Pierre-Paul De Breuck

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

https://pierrepauldb.com

debreuckpp@gmail.com

Languages

French native
Dutch native
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
- Other: bash, C, Java, HTML, CSS, LaTex, Adobe suite.

Hobbies

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

Soft skills

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

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 — **August 2016-2022**
Camp de partage asbl, Belgium
Two-week camp with institutionalized children. Creative activities, emotive communication and conflict handling.
'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
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 — **2014-2017**
Université Catholique de Louvain
Magna Cum Laude

Primary and secondary school — **Summer 2014**
College Paters Jozefieten, Melle

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Teaching

Teaching assistant quantum mechanics (LMAPR 1491) - 3th 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)

Last updated: December, 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 -meta-stable 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)