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

2021–ㅤVisiting Researcher
with Prof Clare Grey (*University of Cambridge*)
 – Data management, analysis software and open APIs for materials chemistry research.

2020–ㅤResearcher
with Prof Gian-Marco Rignanese (*Université catholique de Louvain*)
 – Machine learning for small materials datasets (MODNet).
 – High-throughput workflows for computational materials science.

2016–2020ㅤPhD student: Crystal structure prediction for next-generation energy storage
with Dr Andrew Morris (*University of Cambridge/University of Birmingham*)
 – 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.
 – Active member of the OPTIMADE consortium for materials database interoperability and author of the optimade-python-tools package and odbx implementation.

2019ㅤVisiting 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).

2019ㅤScientific 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, 2015ㅤUG research: Interactions of quantised vortices in superfluid helium
with Dr Paul Walmsley & Prof Andrei Golov (*University of Manchester*)

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

2013ㅤUG 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)

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