Languages

English Fluent
French Native
Dutch Native

Awards

- **2025** IMCN Best Thesis Award
- **2021** F.R.S-FNRS Aspirant Renewal Fund for Scientific Research
- **2019** F.R.S-FNRS Aspirant Fund for Scientific Research
- **2018** Lhoist Berghmans MIT-UCL grant
- **2014** 'Vlaamse Fysica Olympiade' Finalist

Technical Expertise

ML / Deep Learning:
PyTorch, PyTorch Geometric, Lightning, TensorFlow, JAX, scikit-learn; generative models, geometric deep learning, active learning, uncertainty-aware and multi-fidelity modeling

Scientific Computing:
Python, NumPy, pandas, matplotlib, Plotly, high-throughput workflows and scientific data pipelines

Atomistic Simulation:
ABINIT, VASP

Tooling:
Git, GitHub, Bash, Linux, LaTeX

Leadership & Collaboration

- Independent research execution
- Scientific communication, community representation, and meeting facilitation
- Mentoring and team coordination
- Cross-disciplinary problem solving
- Resilience in ambiguous research settings

Hobbies

- Videography with self-built drones
- Tennis
- Music production

PIERRE-PAUL DE BREUCK

Research Scientist in Generative ML for Materials Discovery

pierrepauldb.com
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EXPERIENCE

Postdoctoral Researcher — August 2024 - present
ICAMS, Ruhr University Bochum

Leading generative-ML and atomistic-modelling projects for energy materials, including database infrastructure, model development, and high-throughput discovery workflows for superconductors and hydrides.

ML Research Intern — October 2023 - February 2024
Mila, Quebec Artificial Intelligence Institute, Montreal, Canada

Developed generative models with GFlowNets for crystal-structure design in electrocatalysis and solid-state batteries in Yoshua Bengio's lab.

PhD in Machine Learning for Materials Discovery — 2019-2024
Université Catholique de Louvain, Belgium

Developed and benchmarked uncertainty-aware, multi-fidelity, and active-learning methods for materials-property prediction and accelerated discovery workflows, resulting in 3 first-author publications and 5 conference presentations, including an invited talk.

President of the researchers association (ACIM) — 2021-2023
IMCN institute, Université Catholique de Louvain, Belgium

Represented PhD researchers to institute leadership, led monthly feedback meetings, and organized community-building events.

Research Intern (Graph Neural Networks) — July-August 2018
MIT, Department of Material Science and Engineering, Cambridge USA

Worked on geometric deep-learning methods for materials applications in a collaborative research setting.

EDUCATION

PhD in Machine Learning for Materials Discovery — 2019-2024
Université Catholique de Louvain, Belgium

Dissertation: 'Small datasets, big predictions: learning methods for uncertainty-aware modelling of multi-fidelity material properties'

Master of Engineering Science in applied physics — 2019
Université Catholique de Louvain

Magna Cum Laude with honours. Master Thesis on Machine Learning in Materials Science.

Bachelor of Engineering Science — 2014-2017
Université Catholique de Louvain

Magna Cum Laude

TEACHING

Teaching assistant quantum mechanics (LMAPR 1491) - 3rd year BSc Engineering **2020-2022**
Université Catholique de Louvain

Intro to Supervised Learning, Machine Learning for Electronic Structure Training School **2021-2023**
ICTP-East African Institute for Fundamental Research under the auspices of UNESCO

Intro to Python for 16-18 years old students **Summer 2017**
Technofutur TIC

Mathematics, Physics and Chemistry Tutor - 1st & 2nd year Engineering **2015-2017**
Université Catholique de Louvain

SELECTED PRESENTATIONS

Talk at AI4AM: AI for advanced materials - Madrid, Spain **May 2026**
A generative material transformer using Wyckoff representation

Invited talk at WE-Heraeus Seminar: Machine Learning for Spectroscopy - Brussels, Belgium **May 2025**
Generative Transformer models for the dielectric function

Invited talk at CECAM Machine Learning of First Principle Observables - Berlin, Germany **July 2024**
Property predictions from limited and multi-fidelity datasets

Contributed talk at the APS March Meeting 2022 - Chicago, USA **March 2022**
Bias-imbalance in data- driven materials science: a case study on MODNet

