Matthew Evans

✉ *matthew@ml-evs.science*
ml-evs.science
ml-evs

I am an open source software developer trying to actualise my vision for the future of decentralized data management in the chemical and materials sciences.

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

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)*

EXPERIENCE

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

- Machine learning for small materials datasets (MODNet).
- High-throughput workflows for computational materials discovery and molecular dynamics.
- Continued development of the OPTIMADE API specification and associated software.

2021– **Visiting Researcher**
in the group of Prof Clare Grey (*University of Cambridge*)

- Data management, analysis software and open APIs for materials chemistry research.
- Funded by BIG-MAP External Stakeholder Initiative to develop `datalab`, a data management API and web UI for samples and associated characterisation via electrochemical cycling, NMR and XRD.
- Founder and co-leader of a MaRDA working group on interoperable metadata extractors in materials science and chemistry.

2022 **Postdoctoral Research Associate**
Cambridge Crystallographic Data Centre
2-month contract to implement a recommender system for the Cambridge Structural Database.

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

- 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.

2019 **Visiting Researcher: Machine learning for materials discovery**
with Prof Adam Foster & Prof Patrick Rinke, *Department of Applied Physics, Aalto University*

2019 **Scientific Software Developer (Intern)**
Enthought Inc., Cambridge

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

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

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

COMPUTING

Exposure: **Daily**, Intermittent, *Occasional*.

Languages	**Python**, Javascript, Vue.js, Fortran, Cython, C++	Expertise	Web APIs & databases, HT workflows, ML, Cloud Automation
DFT	**CASTEP**, Quantum Espresso, *GPAW*	Stack	FastAPI, pydantic, Flask, Tensorflow
Tools	**git**, **vim**, **Docker**, **Ansible**, **Terraform**	Practices	**Test-driven development, CI/CD**

(TEACHING + SERVICE)

2022– Founded and co-lead a MaRDA working group on metadata extractors for materials science and chemistry

2020– Co-chair of the Research Data Alliance (RDA) IG *Materials Data, Infrastructure & Interoperability*

2018– Reviewed manuscripts and data for *npj. Computational Materials* (x2), *Scientific Data* (x1), *J. Phys.: Cond. Mat.* (x3), *Scientific Reports* (x1), *Digital Discovery* (x3) and *Journal of Open Source Software* (x4)

2022 Organiser for the CECAM Virtual Workshop *Machine-actionable Data Interoperability for Chemical Sciences* (MADICES)

2021 Lecturer for “Working with Materials Databases” at the ICTP-East African Institute for Fundamental Research Training School *Machine Learning for Electronic Structure and Molecular Dynamics*

2021 Mentor at Acceleration Consortium Hackathon on Scientific Databases

2021 Developed and delivered a 2-day OPTIMADE tutorial for the NOMAD Virtual Tutorial Series.

2016–2020 Active member of TCM `sysadmin` team, Cavendish Laboratory

2019-2021 Demonstrator: Part II Computational Physics, Cavendish Laboratory

- Demonstrated scientific Python to beginners in weekly labs (2019 only).
- Conceptualised and delivered a tutorial on the basics of version control with Git (2019-2021).

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

- Small group teaching, providing detailed feedback on assigned problems.

2016–2019 Demonstrator: 3x Part IB Introduction to Computing (C++), Cavendish Laboratory

2016–2019 Demonstrator: 4x at annual CASTEP workshop, University of Oxford

2017 Volunteer: 2nd Conference of Research Software Engineers, University of Manchester

2016–2017 Volunteer: Key Stage 2 Code Club, Ridgefield Primary School, Cambridge

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

- Provided tuition to small groups and ‘looked after children’ across 15 schools.
- Helped lead a successful pilot to teach primary school children programming using Scratch.

(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).

2019 HPC-Europa 3 funding to visit Aalto University for 7 weeks and associated computing time.

2018 Tier-2 HPC Resource Allocation: PI on project awarded 2 MCPUh, *Crystal structure prediction for next-generation solar absorbers*, **M. L. Evans**, D. O. Scanlon and A. J. Morris.

HPC Midlands+ Substantial Project: awarded 1.3 MCPUh for *High-throughput materials discovery for energy applications*, **M. L. Evans** and A. J. Morris.

2017 Tier-2 HPC Resource Allocation: Co-investigator on project awarded 4 MCPUh, *Ab initio structure prediction for next-generation battery materials*, B. Karasulu, **M. L. Evans** and A. J. Morris.

2015 Tesella Prize for Software, University of Manchester, for the most effective use of software in a final year physics project.

2013, 2014 Undergraduate research bursary for two summers as an undergraduate, totalling £4200.

2011–2015 Means-tested and merit based scholarship to study at the University of Manchester, worth £12,000.

PRESENTATIONS

2023 Invited seminar: *Interoperable data management for fundamental materials chemistry research*, Department of Chemistry, University of Nottingham, United Kingdom.

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

Invited seminar: *Interoperable data management for fundamental battery research*, Conductivity and Catalysis Lab, Technische Universität Berlin, Germany.

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 seminar: *Interoperable data management for fundamental battery research*, Laboratory of Materials Simulation, Paul Scherrer Institut, Switzerland.

Invited talk: *Metadata extractors for interoperable ETL*, MaRDA Alliance Annual Meeting

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

Invited talk: *The OPTIMADE Ecosystem*, DoE Battery Genome Initiative

Invited panel discussion: *Delivery platforms for open marketplaces*, Research Data Alliance (RDA) 17th Virtual Plenary Meeting

2020 Invited talk: *The OPTIMADE Specification*, Research Data Alliance (RDA) 16th Virtual Plenary Meeting: Data Infrastructure for Collaborations in Materials Research

Invited talk and workshop demonstration: *`odbx` & OPTIMADE* and *`optimade-python-tools`*, CECAM Workshop, Open Databases Integration for Materials Design 2020

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

Invited talk: *`matador` & OPTIMADE*, CECAM Workshop, Open Databases Integration for Materials Design 2019, EPFL, Switzerland

2018 Contributed talk: *Sn-P anodes for potassium-ion batteries: insights from crystal structure prediction*, SMARTER6 Conference, Ljubljana, Slovenia

Invited talk: *`matador`: databases and crystal structure prediction* (slides), CECAM Workshop, Open Databases Integration for Materials Design 2018, EPFL, Switzerland

2017 Invited seminar: *Crystal structure prediction for next-generation battery anodes* (slides), Solid State Seminar Series, University of Cambridge

Poster Presentation: 13th RSC Conference in Materials Chemistry (poster), University of Liverpool

2016 Poster Presentation: SMARTER5 Conference, University of Bayreuth, Germany

PUBLICATIONS

Underline indicates (joint) first authorship.

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. *Preprint,* (2024). DOI:`10.48550/arXiv.2402.00572`.
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.**, Yan, Y., Wang, S., Miao, N., Zheng, R., Rignanese, G.-M. & Wang, J. Machine learning-accelerated discovery of A_2BC_2 ternary electrides with diverse anionic electron densities. *Journal of the American Chemical Society* **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., Dwaraknath, S., Scheidgen, M., Fekete, Á. & Winston, D. 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. *Journal of Physics: Condensed Matter* **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`.

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