

# Matthew Evans

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🌐 [ml-evs.science](https://ml-evs.science)  
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*decentralized data management • open science & software  
materials discovery • ab initio calculations*

## RESEARCH INTERESTS

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

## 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 Clare Grey FRS
- 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 spanning <https://psdi.ac.uk>, <https://ccdc.cam.ac.uk>, University of Nottingham, TUBerlin 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
- 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.
- 2016–2020 **PhD student: Crystal structure prediction for next-generation energy storage**  
University of Cambridge, with Dr Andrew Morris
- 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*.

## COMPUTING

Languages	<b>Python</b> , Javascript, Vue.js, Fortran, C++	Tools	<b>git</b> , <b>vim</b> , <b>Docker</b> , <b>Ansible</b> , <b>Terraform</b>
Practices	<b>Test-driven development</b> , <b>CI/CD</b> , <b>Cloud Automation</b> , <b>HPC</b>	Expertise	Web APIs, databases, machine learning, high-throughput workflows

## OTHER EXPERIENCE

- 2021–2025 **Visiting researcher:** Data management platforms for materials chemistry research  
Department of Chemistry, University of Cambridge with Prof Clare Grey
- 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* (x1), *Sci. Rep.* (x1), *Sci. Technol. Adv. Mater.: Methods* (x1).
- 2025 Co-organiser of the CECAM workshop *Open Databases For Materials Design (OPTIMADE)*, Vilnius, Lithuania, September 2025
- 2022–2025 Initiator and organiser of the CECAM Workshop series *Machine-actionable Data Interoperability for Chemical Sciences (MADICES)*, February 2022, April 2024 and upcoming in October 2025)
- 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*. Materials Modelling Discussion Group, University of Birmingham; PSDI Polymer Data Workshop, Loughborough University; Computational Chemistry Seminar Series, University of Warwick; AIChemistry Seminar Series, 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](#)).

### Preprints

15. Zimmermann, Y., Bazgir, A., *et al.* *Reflections from the 2024 Large Language Model (LLM) Hackathon for Applications in Materials Science and Chemistry* (submitted). 2024. [10.48550/arXiv.2411.15221](#).

### Peer-reviewed articles

20. 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.* (accepted), (2025). [10.48550/arXiv.2505.03049](#).
19. 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](#).
18. **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](#).
17. 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](#).
16. **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. Lertkiatrakul, 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](#).