

# 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)
  - 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*)
- 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](#)
  - Contributed to the [CASTEP](#) and [OptaDOS](#) codes.
  - Active member of the [OPTIMADE consortium](#) for materials database interoperability and author and maintainer of [optimade-python-tools](#) packages 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*)

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## COMPUTING

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

Languages **Python**, Fortran, Cython, C++

Databases **MongoDB**, SQL, *Elasticsearch*

Tools **git**, **vim**, **Docker**

Practices **Test-driven development**, CI

## (TEACHING + SERVICE)

- 2020- Co-chair of the Research Data Alliance (RDA) Interest Group "Materials Data, Infrastructure & Interoperability"
- 2018- Reviewed manuscripts for *Scientific Reports*
- 2016–2020 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
- 2016–2019 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)

- 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: *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

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- 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.

11. Andersen, C. *et al.* OPTIMADE: an API for exchanging materials data. (*in preparation*), (2021).
10. **Evans, M. L.** & Andersen, C. W. optimade-python-tools. (*in preparation*), (2021).
9. Ellis, A. W., **Evans, M. L.**, Groh, M., Morris, A. J. & Marbella, L. E. Phase transformations in tin phosphide anodes for K-ion batteries: A solid-state NMR and DFT study. (*in preparation*), (2021).
8. De Breuck, P. and **Evans, M. L.** and Rignanese, G. Robust model benchmarking and bias-imbalance in data-driven materials science: a case study on MODNet. (*submitted*), (2021).
7. **Evans, M. L.** *et al.* Phosphorus anodes for K-ion batteries: insights from *ab initio* structure prediction. (*in preparation*), (2021).
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](#).