€.

Technical and Computational Skills

Computational Methods and Frameworks: DFT (VASP, Quantum ESPRESO), Molecular Dynamics (LAMMPS, VASP, ASE), Phonon Calculations (Phonopy, Phono3py, DynaPhoPy, hiPhive), Crystal Structure Prediction (PyMCSP, CrySPY), Materials Science (Pymatgen, PyXtal, Sumo, easyunfold, Materials Project, VASPKIT, ASE), Machine Learning Interatomic Potentials (MACE, M3GNet), Machine Learning (PyTorch, PyTorch Geometric, TensorFlow, scikit-learn)

Programming: Python, Fortran, Bash

High-Performance Computing: SLURM, parallel workflows, cluster administration basics

Data Analysis and Visualization: pandas, NumPy, SciPy, Excel, Matplotlib, seaborn, VESTA

Open-Source Contributions

Developed and maintained publicly available code repositories on GitHub (only public repositories are listed):

PyMCSP – *Crystal Structure Prediction and Diffraction Analysis*

Open-source code for crystal structure prediction and diffraction studies based on random search algorithms and machine learning interatomic potentials (MLIPs). The package is under active development; it currently supports crystal structure prediction (with and without pressure) for inorganic and molecular crystals and assists in phase discovery from diffraction data.

Repository: https://github.com/polbeni/PyMCSP

Materials Modelling tools – *Automation and Analysis Utilities for Atomistic Simulations*

A collection of tools for computational materials modeling, including input generators (for VASP, Quantum ESPRESSO, etc.), Bash scripts for workflow automation, and Python scripts for pre- and post-processing of simulation data. Features include: plotting phonon and electronic band structures, generating disordered and distorted crystal structures (solid solutions, surfaces, etc.), computing Fröhlich coupling corrections, analyzing XDATCAR files, studying molecular dynamics trajectories, visualizing ion motion, generating Gibbs surface maps as functions of pressure and temperature, among others.

Repository: https://github.com/polbeni/materials-modelling

GNNs for Materials – *Graph Neural Networks for Materials Property Prediction*

Framework for training and evaluating graph neural network (GNN) models to predict materials properties. The repository includes scripts for generating crystal graphs (using cutoff-radius method), retrieving data from the Materials Project database, building custom DFT datasets, training and retraining GNN models, performing hyperparameter studies, and analyzing model performance.

Repository: https://github.com/polbeni/GNN-materials

Teaching and Mentoring Experience

Teaching Assistant, Feb 2023 - Present:

"Physics I: Fundamentals of Mechanics," Bachelor's degree in Engineering

"Physics II: Fundamentals of Electromagnetism," Bachelor's degree in Engineering

Supervision of undergraduate and graduate students on DFT and ML-based projects.

References

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Prof. Edgardo Saucedo
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Prof. Bartomeu Monserrat
Department of Materials Science and Metallurgy, University of Cambridge
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Prof. Teruyasu Mizoguchi
Institute of Industrial Science, The University of Tokyo
teru@iis.u-tokyo.ac.jp

Languages

English: Full Professional Proficiency.

Spanish: Native.

Catalan: Native.