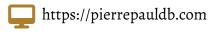
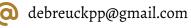


# PIERRE-PAUL DE BREUCK

29 years old computational materials scientist specialized in AI for materials discovery





## EXPERIENCE

#### **Postdoc**

#### August 2024 - present

# ICAMS, Ruhr University Bochum

Group leader in the group of Prof. Miguel Marques. We combine ab-initio and ML methods for energy materials. Current projects involve extending and hosting the Alexandria database, generative methods conditionned on desired properties, chiral semiconductors search (high-throughput screening with VASP) among others.

#### Research intern

## October 2023 - February 2024

# Mila, Quebec Artificial Intelligence Institute, Montreal, Canada

Crystal structure generation with GFlowNets for electrocatalyst design and solid-state batteries in Prof. Yoshua Bengio's lab.

## 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"

My research centers on designing machine learning models for materials property prediction, active learning for DFT, DFPT and experimental speedup, and generative methods. Soft skills include conducting autonomous research in an advanced field, involving problem solving and resilience. Coordinating and supervising younger (international) researchers. Scientific communications: four written publications, three contributed talks and one invited talk.

#### President of the researchers association (ACIM)

2021-2023

#### IMCN institute, Université Catholique de Louvain, Belgium

Responsible of monthly meetings in order to transfer researchers inquires to the institute board (team management) and organize social events.

#### Research intern July-August 2018

MIT, Department of Material Science and Engineering, Cambridge USA. Autonomous and team work on Crystal Graph Convolutional Neural Networks

#### Voluntary work - animator

#### Camp de partage asbl, Belgium

#### August 2016-2022

## Two-week camp with institutionalized children. Creative activities. emotive communication and conflict handling.

Bilingual children camp dealing with different

• Other: bash, C, Java, HTML, CSS,

languages and cultural backgrounds.

'Nasze Miasto - Unsere Stadt', Görlitz,

# Teaching tutor

#### 2015-2022

# Université Catholique de Louvain, Belgium

Teaching Quantum Mechanics, Mathematics, Physics and Chemistry

#### **EDUCATION**

#### Master of Engineering Science in applied physics

#### 2019

#### Université Catholique de Louvain

Magna Cum Laude with honours

Master Thesis on Machine Learning in Material Science

#### **Bachelor of Engineering Science**

#### Université Catholique de Louvain

2014-2017

Magna Cum Laude

Primary and secondary school

#### Summer 2014

College Paters Jozefieten, Melle

Last updated: December, 2025

# native

French native

Dutch

**LANGUAGES** 

**English** professional working proficiency

# 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

# COMPUTER SKILLS

- Python: 8+ years experience, with focus on ML libraries: scikit-learn, pytorch, lightning, tensorflow, pandas, numpy, matplotlib, plotly,...
- Ab-initio: ABINIT, VASP
- Git version control and GitHub
- LaTex, Adobe suite.

# HOBBIES

- Videography with self-built drones
- Tennis player
- Sailor

# SOFT SKILLS

- Versatile problem solving
- Autonomy
- Responsibility Team management
- Determination Resilience

## **TEACHING**

Teaching assistant quantum mechanics (LMAPR 1491) - 3<sup>th</sup> year BSc. Engeneering

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**

Invited talk at WE-Heraeus Seminar: Machine Learning for Spectroscopy

May 2025

Brussels, Belgium

Generative Transformer models for the dielectric function

Invited talk at CECAM Machine Learning of First Principle Observables

July 2024

Berlin, Germany

Property predictions from limited and multi-fidelity datasets

Contributed talk at the APS March Meeting 2022

March 2022

Chicago, USA

Bias-imbalance in data- driven materials science: a case study on MODNet

Contributed talk at the 17th ETSF Young Researchers' Meeting

September 2021

Cagliari, Italy

MODNet: property prediction for limited datasets and the bias-imbalance issue.

Invited talk at CECAM Mixed-Gen workshop.

April 2021

Virtual

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

Virtual

MODNet: property prediction for limited materials datasets by feature selection and joint-learning

#### **JOURNAL PUBLICATIONS**

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.

Under submission.

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 Under submission at npj Comput. Mater.

Generative AI for Crystal Structures: A Review

P.-P. De Breuck, G.M. Rignanese, S. Botti and M.A.L. Marques

npj Comput. Mater. (2025)

# JOURNAL PUBLICATIONS (CONTINUED)

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.

A generative material transformer using Wyckoff representation **P.-P. De Breuck**, H.A. Piracha, G.M. Rignanese and M.A.L. Marques Under submission at npj Comput. Mater.

Optical materials discovery and design with federated databases and machine learning V. Trinquet, Matthew L. Evans, Cameron J. 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 -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)