Matthew Evans

matthew@ml-evs.science
ml-evs.science
ml-evs

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

RESEARCH INTERESTS

My background in computational materials science left me with an overarching research interest in the application of machine learning, open source software and infrastructure, and data management practices to accelerate and enhance scientific workflows in the chemical and materials sciences.

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)*

SELECTED EXPERIENCE

2020– **Postdoctoral Researcher** then **BEWARE Research Fellow** (2022 onwards)
Universitè catholique de Louvain and Matgenix, with Prof Gian-Marco Rignanese

- Co-creator and architect of *datalab*, open source data management software for sample tracking and characterisation, lab management, and machine learning, deployed at several labs internationally.
- High-throughput machine-learning accelerated workflows for materials discovery and design.
- Leading development of the OPTIMADE API specification and associated software.

2021– **Visiting Researcher: Data management platforms for materials chemistry research**
University of Cambridge, with Prof Clare Grey FRS

- Developing bespoke data management platforms for materials chemistry and battery research.
- Supervising development contributions from group members and a part-time software developer.

2024– **Scientific Software Consultant** and **Director** (part-time)
datalab industries ltd.

- Supporting the open source development of OPTIMADE and *datalab* via consultancy services.
- Customisation and deployment of *datalab* for industrial R&D and academic labs.

2016–2020 **PhD student: Crystal structure prediction for next-generation energy storage**
University of Cambridge, with Dr Andrew Morris

- Computional 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`.

COMPUTING

Languages **Python**, Javascript, Vue.js, Fortran, C++

Practices **Test-driven development, CI/CD, Cloud Automation, HPC**

Tools **git**, **vim**, **Docker**, **Ansible**, **Terraform**

Expertise Web APIs, databases, machine learning, high-throughput workflows

OTHER EXPERIENCE

2019 **Visiting Researcher: Machine learning for materials discovery**
Aalto University, with Profs Adam Foster & Patrick Rinke

2019 **Scientific Software Developer (Intern): Multi-objective optimisation**
Enthought Inc., Cambridge

2014, 2015 **UG research: Interactions of quantised vortices in superfluid helium**
University of Manchester, with Dr Paul Walmsley & Prof Andrei Golov

2013 **UG research: Hard sphere packing of nanotube-encapsulated fullerenes**
University of Nottingham, with Dr Ho-Kei Chan & Prof Elena Besley

SELECTED (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).

SELECTED (TEACHING + SERVICE)

2022–2024 Proposed and co-lead a MaRDA working group on metadata extractors for materials science.

2018– Reviewed manuscripts and data for *npj. Comp. Mater.* (x1), *Sci Data* (x1), *J. Phys.: Cond. Mat.* (x4), *Scientific Reports* (x1), *Digital Discovery* (x4), *Machine Learning: Science & Technology* (x2), and *Journal of Open Source Software* (x6)

2022– Organiser of the CECAM Workshop series *Machine-actionable Data Interoperability for Chemical Sciences* (MADICES, February 2022 and April 2024)

2019-2021 Demonstrator: Part II Computational Physics, 3x Part IB Intro to Computing, Cavendish Laboratory

2016–2018 Supervisor: 2x Part IB Electromagnetism, Dynamics and Thermodynamics, Selwyn College

2012–2015 Tutor: GCSE Maths & Key Stage 2 Programming for The Tutor Trust, Manchester

SELECTED RECENT PRESENTATIONS

2024 Invited talk (upcoming): *Decentralized materials research data management, curation and dissemination for accelerated discovery*, Democratizing AI in Materials Science — A Pathway to Broaden the Impact of Materials Research, MRS Fall Meeting, Boston, USA

Contributed paper: *Optical materials discovery and design with federated databases and machine learning*, Faraday Discussions, University of Oxford, United Kingdom.

Invited talk: *Federated, interoperable databases for accelerated materials discovery and design*, CECAM Flagship Workshop on MLIPs and Accessible Databases, Grenoble, France.

2023 Contributed talk: *Interoperable data management for fundamental battery research*, RSC Annual Advanced Battery Materials Symposium, Institute of Physics, United Kingdom.

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

PUBLICATIONS

Underline indicates (joint) first authorship (reordered where appropriate). Full list available at https://ml-evs.science/papers.

16. **Evans, M. L.**, Trinquet, V., Hargreaves, C. J., De Breuck, P.-P. & Rignanese, G.-M. Optical materials discovery and design with federated databases and machine learning. *Faraday Discussions,* (2024). DOI:10.1039/D4FD00092G. arXiv:2405.11393.

15. **Evans, M. L.**, Bergsma, J., Merkys, A., Andersen, C. W., *et al.* Development and application of the OPTIMADE API for materials data exchange and discovery. *Digital Discovery,* (2024). DOI:10.1039/D4DD00039K.

14. Rosen, A. S. *et al.* Jobflow: Computational Workflows Made Simple. *Journal of Open Source Software* **9,** 5995, (2024) ISSN: 2475-9066. DOI:10.21105/joss.05995. (2024).

13. Wang, Z., Gong, Y., **Evans, M. L.**, *et al.* Machine learning-accelerated discovery of A_2BC_2 ternary electrides with diverse anionic electron densities. *J. Amer. Chem. Soc.* **145,** 26412–26424, (2023). DOI:10.1021/jacs.3c10538.

12. Lertkiattrakul, 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. *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., *et al.* 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. **Evans, M. L.**, Andersen, C. W., Armiento, R., Blokhin, E., Conduit, G. J., *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. *J. Phys.: Cond. Mat.* **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/gdq6h4.

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.