Matthew Evans

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

RESEARCH INTEREST

My background in computational materials science has left me with an overarching interest in the application of machine learning, open source software, and data management infrastructure to accelerate and enhance scientific workflows for discovery in the chemical and materials sciences, in particular for energy storage and conversion applications.

EDUCATION

2016–2023 **PhD Physics**, *(submitted July 2023)*, 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

2025– **Leverhulme Trust Early Career Research Fellow**

University of Cambridge, with Prof Dame Clare Grey FRS

- 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.
- Extending *datalab* to support additional domains, user workflows and modalities to enable research data management for automated, autonomous and otherwise data-driven labs.
- Pushing for interoperability in the chemistry and materials science software & data ecosystem via OPTIMADE and community efforts such as MADICES.

2024– **Scientific Software Consultant** and **Director**

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.
- Key stakeholder in projects with partners spanning PSDI, CCDC, Faraday Institution and others.

2020–2025 **Research Assistant** (2020–2022) then **BEWARE Research Fellow** (2022–2025)

IMCN, Université catholique de Louvain and Matgenix SRL., with Prof Gian-Marco Rignanese

- High-throughput machine-learning accelerated workflows for materials discovery and design.
- Leading development of the OPTIMADE API specification and associated software (`optimade-python-tools`, `optimade-maker`).

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`.

OTHER EXPERIENCE

2021–2025 **Visiting researcher**: Data management platforms for materials chemistry research
Department of Chemistry, University of Cambridge with Prof Clare Grey FRS

2022 **Postdoctoral Researcher** Recommender systems for crystal structure search
Cambridge Crystallographic Data Centre, Cambridge, UK

2019 **Visiting Researcher**: Machine learning for materials discovery
Aalto University, Finland, 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)

2025 Leverhulme Trust Early Career Research Fellowship with additional support from Isaac Newton Trust.

2022 BEWARE2 Fellowship from the Wallonia-Brussels Federation (approx. €300,000).

2021 PI for "Interoperable data management for fundamental battery research", BIG-MAP External Stakeholder Initiative (approx. €150,000).

SELECTED (TEACHING + SERVICE)

2018– Reviewed for *Digital Discovery* (x7), *JOSS* (x6), *J. Phys.: Cond. Mat.* (x4), *Mach. Learn.: Sci. Technol.* (x2) (IOP Outstanding Reviewer 2024), *npj. Comp. Mater.* (x1), *Sci Data* (x2), *Sci. Rep.* (x1), *Sci. Technol. Adv. Mater.: Methods* (x1), *Physica Scripta* (x1), *Phys. Chem. Chem. Phys.* (x1)

2022– Initiator and organiser of the CECAM MADICES workshop series in 2022 (virtual), 2024 (Berlin, Germany) and 2025 (Villigen, Switzerland).

2025– Member of the Society of Research Software Engineering UK & co-organiser of the Research Software Engineering East of England (RS-Triple-E) group.

2025– Co-organiser of the CECAM *OPTIMADE* workshop series, 2025 (Vilnius, Lithuania) and 2026 (Grenoble, France).

2025– Member of the steering committee for the Collaborative Computational Project for NMR Crystallography.

2026– Data Champion at the University of Cambridge

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

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

2025 Invited talk: *Decentralized materials research data management, curation and dissemination for accelerated discovery*, Machine Learning for Spectroscopy, Vrije Universiteit Brussel, Belgium.

4x Invited seminars: *Decentralized materials research data management, curation and dissemination for accelerated discovery*. MMDG, Uni. Birmingham; PSDI Polymer Data Workshop, Loughborough Uni.; Comp. Chem. Seminars, Uni. Warwick; AIChemy Seminars, Imperial College London

2024 Invited talk: *Decentralized materials research data management, curation and dissemination for accelerated discovery*, Symposium: Democratizing AI in Materials Science, MRS Fall, Boston, USA

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

PUBLICATIONS

Underline indicates (joint) first authorship (reordered where appropriate). Full list with OA links available online (https://ml-evs.science/papers, ORCiD, Google Scholar).

Peer-reviewed articles

19. Zimmermann, Y., Bazgir, A., *et al.* 32 Examples of LLM Applications in Materials Science and Chemistry: Towards Automation, Assistants, Agents, and Accelerated Scientific Discovery. *Mach. Learn.: Sci. Technol.,* (2025). 10.1088/2632-2153/ae011a.
18. Trinquet, V., **Evans, M. L.** & Rignanese, G.-M. Accelerating the discovery of high-performance nonlinear optical materials using active learning and high-throughput screening. *J. Mat. Chem. C,* (2025). 10.1039/d5tc01335f.
17. **Evans, M. L.**, Rignanese, G.-M., Elbert, D. & Kraus, P. Metadata, automation, and registries for extractor interoperability in the chemical and materials sciences. *MRS Bulletin,* (2025). 10.1557/s43577-025-00925-8.
16. Mroz, A. M., **Evans, M. L.**, *et al.* Cross-disciplinary perspectives on the potential for artificial intelligence across chemistry. *Chemical Society Reviews,* (2025). 10.1039/D5CS00146C.
15. **Evans, M. L.**, Trinquet, V., *et al.* Optical materials discovery and design with federated databases and machine learning. *Faraday Discussions* **256,** 459–482, (2025). 10.1039/D4FD00092G.
14. **Evans, M. L.**, Bergsma, J., Merkys, A., Andersen, C. W., *et al.* Developments and applications of the OPTIMADE API for materials data exchange and discovery. *Digital Discovery* **3,** (2024). 10.1039/D4DD00039K.
13. Rosen, A. S., Gallant, M., *et al.* Jobflow: Computational Workflows Made Simple. *Journal of Open Source Software* **9,** 5995, (2024). 10.21105/joss.05995. (2024).
12. 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). 10.1021/jacs.3c10538.
11. Lertkiattrakul, M., **Evans, M. L.** & Cliffe, M. J. PASCal Python: A Principal Axis Strain Calculator. *Journal of Open Source Software* **8,** 5556, (2023). 10.21105/joss.05556.
10. Jablonka, K. M., Ai, Q., *et al.* 14 Examples of How LLMs Can Transform Materials Science and Chemistry: A Reflection on a Large Language Model Hackathon. *Digital Discovery,* (2023). 10/gswbnx.
9. 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). 10/h69d.
8. **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). 10/gn3w9f.
7. **Evans, M. L.**, Andersen, C. W., *et al.* OPTIMADE, an API for exchanging materials data. *Scientific Data* **8,** 217, (2021). 10/gmnrxj.
6. 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). 10/gpw93d.
5. **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). 10/gmf4mv.
4. 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). 10/gg5sx3.
3. Harper, A. F., **Evans, M. L.**, *et al.* Ab initio Structure Prediction Methods for Battery Materials. *Johnson Matthey Technology Review* **64,** 103–118, (2020). 10/ggrmgf.
2. Marbella, L. E., **Evans, M. L.**, *et al.* Sodiation and Desodiation via Helical Phosphorus Intermediates in High-Capacity Anodes for Sodium-Ion Batteries. *J. Amer. Chem. Soc.* **140,** 7994–8004, (2018). 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). 10/gf2529.