

materials discovery • ab initio calculations
data management and APIs • open science & software

EDUCATION

- 2016–2023
- PhD Physics, Theory of Condensed Matter Group, University of Cambridge
- 2015–2016
- MPhil Scientific Computing, University of Cambridge, *Pass with distinction*
- 2011–2015
- MPhys Physics with Theoretical Physics, University of Manchester, *First Class (Hons)*

EXPERIENCE

- 2020–
- Researcher then BEWARE Research Fellow (jointly at Matgenix, 2022 onwards)
with Prof Gian-Marco Rignanese (*Université catholique de Louvain*)
 - Machine learning for small materials datasets (MODNet).
 - High-throughput workflows for computational materials discovery and molecular dynamics.
 - Continued development of the OPTIMADE API specification and associated software.
- 2021–
- Visiting Researcher
in the group of Prof Clare Grey (*University of Cambridge*)
 - Data management, analysis software and open APIs for materials chemistry research.
 - Funded by BIG-MAP External Stakeholder Initiative to develop [dataLab](#), a data management API and web UI for samples and associated characterisation via electrochemical cycling, NMR and XRD.
 - Founder and co-leader of a [MaRDA](#) working group on interoperable [metadata extractors](#) in materials science and chemistry.
- 2022
- Postdoctoral Research Associate
Cambridge Crystallographic Data Centre
2-month contract to implement a recommender system for the Cambridge Structural Database.
- 2016–2020
- PhD student: Crystal structure prediction for next-generation energy storage
with Dr Andrew Morris (*University of Cambridge*)
 - Computational materials discovery for conversion anodes for Li, Na and K-ion batteries.
 - Author of two open-source Python packages: database approaches for high-throughput calculations and materials design with [matador](#) and crystal structure prediction with [ilustrado](#).
 - Active member of the [OPTIMADE consortium](#) for materials database interoperability and author of the [optimade-python-tools](#) package (used in production by The Materials Project, NOMAD, Materials Cloud and others) and [odbx](#) implementation.
- 2019
- Visiting Researcher
Department of Applied Physics, Aalto University

Received HPC-Europa funding to visit the group of Prof Adam Foster for 7 weeks, with computational resources provided by the Finnish IT center for science (CSC).
- 2019
- Scientific Software Developer (Intern)
Enthought Inc., Cambridge

Worked on the open source, Horizon 2020 [FORCE project](#), adding functionality to a workflow manager for multi-criteria optimisations. Helped develop Cython bindings for the ACADO toolkit.
- 2014, 2015
- UG research: Interactions of quantised vortices in superfluid helium
with Dr Paul Walmsley & Prof Andrei Golov (*University of Manchester*)
- 2014–2015
- MPhys project: Electronic structure of defects in graphene superlattices
with Prof Francisco Guinea (*University of Manchester*)
- 2013
- UG research: Hard sphere packing of nanotube-encapsulated fullerenes
with Dr Ho-Kei Chan & Prof Elena Besley (*University of Nottingham*)

COMPUTING

	Exposure: Daily , Intermittent, <i>Occasional</i> .		
Languages	Python , Javascript, Vue.js, Fortran, Cython, C++	Expertise	Web APIs & databases, HT workflows, ML
DFT	CASTEP , Quantum Espresso, <i>GPAW</i>	Stack	FastAPI, pydantic, Flask, Tensorflow
Tools	git , vim , Docker	Practices	Test-driven development , CI

(TEACHING + SERVICE)

- 2022–
- Founded and co-lead a [MaRDA](#) working group on [metadata extractors](#) for materials science and chemistry
- 2020–
- Co-chair of the Research Data Alliance (RDA) IG *Materials Data, Infrastructure & Interoperability*
- 2018–
- Reviewed manuscripts and data for *npj. Computational Materials* (x2), *Scientific Data* (x1), *J. Phys.: Cond. Mat.* (x1), *Scientific Reports* (x1), *Digital Discovery* (x2) and *Journal of Open Source Software* (x4)
- 2022
- Organiser for the CECAM Virtual Workshop *Machine-actionable Data Interoperability for Chemical Sciences* ([MADICES](#))
- 2021
- Lecturer for “Working with Materials Databases” at the ICTP-East African Institute for Fundamental Research Training School *Machine Learning for Electronic Structure and Molecular Dynamics*
- 2021
- Mentor at Acceleration Consortium Hackathon on Scientific Databases
- 2021
- Developed and delivered a **2-day OPTIMADE tutorial** for the NOMAD Virtual Tutorial Series.
- 2016–2020
- Active member of TCM sysadmin team, Cavendish Laboratory
- 2019-2021
- Demonstrator: Part II Computational Physics, Cavendish Laboratory
 - Demonstrated scientific Python to beginners in weekly labs (2019 only).
 - Conceptualised and delivered a tutorial on the basics of [version control with Git](#) (2019-2021).
- 2016–2018
- Supervisor: 2x Part IB Electromagnetism, Dynamics and Thermodynamics, Selwyn College
 - Small group teaching, providing detailed feedback on assigned problems.
- 2016–2019
- Demonstrator: 3x Part IB Introduction to Computing (C++), Cavendish Laboratory
- 2016–2019
- Demonstrator: 4x at annual CASTEP workshop, University of Oxford
- 2017
- Volunteer: 2nd Conference of Research Software Engineers, University of Manchester
- 2016–2017
- Volunteer: Key Stage 2 Code Club, Ridgfield Primary School, Cambridge
- 2012–2015
- Tutor: GCSE Maths & Key Stage 2 Programming for [The Tutor Trust](#), Manchester
 - Provided tuition to small groups and ‘looked after children’ across 15 schools.
 - Helped lead a successful pilot to teach primary school children programming using Scratch.
- (AWARDS + HONOURS)
- 2022

