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Martin Uhrín

With a background in physics and computer science, I specialize in high-throughput DFT calculations combined with machine learning for materials discovery. My current work focuses on developing explainable, physics-informed machine learning methods, especially generative models for inverse design—enabling the prediction of materials from desired properties and reshaping experimental characterisation.

Personal Information

Date of Birth	1st May, 1985	Citizenship	British and Slovak (EU)
Languages	English - native Slovak - native French - B2 German - basic		
OrcID	0000-0001-6902-1289	Scholar ID	coQ8EwwAAAAJ

Education

Sept 2010 - Dec 2014 **PhD, Computational Condensed Matter**, *UCL*, UK — *Advisor* Chris Pickard
Defense date 19/06/2015
Title: Understanding the Structure of Materials at the Intersection of Rationalisation, Prediction and Big Data

2003 - 2007, 2008 - 2009 **M.Phys Hons Computational Physics**, *University of Edinburgh*, UK,
1st class. Class medal for highest grade in class.
Five year integrated masters program plus self organised year in industry (2007/8)
Title: Initial Stages of Planetary Formation: Simulation of Dust Cluster Growth and Collision

Employment History

Nov 2023 - **MIAI Research Chair**, *Université Grenoble Alpes*, France
Holder of an inteternational chair from the Multidisciplinary Institute in Artificial Intelligence, I lead a team conducting research into the development of machine learning methods to accelerate materials modelling and enable inverse design using generative models.

Mar 2021 - Sept 2023 **Scientist**, *EPFL*, Switzerland — *Advisor* Nicola Marzari
Hosted in the group of Prof. Nicola Marzari, I conduct independent research on machine learning methods for materials and molecules, focusing on the development of physics inspired methods for property prediction and inverse design. I was also responsible for EPFL's contribution to pan-European 'DOME 4.0: Digital Marketplaces Ecosystem' project.

Oct 2019 - Mar 2021 **Postdoctoral researcher**, *DTU*, Denmark — *Advisors* Jin Chang and Tejs Vegge
My work focused on the computational discovery of cathodes and electrolytes for metal-air batteries, using high-throughput quantum chemistry and machine learning to predict the conductivity of ionic liquids.

Jan 2015 - Jan 2019 **Postdoctoral researcher**, *EPFL*, Switzerland — *Advisor* Nicola Marzari
I was lead author of the AiiDA workflow engine, enabling high-throughput simulations for large-scale materials discovery, including efforts to map properties of known and hypothetical binary compounds.

Jul 2007 - Jun 2008 **Software Engineer**, *Microsoft Game Studios (Rare)*, UK
Software engineer on the Xbox 360 game 'Banjo-Kazooie: Nuts & Bolts'; tasked with writing high-performance C++ gameplay and physics code as part of large team.

Approved Research Projects

As PI

2025 - 2029 ANR project LUMEN, €170k (€900k total) for "Liquid structure understanding for microstructure engineering with novel upscaling assisted by artificial intelligence"

2025 - 2028 Carnot Energie/IMEP^2 doctoral school, €150k for "Machine Learning for elasto-caloric materials discovery"

2024 - 2028 ANR project AMADEUS, €80k (€900k total) for "Automated and machine learning driven design and discovery of high entropy ceramics perovskite oxides for energy applications"

2023 - 2027 MIAI International Chair, €600k for "From Edisonian trial and error to the inverse design of materials and molecules"

As participant

2022 - 2026 CSCS Compute allocation: 5.3M node hours for "High-throughput screening of novel Li-ion cathodes at finite temperature"

2021 - 2024 CSCS Compute allocation: 2.1M node hours for "Materials for energy"

2021 - 2024 Horizon 2020 "Battery Interface Genome - Materials Acceleration Platform" (€20M, 34 partners, PI: Tejs Vegge)

2017 - 2020 Horizon 20202: "Materials Modelling Marketplace for Increased Industrial Innovation" (€9.2M total, 18 partners, PI: Adham Hashibon)

Supervision of Junior Researchers

Postdoc

Mar 2025 - Giovanni Trezza, Next-generation equivariant generative machine learning models for the inverse design of materials and molecules

