SANDER VANDENHAUTE

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EDUCATION

PhD in Engineering Physics Ghent University (BE) JUN 2019 – DEC 2024
additional coursework in computer architecture and parallel programming

MS in Electrical Engineering Columbia University (US) SEP 2018 – MAY 2019
deep learning (vision/speech), convex optimization, sparse representations, probabilistic programming

BS/MS in Engineering Physics Ghent University (BE) SEP 2013 – JUN 2018
additional coursework in macro-economics, modern history, epistemology, and ethics

EXPERIENCE

Postdoctoral Researcher Stanford University (US) OCT 2025 – PRESENT

- Riemannian flow matching for fast and efficient rate calculations of chemical and physical transformations
  integrating concepts from optimal control theory and differential geometry with equivariant GNNs to predict physical properties using nonequilibrium statistical mechanics.

AI Researcher Orbital Materials (UK) JAN 2025 – AUG 2025

- core developer of Orb-v3; a fast and scalable universal interatomic potential
  developed equigrad, an efficient regularization strategy that incentivizes equivariance, along with various other architectural improvements (**paper**)
- designed and trained GNNs to experimental datasets of small molecule thermodynamic properties
  models were used to design and synthesize new molecules for chip cooling; a patent application has been submitted for selected candidates after successful experimental validation

PhD in Engineering Physics Ghent University (BE) JUN 2019 – DEC 2024

- `psiflow`: scalable & asynchronous execution of free energy calculations with ML potentials
  biased sampling and replica exchange; on-the-fly learning of (equivariant) graph neural network potentials; thermodynamic integration and MBAR; asynchronous execution on thousands of nodes (**paper**, **code**)
- transfer learned reaction coordinates for efficient rare event sampling
  learned coordinates are by construction invariant with respect to translations, rotations, and permutations. Data efficiency exceeds SOTA because it exploits the learned feature representation of GNN potentials (**paper**)
- fine-tuning of pretrained GNN potentials using energy corrections with respect to high-level QM data
  the base GNN is augmented with an additional ΔE readout which is trained using energies *only* (**paper**)
- GPU-accelerated simulation of disordered phase transitions in soft porous crystals
  I developed and implemented a fully anisotropic energy-only pressure control algorithm (**code**)

Research Intern Camlin Technologies (CH) JUN 2017 – DEC 2017

- implemented a quantum mechanical model to predict emission spectra of layered semiconductor structures used in tunable IR lasers
- performed photoluminescence and transmission measurements of the structures at cryogenic temperatures using FTIR spectroscopy, and improved the accuracy of the experimental setup

Research Intern Trinity College Dublin (IE) JUN 2016 – SEP 2016
developed and built a pulsed LED system for high-dynamic range particle imaging velocimetry using custom PCBs with high-power picosecond pulses

PERSONAL

funding	MS scholarschip from the Belgian American Educational Foundation (BAEF; tuition + stipend) PhD fellowship from Fonds Wetenschappelijk Onderzoek Flanders (FWO)
skills	Python (PyTorch/JAX), asynchronous execution, bash, Docker/Apptainer, Inkscape, Blender
teaching	undergraduate quantum mechanics & statistical mechanics
hobbies	music production, swimming, tennis
languages	Dutch (native), English (excellent), French (good), German (basic)

PUBLICATIONS

1 **A Novel NPT Thermodynamic Integration Scheme to Derive Rigorous Gibbs Free Energies for Crystalline Solids**
Karel LK De Witte, Tom Braeckevelt, Massimo Bocus, Sander Vandenhaute, Veronique Van Speybroeck
arXiv:2602.20738, **2026**

2 **The effect of the A-site cation on the phase transition temperature of metal halide perovskites**
Tom Braeckevelt, Sander Vandenhaute, Sven MJ Rogge, Johan Hofkens, Veronique Van Speybroeck
arXiv:2602.20058, **2026**

3 **Cluster-based machine learning potentials to describe disordered metal–organic frameworks up to the mesoscale**
Pieter Dobbelaere, Sander Vandenhaute, Veronique Van Speybroeck
Chemistry of Materials 37 (15), 5696-5709, **2025**

4 **Orb-v3: atomistic simulation at scale**
Benjamin Rhodes[†], Sander Vandenhaute[†], Vaidotas Šimkus, James Gin, Jonathan Godwin, Tim Duignan, Mark Neumann
[†]: these authors contributed equally
arXiv:2504.06231, **2025**

