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

- Funded by BIG-MAP External Stakeholder Initiative to develop `datalab`, a data management platform for tracking samples, devices and associated characterisation.
- Founder and co-leader of a MaRDA working group on interoperable metadata extractors in materials science and 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

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.*, *Sci Data* (x1), *J. Phys.: Cond. Mat.* (x4), *Scientific Reports* (x1), *Digital Discovery* (x4) and *Journal of Open Source Software* (x4)

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

SELECTED RECENT PUBLICATIONS

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

1. **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 (accepted)*, (2024). DOI:10.48550/arXiv.2402.00572.
2. 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.
3. 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.
4. **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.
5. 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.
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). DOI:10/gpw93d.