ANDRIJ VASYLENKO

Computational Materials Scientist | AI-Driven Discovery

andrij@liverpool.ac.uk | URL | GitHub | GoogleScholar

EDUCATION

2013–2015

PhD Physics Adam Mickiewicz University, Poznań

Marie Sklodowska-Curie Doctoral Fellowship (Eminence Programme)
Nonequilibrium statistical theory and ab initio modelling of electron–ionic systems.
Advisors: Prof. Dr Sci. Mykhailo Tokarchuk & Prof. dr hab. Stefan Jurga

POSITIONS HELD & INDUSTRY COLLABORATIONS

2018–Present

Research Associate, University of Liverpool (UoL)

Lead development of computational and machine-learning workflows for materials discovery; contribute to project strategy, workflow design, and informal supervision of PhD students and postdoctoral researchers across chemistry and computer science.

2022–2024

Research Consultant, Ceres Power via UoL

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.

2015–2018

Research Fellow, University of Warwick

Led high-throughput DFT-based crystal-structure prediction of nanoconfined materials, including modification of CASTEP to model steric confinement effects. Developed predictive models validated experimentally, resulting in first-author publications in leading condensed-matter and materials-science journals.

SELECTED OUTPUTS

Science ***383****, 739 (2024)*

Discovery of a superionic lithium conductor through multi-anion structural design

Identified a new Li-ion conductor using AI-guided analysis and *ab initio* simulation. Demonstrated predictive link between element combination and synthetic accessibility enabling discovery of a novel solid electrolyte.

Nat. Commun. ***12****, 5561 (2021)*

Unsupervised learning for element selection in crystalline solids

Introduced an unsupervised representation of chemical space to rank unexplored elemental combinations, forming the basis for synthesis-aware AI now proposed in this Fellowship.

J. Chem. Phys. ***160****, 054110 (2024)*

Bayesian optimisation for inorganic exploration

Developed an active-learning framework coupling Bayesian optimisation with *ab initio* techniques, accelerating exploration of compositional space with uncertainty estimates.

UK Patent GB2627468A

Lithium-ion conductor materials

Invented and computationally validated a novel Li-ion conductor, incorporated into Liverpool's experimental screening of candidate solid electrolytes.

Preprint arXiv:2510.23181 (2025)

Physics-informed diffusion models for crystal generation

Proposes a physics-grounded generative model capable of extrapolating stable crystal structures beyond known motifs, expanding AI reach to uncharted chemical space.

RESEARCH FUNDING

AIchemy Collaborative Fund — PRINCIPAL INVESTIGATOR

2025–2026 Initiated collaboration with Empa (Switzerland) on AI-guided synthesis of polar nitrides.

Isambard-AI HPC Computational Grant — PRINCIPAL INVESTIGATOR

2025 36,000 GPU-hours for AI-driven materials design.

EPSRC HPC National Resource — CO- INVESTIGATOR

2024–2025 1.38M CU hours for high-throughput materials simulations.

UKRI EPSRC Open Fellowship — PRINCIPAL INVESTIGATOR

2024 Unfunded; proposal submitted under the EPSRC Energy theme and reclassified to the Physical Sciences theme, which was not funded in that call. The Physical Sciences panel recommended resubmission of the programme under the *UKRI Future Leaders Fellowship* scheme.

Royal Society International Exchange — PRINCIPAL INVESTIGATOR

2026 (under review) Collaboration with ETH Zurich on AI-guided synthesis of luminescent nanomaterials.

National Science Centre (Poland) — RESEARCHER CO-INVESTIGATOR

2015–2021 Two grants on nanostructures and high-entropy alloys.

TEACHING & SUPERVISION

Centre for Responsible AI, NEW YORK UNIVERSITY

2025 Lead a semester-long generative-AI project for materials modelling within the Centre's fellows programme, supervising three PhD-level researchers (remote) on model design and evaluation, with the option to extend into subsequent semesters.

University of Liverpool

2021–Present Provide informal co-supervision and onboarding support for Master's, PhD and postdoctoral researchers in Computer Science and Chemistry working on computational materials and AI, including guidance on project definition, HPC proposals, and implementation of ML and simulation workflows.

PRIZES, AWARDS & RECOGNITION

2025 UK Department for Science & Technology feature – EIMCRYSTAL project showcased to the Secretary of State.

2025 Invited Speaker, Empa (Switzerland).

2017 Warwick Awards for Teaching Excellence, *Faculty Award*, University of Warwick.

2013-15 Marie Sklodowska-Curie Fellowship.

COLLABORATIONS & EXTERNAL ENGAGEMENT

2022–Present Active collaborations with Empa, ETH Zurich, Ceres Power Ltd, the Centre for Responsible AI at NYU, and internal partners at the Materials Innovation Factory and Department of Computer Science. Contribute to external visibility of AI for Science through national communication campaigns and public-facing presentations.

LEADERSHIP, TRAINING & MENTORING

2021–Present Mentor early-career researchers in ML and data-driven discovery, including informal co-supervision of students at Liverpool and supervision of three PhD-level research fellows through the NYU Responsible AI #RAIforUkraine programme, which supports Ukrainian students whose studies have been disrupted by the war. Contribute to interdisciplinary training in AI, chemistry, and HPC, and promote transparent, reproducible and inclusive AI practices in collaborative projects.