5 **Water motifs in zirconium metal-organic frameworks induced by nanoconfinement and hydrophilic adsorption sites**
Aran Lamaire, Jelle Wieme, Sander Vandenhaute, Ruben Goeminne, Sven M. J. Rogge, Veronique Van Speybroeck
Nature Communications , **2024**, 15, 9997

6 **The Operando Nature of Isobutene Adsorbed in Zeolite H-SSZ-13 Unraveled by Machine Learning Potentials Beyond DFT Accuracy**
Massimo Bocus[†], Sander Vandenhaute[†], Veronique Van Speybroeck
[†]: these authors contributed equally
Angewandte Chemie Int. Ed. **2024**, e202413637

7 **Rare Event Sampling using Smooth Basin Classification**
Sander Vandenhaute, Tom Braeckevelt, Pieter Dobbelaere, Massimo Bocus, Veronique Van Speybroeck
arXiv:2404.03777, **2024**

8 **Machine learning potentials for metal-organic frameworks using an incremental learning approach**
Sander Vandenhaute, Maarten Cools-Ceuppens, Simon DeKeyser, Toon Verstraelen, Veronique Van Speybroeck
npj Computational Materials, **2023**, *9*, 19

9 **Accurately Determining the Phase Transition Temperature of CsPbI3 via Random-Phase Approximation Calculations and Phase-Transferable Machine Learning Potentials**
Tom Braeckevelt, Ruben Goeminne, Sander Vandenhaute, Sander Borgmans, Toon Verstraelen, Julian A. Steele, Maarten B. J. Roeffaers, Johan Hofkens, Sven M. J. Rogge, Veronique Van Speybroeck
Chemistry of Materials, **2022**, *34*, 8561–8576

10 **Large-Scale Molecular Dynamics Simulations Reveal New Insights Into the Phase Transition Mechanisms in MIL-53(Al)**

Sander Vandenhaute, Sven M. J. Rogge, Veronique Van Speybroeck
Frontiers in Chemistry, **2021**, *9*, 718920

11 **Towards modeling spatiotemporal processes in metal–organic frameworks**
Veronique Van Speybroeck, Sander Vandenhaute, Alexander E. J. Hoffman, Sven M. J. Rogge
Trends in Chemistry, **2021**, *3*, 605-619

CONFERENCE CONTRIBUTIONS

1 **(invited) Pushing the Limits of Computational Chemistry**
Sander Vandenhaute, Tom Braeckevelt, Veronique Van Speybroeck
LUMI-BE User Day, November 2024 (Charleroi, BE)

2 **Learned Rare Event Sampling at the Top of Jacob's Ladder**
Sander Vandenhaute, Massimo Bocus, Veronique Van Speybroeck
Advances in catalytic reactivity simulations under operando conditions, October 2024 (Varigotti, IT)

3 **Scalable Molecular Simulation with psiflow**
Sander Vandenhaute, Veronique Van Speybroeck
ParslFest, September 2024 (Chicago, US)

4 **(invited) Tutorial: Scalable Molecular Simulation with psiflow**
Sander Vandenhaute, Veronique Van Speybroeck
Machine Learning Interatomic Potentials: Theory and Practice, November 2023 (Helsinki, FI)

5 **(invited) Free Energy Calculations at the Top of Jacob's Ladder**
Sander Vandenhaute, Massimo Bocus, Veronique Van Speybroeck
Machine Learning Interatomic Potentials: Theory and Practice, November 2023 (Helsinki, FI)

6 **Scalable Molecular Simulation with psiflow**
Sander Vandenhaute, Veronique Van Speybroeck
ParslFest, October 2023 (Chicago, US)

7 **Free Energy Calculations at the Top of Jacob's Ladder**
Sander Vandenhaute, Massimo Bocus, Veronique Van Speybroeck
EuroHPC User Day, October 2023 (Brussels, BE)

8 **On-the-fly Learning for Activated Processes**
Sander Vandenhaute, Maarten Cools-Ceuppens, Simon DeKeyser, Toon Verstraelen, Veronique Van Speybroeck
Swiss Equivariant Learning Workshop, July 2022 (Lausanne, CH)

9 **Large-Scale Molecular Simulations for Metal-Organic Frameworks**
Sander Vandenhaute, Sven M. J. Rogge, Toon Verstraelen, Veronique Van Speybroeck
The Influence of Crystal Size and Morphology on Framework Materials, Februari 2022 (online)

10 **Systematic Coarse-Graining in Metal-Organic Frameworks**
Sander Vandenhaute, Sven M. J. Rogge, Veronique Van Speybroeck
EuroMAT, September 2021 (online)