PhD

Dec 2025 - Zhiyi Wang, Machine learning-enhanced atomic simulations for the discovery of novel elastocaloric materials

Dec 2023 - Mattia Ragni, Development of physics-based machine learning models for accelerated discovery of materials

Mar 2021 – Jun 2025 Austin Zadoks (co-advisors Nicola Marzari, Antimo Marrazzo), Development of equivariant neural network models for the prediction of tensorial quantities of materials

Master's

Jul 2026 Aditi Chauhan, Magnetic exchange integrals in cuprate superconductors by machine learning

May 2026 Aycha Couchene, Machine Learning of Electro-Optical Properties with Graph Neural Networks

Sept 2022 Anna Paulish, Variational Autoencoder for generating novel glassy structures

Mar 2023 Alessandro D'Urso, Equivariant models for predicting tensorial properties of materials

Sept 2022 Zhiyi Wang, Machine learning interaction potentials for solid electrolytes

Teaching Activities

Autumn 2025 **Modélisation des matériaux**, *Project supervisor*

August 2025 **DIADEM Summer School**, *Lecturer*, Physics-Informed Machine Learning at the Atomic Scale

August 2025 **CECAM School on Machine Learning for Molecules and Materials Research**, *Lecturer*, Physics-Informed Machine Learning of Response Properties

Autumn 2024 **Modélisation des matériaux**, *Project supervisor*

Summer 2024 **Modélisation des matériaux summer school**, *Lecturer*, Introduction to machine learning for materials

May 2020 Developed and taught virtual Atomic Simulation Environment tutorial to 50+ BIG-MAP members.

Autumn 2016 **Modélisation des matériaux**, *Teaching assistant*
MSE-370 course at EPFL - Responsible for giving tutorials on materials modelling using C++

Jul 2012 - Dec 2013 **Introduction to Scientific Computing with C++**, *Lecturer*
Created new course taken by incoming PhD students at UCL. Taught over 65 students in 4 sessions.

Recent talks

2026

invited ENS Physics Department seminar Equivariant Neural Networks: A General Framework for Learning in Physical Systems

2025

invited School on Machine Learning for Molecules and Materials Research Physics-Informed Machine Learning of Response Properties

invited SISSA seminar Physics-Informed Machine Learning of Response Properties

invited MaterialsDay Accelerating the Path to Novel Materials: Physics based machine learning...

2024

invited Paul Scherrer Institute department seminar Physics inspired machine learning at the atomic scale

invited CINaM department seminar Physics inspired machine learning at the atomic scale

invited DIADEM GenAI, NumpEX trans-PEPR discussion, Paris When GenAI meets Materials Science

invited Universidade Federal Fluminense physics department seminar, Brazil Physics inspired machine learning at the atomic scale

invited Ilum Escola de Ciência seminar, Brazil Physics inspired machine learning at the atomic scale

invited Interdisciplinary collaborative meeting, São Carlos, Brazil Symmetry-aware generative model for glassy motifs

Brazilian Materials Research Society Meeting, Santos Symmetry-aware models beyond energies and forces

invited Machine Learning Interatomic Potentials and Accessible Databases, Grenoble, FR Symmetry-aware models beyond energies and forces

Journées plénières GDR IAMAT 2024, Toulouse, FR Equivariant machine learning: A natural and highly data-efficient tool for predicting physical quantities

Machine Learning Modalities for Materials Science, Ljubljana, SLO, Symmetry-aware generative model for glassy motifs

2023

invited Univ. Ulm Institute of Theoretical Chemistry seminar Machine learning self-consistent Hubbard parameters using equivariant neural networks

Professional Service

Projects PEPR DIADEM - French national project dedicated to accelerating materials discovery, management team

Data-driven Applications towards the Engineering of Functional Materials COST Action working group co-lead

Journals Associate editor, AI for Science (IOPScience)

Refereeing ○ Physical Review Letters ○ Physical Review B. ○ Computer Physics Communications ○ Nature Machine Intelligence ○ npj computational materials ○ JACS ○ JOSS

Organisation of Conferences

Oct 2024 **Condensed Matter Days 2024**, *Marseille, France*
Organised mini-colloquium: *Advanced in machine learning for materials modelling*

