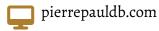


# PIERRE-PAUL DE BREUCK

26 years old computational materials scientist specialized in Machine Learning for materials discovery





#### EXPERIENCE

#### 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

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

#### August 2016-2022

#### 'Nasze Miasto - Unsere Stadt', Görlitz, Germany

Bilingual children camp dealing with different languages and cultural backgrounds.

### Teaching tutor

2015-2022

#### Université Catholique de Louvain, Belgium

Instruct Quantum Mechanics, Mathematics, Physics and Chemistry by connecting advanced concepts to the subject of interest.

#### **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**

2014-2017

#### Université Catholique de Louvain

Magna Cum Laude

#### Primary and secondary school

Summer 2014

College Paters Jozefieten, Melle

### **LANGUAGES**

French native Dutch

native

**English** professional working proficiency

### AWARDS

- **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: 5+ years experience, with focus on datascience libraries: scikitlearn, tensorflow, pytorch, pandas, numpy, matplotlib, plotly.
- Git version control
- Other: bash, C, Java, HTML, CSS, LaTex, Adobe suite.

## HOBBIES

- Videography with self-built drones
- Advanced tennis player
- Skilled 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
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**

### 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

#### Poster presentation at the 2020 Virtual MRS Fall Meeting, November 27 – December 4

November 2020

Virtual- Symposium: Data Science and Automation to Accelerate Materials Machine Learning Materials Properties for Small Datasets

#### **PUBLICATIONS**

Combination of ab initio descriptors and machine learning approach for the prediction of the plasticity mechanisms in  $\beta$ -metastable Ti alloys

M. Coffigniez, **P.-P. De Breuck** et al., 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)

Last updated: May, 2024