ANDRIJ VASYLENKO

Computational Materials Scientist | AI-Driven Discovery

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Computational materials scientist integrating DFT, machine learning, and high-throughput simulation workflows for autonomous materials discovery. Over a decade of experience bridging condensed-matter physics, solid-state chemistry, and AI. Developer of Bayesian-optimisation frameworks that accelerate first-principles screening; contributor to open-source tools (e.g., PyOD >16 M downloads). Proven record of mentoring researchers, managing HPC resources, and translating AI-driven models into experimentally validated discoveries (*Science*, *Nature Communications*, UK patent GB2627468).

POSITIONS HELD & INDUSTRY COLLABORATIONS

Research Associate (Permanent), University of Liverpool (UoL)

2024–Present Lead computational materials modelling and machine-learning method development; responsible for project strategy, workflow design, and supervision of PhD students and postdoctoral researchers in AI-driven materials discovery across chemistry and computer science.

Research Consultant, Ceres Power via UoL

2022–Present Collaborate with Prof. Matthew Rosseinsky, OBE FRS, to design and optimise functional materials for energy applications. Developed DFT- and ML-driven workflows linking simulation with experimental validation; contributed to materials selection strategy and high-throughput screening pipelines for industrial deployment.

Research Associate, University of Liverpool

2018–2024 Developed supervised, semi-supervised, and unsupervised ML algorithms for materials representation, discovery, and functional optimisation. Led large-scale first-principles modelling of condensed-matter systems using VASP and ASE; integrated active-learning approaches for accelerated phase-field exploration.

Research Fellow, University of Warwick

2015–2018 Led high-throughput DFT-based crystal structure prediction of nanoconfined materials, including modification of VASP to model steric confinement effects. Developed predictive models validated experimentally, resulting in first-author publications in *ACS Nano*, *Physical Review B*, and *Physical Review Materials*.

EDUCATION

PhD Physics Adam Mickiewicz University, Poznań

2013–2015 PhD in Physics — Adam Mickiewicz University, Poznań
Marie Sk lodowska-Curie Doctoral Fellowship (Eminence Programme)
Thesis: *Nonequilibrium statistical theory and ab initio modelling of electron–ionic systems.*
Advisors: Prof. Dr Sci. Mykhailo Tokarchuk & Prof. dr hab. Stefan Jurga

AWARDS & GRANTS (SELECTED)

2025–2026 UK AIchemy Collaborative Travel Fund, *Principal Investigator*. Initiated collaboration with Empa Dübendorf on high-throughput computational–experimental integration.

2025 UK National Supercomputing Service (Isambard AI), *Principal Investigator*. Competitive allocation of 36,000 GPU-hours for AI-driven materials design.

2024–2025	UK EPSRC HPC National computational resource, *Principal Investigator*. Allocation of 1,382,400 CU hours for high-throughput materials simulation.
2018–2021	National Science Centre (NCN) (Poland), *Researcher Co-Investigator*, High-entropy alloys via high-power pulsed hybrid magnetron sputtering: modelling, synthesis, and investigation of functional properties.
2015–2018	NCN (Poland), *Researcher Co-Investigator*, Modelling and design of metal and transition metal oxides nanostructures on graphene for functional materials applications.
2013–2015	EU Marie Sk lodowska-Curie Doctoral Fellowship , *PhD Fellow*. Awarded under the Eminence programme for doctoral research in theoretical condensed matter physics.

SCIENTIFIC COMPUTING

Programming	Python, Fortran, C
Parallel & HPC	MPI, OpenMP, Slurm, PyTorch Distributed (DDP)
Machine Learning	PyTorch, Scikit-Learn
Automation	ASE, Pymatgen
Data Handling	NumPy, Pandas, Matplotlib
Atomisitics	VASP, Quantum ESPRESSO, LAMMPS, GULP
Version Control	Git, Docker

SELECTED PUBLICATIONS & PATENTS

A. Vasylenko, et al. *Physics-informed diffusion models for extrapolating crystal structures beyond known motifs*, *Preprint*, arXiv:2501.23181 (2025). Introduces a physics-informed generative model and chemically grounded diversity metric that condition diffusion sampling beyond training distributions, producing novel, stable frameworks.

Z. Ursani, D. Antypov, K. Atkinson, M. Dyer, M. Rosseinsky, S. Schewe, and A. Vasylenko. *Protocol for Generating New Patterns Using Monte Carlo Ensemble of Hierarchical Models*, *AIPR* (2025), ID:AP0121. *Best Paper Award*. Introduces a probabilistic ensemble framework for pattern generation, linking hierarchical modelling with generative AI concepts.

G. Han, M. J. Rosseinsky, A. Vasylenko, et al. *UK Patent Application, University of Liverpool. GB2627468A - Lithium-Ion conductor materials*

G. Han, A. Vasylenko, L. M. Daniels, et al. *Superionic lithium transport via multiple coordination environments defined by two anion packing*, *Science*, 383 (6684), 739–744 (2024). Integrates AI-guided analysis with high-throughput DFT and AIMD simulations to identify and validate a novel superionic solid electrolyte.

A. Vasylenko, B. Asher, C. M. Collins, et al. *Inferring energy–composition relationships with Bayesian optimisation for enhanced exploration of inorganic materials*, *J. Chem. Phys.*, 160, 054110 (2024). Develops an active-learning framework coupling Bayesian optimisation with ab-initio data for accelerated phase-field exploration.

A. Vasylenko, J. Gamon, B. B. Duff, et al. *Element selection for crystalline inorganic solid discovery guided by unsupervised machine learning of experimentally explored chemistry*, *Nat. Commun.*, 12, 5561 (2021). Applies unsupervised representation learning to map chemical space and identify unexplored stable element combinations.