Jun 2022 **Swiss Equivariant Learning Workshop**, *Lausanne, Switzerland*, 100 participants
I was lead organiser of first European workshop dedicated to equivariant methods in machine learning with 17k Fr budget

Dec 2021 **Symmetry-Aware Neural Networks for the Material Sciences**, *Boston, USA*, ∼30 participants
Developed and delivered tutorial on "Analyzing geometry and structure of atomic configurations with equivariant and invariant functions" using e3nn

May 2018 **PRACE-MaX Tutorial on high-throughput computations: general methods and applications using AiiDA**, *Bologna, Italy*

May 2017 **2nd MARVEL/Psi-k/MaX tutorial on high-throughput computations**, *Lausanne, Switzerland*, ∼50 participants

Mar 2017 **MARVEL/MaX advanced AiiDA tutorial**, *Lausanne, Switzerland*, ∼20 participants

Jan 2017 **College on Multiscale Computational Modeling of Materials for Energy Applications** **AiiDA tutorial**, *Trieste, Italy*, ∼50 participants

Dec 2016 & Oct 2017 **AiiDA Coding Weeks**, *Switzerland*, ∼20 participants
Organisation of an intensive week of coding with collaborators from Switzerland and abroad

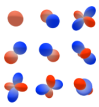
Jun 2016 **1st MARVEL/Psi-k/MaX tutorial on high-throughput computations**, *Lausanne, Switzerland*, ∼50 participants
Organisation, development and delivery of tutorial material

Other artefacts with documented use

Software

Library to generate invertible atomic fingerprints and create neural networks for machine learning interaction potentials
Lead author ○ `https://github.com/muhrin/milad/`

A scalable computational infrastructure for automated reproducible workflows and data provenance
downloads 36k/month Lead author of workflow engine ○ `https://aiida.readthedocs.io`



e3nn: A modular framework for neural networks with Euclidean symmetry
downloads 426k/month Developer ○ `https://docs.e3nn.org`
Mario Geiger, Tess Smidt, . . . , **MU** et al. (2022). e3nn/e3nn: 2022-04-13 (0.5.0). Zenodo.

mincePy: A python library to store scientific data types in a MongoDB database
downloads 1.3k/month Lead author ○ `https://mincepy.readthedocs.io`

pyOS: An easy-to-use tool for working collaboratively on scientific python data
downloads 886/month Lead author ○ `https://pyos.readthedocs.io`

kiwiPy: A robust, high-throughput queuing system for managing scientific jobs
downloads 59k/month Lead author ○ `https://kiwipy.readthedocs.io`

plumPy: A general purpose python workflow library that powers AiiDA
downloads 63k/month Lead author ○ https://plumpy.readthedocs.io

Standards

OPTIMADE: A standard for accessing and querying databases of atomic structures
Contributed to the standardisation process at regular meetings
http://www.optimade.org/

BattINFO A battery interface domain ontology based on the European Materials Modelling Ontology
Contributed expertise on metal-air battery anodes and electrolytes
https://github.com/BIG-MAP/BattINFO

Collaborators

- Prof. Nicola Marzari, University of Cambridge
- Prof. Michele Ceriotti, EPFL
- Prof. Tess Smidt, Massachusetts Institute of Technology
- Prof. Eliodoro Chiavazzo, University of Turin
- Dr. Assil Bouzid, IRCER, Limoges
- Dr. Lorenzo Monacelli, Sapienza University of Rome

Publications

Preprints and in preparation

M. Ragni and **M. Uhrin**, "Physics-informed machine learning of NMR spectra", In preparation.

M. Ragni, L. Bastonero, I. Timrov, and **M. Uhrin**, "A Unified Equivariant Framework for Physics-Based Prediction of Atomistic Response Functions", In preparation.

Z. Wang, S. Muy, N. Marzari, and **M. Uhrin**, "Using equivariant machine learning potentials to study Li_6PS_5Cl Argyrodite solid electrolytes for all-solid-state batteries", In preparation.

M. Uhrin, J. P. A. Martins, and L. T. Costa, "Predicting experimental properties of ionic liquids using equivariant graph neural networks", In preparation.

