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

2020– **Postdoctoral Researcher**

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

- Machine learning for small materials datasets (MODNet),
- Continuing work on the OPTIMADE API,
- High-throughput workflows for computational materials science.

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 [9, 5, 4, 2]
- Author of two open-source Python packages: database approaches for high-throughput calculations and materials design with `matador` [6] and crystal structure prediction with `ilustrado`.
- Contributed to the CASTEP and OptaDOS codes.
- Active member of the OPTIMADE consortium for materials database interoperation [8] and author and maintainer of `optimade-python-tools` package [7] 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, with a focus on adding functionality to the 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*
DFT	**CASTEP**, Quantum Espresso, GPAW	Packages	**NumPy, SciPy, matplotlib**, scikit-learn
Tools	**git**, **vim**, **Docker**	Practices	**Test-driven development, CI**

(TEACHING + SERVICE)

2018– Reviewed manuscripts for *Scientific Reports*

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

2019 Demonstrator: Part II Computational Physics, Cavendish Laboratory
- Demonstrated scientific Python to beginners in weekly labs.
- Wrote and delivered a tutorial on the basics of version control with Git.

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– 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)

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

2015– Presented posters and talks at over 20 conferences and workshops both nationally and internationally. Selected works can be found on my personal website.

2020 Invited talk and 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: in preparation, preprint, published.

9. **Evans, M. L.** *et al.* Phosphorus anodes for K-ion batteries: insights from *ab initio* structure prediction. *(in preparation),* (2020).
8. Andersen, C. *et al.* OPTIMADE: an API for exchanging materials data. *(in preparation),* (2020).
7. Andersen, C. & **Evans, M. L.** optimade-python-tools. *(in preparation),* (2020).
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,* (2020). DOI:10.21105/joss.02563.
5. Harper, A. F., **Evans, M. L.** & Morris, A. J. Phases of Copper Phosphides from Computational Structure Searches. *Chem. Mater.* **32,** (2020). DOI:10.1021/acs.chemmater.0c02054. arXiv:2005.05375.
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. *Chem. Mater.* **30,** (2018). DOI:10.1021/acs.chemmater.8b02803.
2. Marbella, L. E., **Evans, M. L.**, Groh, M. F., Nelson, J., Griffith, K. J., Morris, A. J. & Grey, C. P. (De)Sodiation via Helical Phosphorus Intermediates in High Capacity Anodes for Sodium-ion Batteries. *J. Am. Chem. Soc.* **140,** 7994–8004, (2018). DOI:10.1021/jacs.8b04183.
1. Zhu, T., **Evans, M. L.**, Brown, R. A., Walmsley, P. M. & Golov, A. I. Interactions between unidirectional quantized vortex rings. *Phys. Rev. Fluids* **1,** 044502, (2016). DOI:10.1103/PhysRevFluids.1.044502. arXiv:1603.04313.

REFEREES

Dr Andrew Morris, University of Birmingham; a.j.morris.1@bham.ac.uk

Prof Mike Payne, University of Cambridge; mcp1@cam.ac.uk

Dr Paul Walmsley, University of Manchester; paul.walmsley@manchester.ac.uk

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