BEWARE2 Fellowship from the Wallonia-Brussels Federation to fund 3 years of postdoctoral work (approx. €300,000).

2021

PI for “Interoperable data management for fundamental battery research”, BIG-MAP External Stakeholder Initiative, total funding €150,000 (personal allocation €50,000).

2019

HPC-Europa 3 funding to visit Aalto University for 7 weeks and associated computing time.

2018

Tier-2 HPC Resource Allocation: PI on project awarded 2 MCPUh, *Crystal structure prediction for next-generation solar absorbers*, **M. L. Evans**, D. O. Scanlon and A. J. Morris.

HPC Midlands+ Substantial Project: awarded 1.3 MCPUh for *High-throughput materials discovery for energy applications*, **M. L. Evans** and A. J. Morris.

2017

Tier-2 HPC Resource Allocation: Co-investigator on project awarded 4 MCPUh, *Ab initio structure prediction for next-generation battery materials*, B. Karasulu, **M. L. Evans** and A. J. Morris.

2015

Tesella Prize for Software, University of Manchester, for the most effective use of software in a final year physics project.

2013, 2014

Undergraduate research bursary for two summers as an undergraduate, totalling £4200.

2011–2015

Means-tested and merit based scholarship to study at the University of Manchester, worth £12,000.

PRESENTATIONS

2023

Invited seminar: *Interoperable data management for fundamental materials chemistry research*, Department of Chemistry, University of Nottingham, United Kingdom.

Contributed talk: *Interoperable data management for fundamental battery research*, RSC Annual Advanced Battery Materials Symposium, Institute of Physics, United Kingdom.

Invited seminar: *Interoperable data management for fundamental battery research*, Conductivity and Catalysis Lab, Technische Universität Berlin, Germany.

Invited talk: *Open Databases Integration for Materials Design* at the CECAM Flagship Workshop for FAIR and TRUE Soft Matter Simulations, Max Planck Institute for Polymer Research, Germany.

Invited seminar: *Interoperable data management for fundamental battery research*, Laboratory of Materials Simulation, Paul Scherrer Institut, Switzerland.

Invited talk: *Metadata extractors for interoperable ETL*, MaRDA Alliance Annual Meeting

Invited talk: *Open Databases Integration for Materials Design* at the Actively Learning Materials Science (AL4MS2023) workshop, Aalto University, Finland.

2021

Invited panel discussions: *International Materials Data: Joint Meeting and Metadata for Data Indexing and Discovery in Materials Science*, Research Data Alliance (RDA) 18th Virtual Plenary Meeting

Invited talk: *The OPTIMADE Ecosystem*, DoE Battery Genome Initiative

Invited panel discussion: *Delivery platforms for open marketplaces*, Research Data Alliance (RDA) 17th Virtual Plenary Meeting

2020

Invited talk: *The OPTIMADE Specification*, Research Data Alliance (RDA) 16th Virtual Plenary Meeting: Data Infrastructure for Collaborations in Materials Research

Invited talk and workshop demonstration: *odbx & OPTIMADE* and *optimade-python-tools*, CECAM Workshop, Open Databases Integration for Materials Design 2020

2019

Contributed talk: *Phosphorus anodes for potassium-ion batteries: insights from crystal structure prediction*, EMRS Spring 2019, Nice, France

Invited talk: *matador & OPTIMADE*, CECAM Workshop, Open Databases Integration for Materials Design 2019, EPFL, Switzerland

2018

Contributed talk: *Sn-P anodes for potassium-ion batteries: insights from crystal structure prediction*, SMARTER6 Conference, Ljubljana, Slovenia

Invited talk: *matador: databases and crystal structure prediction* ([slides](#)), CECAM Workshop, Open Databases Integration for Materials Design 2018, EPFL, Switzerland

2017

Invited seminar: *Crystal structure prediction for next-generation battery anodes* ([slides](#)), Solid State Seminar Series, University of Cambridge

Poster Presentation: 13th RSC Conference in Materials Chemistry ([poster](#)), University of Liverpool

2016

Poster Presentation: SMARTER5 Conference, University of Bayreuth, Germany

PUBLICATIONS

Underline indicates (joint) first authorship.