Contributed talk at the 17th ETSF Young Researchers' Meeting - Cagliari, Italy **September 2021**
MODNet: property prediction for limited datasets and the bias-imbalance issue

Invited talk at CECAM Mixed-Gen workshop **April 2021**
Accurate and interpretable property prediction for limited materials datasets by feature selection and joint-learning

Contributed talk at the APS Online March Meeting 2021 **March 2021**
MODNet: property prediction for limited materials datasets by feature selection and joint-learning

Poster presentation at the 2020 Virtual MRS Fall Meeting **November 2020**
Machine Learning Materials Properties for Small Datasets. Symposium: Data Science and Automation to Accelerate Materials Development and Discovery

PUBLICATIONS

Machine learning driven exploration of hydride superconductors at ambient pressure
P. R. Pires, T. H. B. Da Silva, K. Gao, K. H. Hiorth, T. F. T. Cerqueira, T. Cavignac, **P.-P. De Breuck**, H.-C. Wang, Đ. Dangić, Y.-W. Fang, A. Sanna, W. Cui, I. Errea, P. Törmä, and M. A. L. Marques
Computational Materials Today, 100052 (2026)

AI-Driven Expansion and Application of the Alexandria Database
T. Cavignac, J. Schmidt, **P.-P. De Breuck**, A. Loew, T. F. T. Cerqueira, H.-C. Wang, A. Bochkarev, Y. Lysogorskiy, A. H. Romero, R. Drautz, S. Botti, and M. A. L. Marques.
[Submitted for publication]

A generative material transformer using Wyckoff representation
P.-P. De Breuck, H.A. Piracha and M.A.L. Marques
npj. Comput. Mater. (2026)

Combining feature-based approaches with graph neural networks and symbolic regression for synergistic performance and interpretability
R. A. Gouvêa, **P.-P. De Breuck**, T. Pretto, G.-M. Rignanese, and M. J. L. Santos
npj. Comput. Mater. (2025)

Generative AI for Crystal Structures: A Review
P.-P. De Breuck, H.-C. Wang, G.-M. Rignanese, S. Botti and M.A.L. Marques
npj. Comput. Mater. (2025)

High-Throughput Search for Cubic Chiral Semiconductors: Structural Insights,Database and Stability Trends
P.-P. De Breuck, H.-C Wang, A. Tellez-Mora, M.A.L. Marques and A. H. Romero
[Under preparation]

Optical materials discovery and design via federated databases and machine learning
V. Trinquet, M. Evans, C. Hargreaves, **P.-P. De Breuck**, and G.-M. Rignanese
Faraday Discuss. (2024)

Combination of ab initio descriptors and machine learning approach for the prediction of the plasticity mechanisms in β-metastable Ti alloys
M. Coffigniez, **P.-P. De Breuck**, L. Choisez, M. Marteleur, M. J. Van Setten, G. Petretto, G.-M. Rignanese, and P. J. Jacques
Materials & Design 239, 112801 (2024)

Influence of roughness and coating on the rebound of droplets on fabrics
P. J. Cruz, **P.-P. De Breuck**, G.-M. Rignanese, K. Glinel, A. M. Jonas
Surfaces and Interfaces 36, 102524 (2023)

A simple denoising approach to exploit multi-fidelity data for machine learning materials properties
X. Liu, **P.-P. De Breuck**, L. Wang, G.-M. Rignanese
npj Comput. Mater. 8, 233 (2022)

Accurate experimental band gap predictions with multifidelity correction learning
P.-P. De Breuck, G. Heymans, G.-M. Rignanese
J Mater. Inf. 2, 10 (2022)

Robust model benchmarking and bias-imbalance in data-driven materials science: a case study on MODNet
P.-P. De Breuck, M. L. Evans, G.-M. Rignanese
J. Phys.: Condens. Matter 33, 404002 (2021)

Materials property prediction for limited datasets enabled by feature selection and joint learning with MODNet
P.-P. De Breuck, G. Hautier, G.-M. Rignanese
npj Comput. Mater. 7, 83 (2021)

Vibrational properties of solids : a machine learning approach
P.-P. De Breuck, G.-M. Rignanese
Master Thesis (2019)