# Matthew Evans

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ml-evs

*energy storage · 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

2016–2020 **Crystal structure prediction for next-generation energy storage applications**

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

Discovery and computational characterisation of high-capacity 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`. Contributed to the CASTEP and OptaDOS codes. Active member of the OPTIMADE consortium for materials database interoperation and author and maintainer of `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**

Internship 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, including developing a Bayesian optimisation plugin. Helped develop Cython bindings for the ACADO toolkit.

2014, 2015 **Interactions of quantised vortices in superfluid helium**

UG with Dr Paul Walmsley & Prof Andrei Golov *(University of Manchester)*

2014–2015 **Electronic structure of defects in graphene superlattices**

MPhys with Prof Francisco Guinea *(University of Manchester)*

2013 **Hard sphere packing of nanotube-encapsulated fullerenes**

UG 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 4 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 20 conferences and workshops both nationally and internationally. Selected works can be found on my personal website.

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

## PUBLICATIONS

Status: in preparation, preprint, published.

7. **Evans, M. L.** *et al.* Phosphorus anodes for K-ion batteries: insights from *ab initio* structure prediction. *(in preparation),* (2020).
6. **Evans, M. L.** matador: database and analysis software for high-throughput atomistic calculations. *(in preparation),* (2020).
5. Harper, A. F., **Evans, M. L.** & Morris, A. J. Novel Phases of Copper Phosphides from Computational Structure Searches, (2020). 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:10.1595/205651320X15742491027978.
3. 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.
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. 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.,* (2018). DOI:10.1021/acs.chemmater.8b02803.

## REFEREES

References available on request.