13.

Wang, Z., Gong, Y., **Evans, M. L.**, Yan, Y., Wang, S., Miao, N., Zheng, R., Rignanese, G.-M. & Wang, J. Machine learning-accelerated discovery of A_2BC_2 ternary electrides with diverse anionic electron densities. *Journal of the American Chemical Society* **145**, 26412–26424, (2023). DOI:[10.1021/jacs.3c10538](#).

12.

Lertkiatrakul, M., **Evans, M. L.** & Cliffe, M. J. PASCAL Python: A Principal Axis Strain Calculator. *Journal of Open Source Software* **8**, 5556, (2023). DOI:[10.21105/joss.05556](#).

11.

Jablonka, K. M., Ai, Q., Al-Feghali, A., Badhwar, S., Bocarsly, J. D., M., A., Bringuier, S., Brinson, L. C., Choudhary, K., Ciroi, D., *et al.* 14 Examples of How LLMs Can Transform Materials Science and Chemistry: A Reflection on a Large Language Model Hackathon. *Digital Discovery*, (2023). DOI:[10/gswbnx](#).

10.

Ells, A. W., **Evans, M. L.**, Groh, M., Morris, A. J. & Marbella, L. E. Phase transformations and phase segregation during potassiation of Sn_xP_y anodes. *Chemistry of Materials*, (2022). DOI:[10/h69d](#).

9.

Evans, M. L., Andersen, C. W., Dwaraknath, S., Scheidgen, M., Fekete, Á. & Winston, D. optimade-python-tools: a Python library for serving and consuming materials data via OPTIMADE APIs. *Journal of Open Source Software* **6**, 3458, (2021). DOI:[10/gn3w9f](#).

8.

Andersen, C. W., Armiento, R., Blokhin, E., Conduit, G. J., Dwaraknath, S., **Evans, M. L.**, Fekete, Á., Gopakumar, A., Gražulis, S., Merkys, A., *et al.* OPTIMADE, an API for exchanging materials data. *Scientific Data* **8**, 217, (2021). DOI:[10/gmnrxj](#).

7.

Breuck, P.-P. D., **Evans, M. L.** & Rignanese, G.-M. Robust model benchmarking and bias-imbalance in data-driven materials science: a case study on MODNet. *Journal of Physics: Condensed Matter* **33**, 404002, (2021). DOI:[10/gpw93d](#).

6.

Evans, M. L. & Morris, A. J. matador: a Python library for analysing, curating and performing high-throughput density-functional theory calculations. *Journal of Open Source Software* **5**, 2563, (2020). DOI:[10/gmf4mv](#).

5.

Harper, A. F., **Evans, M. L.** & Morris, A. J. Computational Investigation of Copper Phosphides as Conversion Anodes for Lithium-Ion Batteries. *Chemistry of Materials*, (2020). DOI:[10/gg5sx3](#).

4.

Harper, A. F., **Evans, M. L.**, Darby, J. P., Karasulu, B., Koçer, C. P., Nelson, J. R. & Morris, A. J. Ab initio Structure Prediction Methods for Battery Materials : A review of recent computational efforts to predict the atomic level structure and bonding in materials for rechargeable batteries. *Johnson Matthey Technology Review* **64**, 103–118, (2020). DOI:[10/ggrmgf](#).

3.

Mayo, M., Darby, J. P., **Evans, M. L.**, Nelson, J. R. & Morris, A. J. Correction to Structure Prediction of Li–Sn and Li–Sb Intermetallics for Lithium-Ion Batteries Anodes. *Chemistry of Materials*, (2018). DOI:[10/gf25zc](#).

2.

Marbella, L. E., **Evans, M. L.**, Groh, M. F., Nelson, J., Griffith, K. J., Morris, A. J. & Grey, C. P. Sodiation and Desodiation via Helical Phosphorus Intermediates in High-Capacity Anodes for Sodium-Ion Batteries. *Journal of the American Chemical Society* **140**, 7994–8004, (2018). DOI:[10/gdc6h4](#).

1.

Zhu, T., **Evans, M. L.**, Brown, R. A., Walmsley, P. M. & Golov, A. I. Interactions between unidirectional quantized vortex rings. *Physical Review Fluids* **1**, 044502, (2016). DOI:[10/gf2529](#).

Last modified: December 21, 2023