

# Matthew Evans

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*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

- PhD **Crystal structure prediction for next-generation energy storage applications**  
with Dr Andrew Morris (*University of Cambridge/University of Birmingham*)  
Discovery and computational characterisation of novel high-capacity anode materials 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](#) package. Contributed to the CASTEP and OptaDOS codes. Active member of the OPTiMaDe consortium for materials database interoperation. PhD research undertaken as a member of the EPSRC CDT for Computational Methods in Materials Science.
- Visiting Researcher**  
2019 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).
- Internship **Scientific Software Developer**  
2019 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.
- UG **Interactions of quantised vortices in superfluid helium**  
2014, 2015 with Dr Paul Walmsley & Prof Andrei Golov (*University of Manchester*)
- MPhys **Electronic structure of defects in graphene superlattices**  
2014–2015 with Prof Francisco Guinea (*University of Manchester*)
- UG **Hard sphere packing of nanotube-encapsulated fullerenes**  
2013 with Dr Ho-Kei Chan & Prof Elena Besley (*University of Nottingham*)

## COMPUTING

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

|           |   |           |  |
|-----------|---|-----------|--|
| Languages | <b>Python</b> , Fortran, Cython, C++    | Databases | <b>MongoDB</b> , SQL                               |
| DFT       | <b>CASTEP</b> , Quantum Espresso, GPAW  | Packages  | <b>NumPy</b> , <b>SciPy</b> , spglib, scikit-learn |
| Tools     | <b>git</b> , <b>vim</b> , <i>Docker</i> | Practices | <b>Test-driven development</b> , <b>CI</b>         |

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## (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.

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## (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.

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## 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

5. **Evans, M. L.**, Griffith, K. J. & Morris, A. J. Sn-P anodes for K-ion batteries: insights from *ab initio* structure prediction. (*in preparation*), (2019).
4. **Evans, M. L.** matador: database and analysis software for high-throughput atomistic calculations. (*in preparation*), (2019).
3. 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](https://doi.org/10.1021/jacs.8b04183).
2. 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](https://doi.org/10.1021/acs.chemmater.8b02803).
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](https://doi.org/10.1103/PhysRevFluids.1.044502). arXiv:[1603.04313](https://arxiv.org/abs/1603.04313).

## REFEREES

Dr Andrew Morris, University of Birmingham; [a.j.morris.1@bham.ac.uk](mailto:a.j.morris.1@bham.ac.uk)

Prof Mike Payne, University of Cambridge; [mcp1@cam.ac.uk](mailto:mcp1@cam.ac.uk)

Dr Paul Walmsley, University of Manchester; [paul.walmsley@manchester.ac.uk](mailto:paul.walmsley@manchester.ac.uk)