+44 7854 246 463
martin.uhrin.10@ucl.ac.uk
www.digitalbaker.net
martin.uhrin
muhrin

Martin Uhrín

I have a mixed physics/computer science background and steer my research to topics that can benefit from a fusion of explainable, physics inspired, models, and advanced methods from computer science and mathematics such as deep learning and equivariant representations. A big driver of my research is a desire to understand the interplay between energy and geometry which is at the heart of explaining why nature prefers certain atomic arrangements over others.

Personal Information

Date of Birth	1st May, 1985	Citizenship	British and Slovak
Languages	English - native French - C1	Slovak - native German - basic	Work Permit	Swiss "B" permit

Professional Experience

2021 - present **Scientist**, EPFL, Switzerland - Nicola Marzari.
Hosted in the group of Prof. Nicola Marzari I am responsible for EPFL's contribution to pan-European 'DOME 4.0: Digital Marketplaces Ecosystem' project. In addition to leading a work package my main contribution centres around developing and making accessible supervised and unsupervised machine learning methods.

2019 - 2021 **Postdoctoral researcher**, DTU, Denmark - Jin Chang and Tejs Vegge.
My work focused on the computational discovery of metal-air batteries cathodes and electrolytes. Using results from high-throughput quantum chemistry simulations we develop a machine learning model to predict the conductivity of ionic liquids.

2015 - 2019 **Postdoctoral researcher**, EPFL, Switzerland - Nicola Marzari.
I was the lead author of the AiiDA workflow engine, a widely used materials informatics platform for reliably carrying out tens of thousands of materials simulations. My research centred around high-throughput materials discovery and was part of an effort to determine the basic properties of all the known, and yet unknown, binary compounds.

2007 - 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.

Education

2010 - 2014 **PhD, Computational Condensed Matter - University College London**.
Supervisor Prof. Chris J. Pickard
Thesis Understanding the Structure of Materials at the Intersection of Rationalisation, Prediction and Big Data

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

Awards and Grants

2020
- Contributed to the successful "Battery Interface Genome - Materials Acceleration Platform" proposal (3 years, €20M, 34 partners)

2017
- PRACE Tier-0 allocation of 1M node hours for high-throughput simulation of all binary phases
- Contributed to the successful "MARKETPLACE - Materials Modelling Marketplace for Increased Industrial Innovation" proposal (€9.2M total)

2014
- Thomas Young Centre Student Day best thesis talk

2010
- Wingate Scholarship for independent research

2009
- M.Phys thesis awarded 90% - highest grade ever given by department
- Edinburgh University class medal 2009
- Marian A. S. Ross Prize for excellent performance
- Department nomination for UK Science, Engineering and Technology awards
- Royal Society of Edinburgh Cormack Vacation Research Scholarship

Collegial

PhD Students

2021 - present Austin Zadoks (Co-advising with Nicola Marzari)

Project Students

Summer 2018 Austin Zadoks (Materials Science)

Summer 2016 Yuntong Zhu (Materials Science)

Summer 2015 Vojislav Dukic (CS)

Teaching

2020 Virtual ASE tutorial to 50+ BIG-MAP members.

2018 Co-developed and lectured two week course on molecular dynamics simulations for 16-17 year old students.

2015 - 2018 Co-developed and delivered numerous AiiDA tutorials (~4 per year, 25-50 students each).

2012 - 2014 Created 3-day "Introduction to Scientific Computing with C++" taken by incoming PhD students at UCL. Taught over 65 students in 4 sessions.

Other Professional Activities

Author of over seven community codes and contributor to many more, currently totalling **~18k downloads/month**.

2015 - present Referee to APS journals PRL and PRB.

Outreach

Created 'CrystalExplorer' Android app bringing crystal structure prediction to the public.
Participated in 'A matter of substance' art exhibition displaying 3D printed crystal structures.

Computational Skills

I have many years of professional experience using several programming languages and expert knowledge of algorithm and data structures as well as best coding practices.

Programming Python, C/C++, Java, PHP, Fortran, C#, Perl

Machine learning PyTorch, TensorFlow and TFLearn, e3nn

Parallelisation CUDA, OpenMP, MPI, Co-array Fortran, Unified Parallel C, pthreads

Web/Data RabbitMQ (AMQP), MongoDB, SQL, REST, HTML, CSS, JavaScript

Codes CASTEP, Quantum ESPRESSO, MOLDY, Amsterdam Density Functional, VASP

Publications

2021 C. W. Andersen et al., "OPTIMADE: an API for exchanging materials data", Submitted to Scientific Data, 1–11 2021, arXiv:2103.02068.

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

M. Uhrin et al., "Workflows in AiiDA: Engineering a high-throughput, event-based engine for robust and modular computational workflows", Computational Materials Science **187**, 110086 2021, eprint: 2007.10312.

2020 S. P. Huber et al., "AiiDA 1.0, a scalable computational infrastructure for automated reproducible workflows and data provenance", Scientific Data **7**, 300 2020, eprint: 2003.12476.

L. Talirz et al., "Materials Cloud, a platform for open computational science", Scientific Data **7**, 299 2020, eprint: 2003.12510.

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.

2019 M. Uhrin et al., "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.

2016 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, arXiv:1604.04115.

2015 M. Uhrin, "Understanding the Structure of Materials at the Intersection of Rationalisation, Prediction and Big Data", PhD thesis (University College London).

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

2011 G. Ackland et al., "The MOLDY short-range molecular dynamics package", Computer Physics Communications **182**, 2587–2604 2011.

In preparation

S. P. Huber et al., "Common workflows for computing material properties using different quantum engines",

M. Uhrin and C. Pickard, "Structure prediction beyond the periodic table using the Lnnard-Jones potential",

M. Uhrin and C. Pickard, "The phases of Lennard-Jones crystals from high-throughput structure prediction",

References

Nicola Marzari
EPFL
nicola.marzari@epfl.ch
+41 21 693 11 29

Tejs Vegge
Danish Technical University
teve@dtu.dk
+45 45 25 82 01

Chris J. Pickard
University of Cambridge
cjp20@cam.ac.uk
+44 122 333 4338