A. Jose, E. Devijver, **M. Uhrin**, N. Jakse, and R. Poloni, "Predicting spin-crossover behavior in metal-organic frameworks from limited and noisy data using quantile active learning", Submitted to npj Computational Materials .

Peer-reviewed

D. Bissuel, L. Orveillon, B. Arrondeau, P. A. D. Mendonça, I. Piazza, **M. Uhrin**, et al., "Reproducible container solutions for codes and workflows in materials science", Advanced Engineering Materials, Accepted 2025.

S. P. Huber, M. Minotakis, M. Bercx, T. Reents, K. Eimre, N. Paulish, N. Hörmann, **M. Uhrin**, N. Marzari, and G. Pizzi, "Mc3d: the materials cloud computational database of experimentally known stoichiometric inorganics", Digital Discovery **5**, 1114–1131 2026.

M. Uhrin, A. Zadoks, L. Binci, N. Marzari, and I. Timrov, "Machine learning hubbard parameters with equivariant neural networks", npj Computational Materials **11**, 19 2025.

S. Clark, F. L. Bleken, S. Stier, E. Flores, C. W. Andersen, M. Marcinek, A. Szczesna-Chrzan, M. Gaberscek, M. R. Palacin, **M. Uhrin**, and J. Friis, "Toward a unified description of battery data", Advanced Energy Materials **12**, 2102702 2022.

M. Uhrin, "Through the eyes of a descriptor: Constructing complete, invertible descriptions of atomic environments", Physical Review B **104**, 144110 2021, arXiv:2104.09319.

I. E. Castelli, D. J. Arismendi-Arrieta, A. Bhowmik, I. Cekic-Laskovic, S. Clark, R. Dominko, et al., "Data Management Plans: the Importance of Data Management in the BIG-MAP Project", Batteries & Supercaps (Wiley), batt.202100117 2021, arXiv:2106.01616.

S. P. Huber, E. Bosoni, M. Bercx, J. Bröder, A. Degomme, V. Dikan, et al., "Common workflows for computing material properties using different quantum engines", npj Computational Materials **7** (Springer Nature), 136 2021, arXiv:2105.05063.

C. W. Andersen, R. Armiento, E. Blokhin, G. J. Conduit, S. Dwaraknath, M. L. Evans, et al., "OPTIMADE, an API for exchanging materials data", Scientific Data **8** (Springer Nature), 217 2021, arXiv:2103.02068.

M. Uhrin, S. P. Huber, J. Yu, N. Marzari, and G. Pizzi, "Workflows in AiiDA: Engineering a high-throughput, event-based engine for robust and modular computational workflows", Computational Materials Science **187** (Elsevier), 110086 2021.

L. Talirz, S. Kumbhar, E. Passaro, A. V. Yakutovich, V. Granata, F. Gargiulo, et al., "Materials Cloud, a platform for open computational science", Scientific Data **7** (Springer Nature), 299 2020.

S. P. Huber, S. Zoupanos, **M. Uhrin**, L. Talirz, L. Kahle, R. Häuselmann, et al., "AiiDA 1.0, a scalable computational infrastructure for automated reproducible workflows and data provenance", Scientific Data **7** (Springer Nature), 300 2020.

M. Uhrin and S. Huber, "kiwiPy: Robust, high-volume, messaging for big-data and computational science workflows", Journal of Open Source Software **5**, 2351 2020.

G. Schusteritsch, **M. Uhrin**, and C. Pickard, "Single-Layered Hittorf's Phosphorus: A Wide-Bandgap High Mobility 2D Material", Nano Letters **16**, 2975–2980 2016.

G. A T Pender and **M. Uhrin**, "Predicting non-square 2D dice probabilities", European Journal of Physics **35** (IOP Publishing), 045028 2014.

G. Ackland, K. D'Mellow, S. Daraszewicz, D. Hepburn, **M. Uhrin**, and K. Stratford, "The MOLDY short-range molecular dynamics package", Computer Physics Communications **182** (Elsevier), 2587–2604 2011.

Contributions to books

M. Uhrin, G. Pizzi, N. Mounet, N. Marzari, and P. Villars, "A High-Throughput Computational Study Driven by the AiiDA Materials Informatics Framework and the PAULING FILE as Reference Database", in *Materials informatics* (Wiley), pp. 149–170.

References

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