# Matthew Evans

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ml-evs

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

## RESEARCH INTERESTS

My background in computational materials science has left me with an overarching research interest in the application of machine learning, collaborative open source software and infrastructure, and digital 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)

Université catholique de Louvain and Matgenix, 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.

2021– **Visiting Researcher: Data management platforms for materials chemistry research**

University of Cambridge, with Prof Clare Grey FRS

- Leading development of `datalab`, a data management API and web UI for samples and associated characterisation via electrochemical cycling, NMR, XRD, etc, deployed at several labs internationally.
- Founder and co-leader of a MaRDA working group on interoperable metadata extractors in chemistry.

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`.
- 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.

## COMPUTING

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

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

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

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

## OTHER EXPERIENCE

2022 **Postdoctoral Research Associate: Recommender systems**
*Cambridge Crystallographic Data Centre*

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

2014–2015 **MPhys project: Electronic structure of defects in graphene superlattices**
University of Manchester, with Prof Francisco Guinea

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– 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* (x5)

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

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.

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

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

## PUBLICATIONS

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

16. Trinquet, V., **Evans, M. L.**, 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., Gallant, M., George, J., Riebesell, J., Sahasrabuddhe, H., Shen, J.-X., Wen, M., **Evans, M. L.**, Petretto, G., Waroquiers, D., Rignanese, G.-M., Persson, K. A., Jain, A. & Ganose, A. M. 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., Ai, Q., Al-Feghali, A., Badhwar, S., Bocarsly, J. D., M., A., Bringuier, S., Brinson, L. C., Choudhary, K., Circi, 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., *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. 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. *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.