Matthew Evans

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energy storage materials • ab initio calculations
crystal structure databases • open science & software

EDUCATION

2016– **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

2022 **Postdoctoral Research Associate**

Cambrige Crystallographic Data Centre

2-month contract to implement a recommender system for the Cambridge Structural Database.

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 implement functionality for electrochemical cycling, NMR and XRD data management.

2020–2022 **Researcher**

with Prof Gian-Marco Rignanese (*Universitè catholique de Louvain*)

- Machine learning for small materials datasets (MODNet).
- Continued development of the OPTIMADE API specification and associated software.

2016–2020 **PhD student: Crystal structure prediction for next-generation energy storage**

with Dr Andrew Morris *(University of Cambridge/University of Birmingham)*

- 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 and `odbx` implementation.

2019 **Visiting Researcher**

Department of Applied Physics, Aalto University

Received HPC-Europa funding to visit the group of Prof Adam Foster for 7 weeks, with computational resources provided by the Finnish IT center for science (CSC).

2019 **Scientific Software Developer (Intern)**

Enthought Inc., Cambridge

Worked on the open source, Horizon 2020 FORCE project, adding functionality to a workflow manager for multi-criteria optimisations. Helped develop Cython bindings for the ACADO toolkit.

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**, Fortran, Cython, C++	Databases	**MongoDB**, SQL, Elasticsearch
DFT	**CASTEP**, Quantum Espresso, *GPAW*	Packages	**NumPy, SciPy, matplotlib, scikit-learn, FastAPI**, Tensorflow
Tools	**git**, **vim**, **Docker**	Practices	**Test-driven development, CI**

(TEACHING + SERVICE)

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

2018– Reviewed manuscripts for *npj. Computational Materials*, *J. Phys.: Cond. Mat.*, *Scientific Reports* and *Journal of Open Source Software*

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.

SELECTED PRESENTATIONS

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 talk: *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

Status: preprint, published. Underline indicates (joint) first authorship.

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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