

# Matthew Evans

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*ab initio calculations · energy storage  
crystal structure databases · software development*

## EDUCATION

- 2016– **PhD Physics**, *Theory of Condensed Matter Group*, University of Cambridge, *expected 2019*.  
2015–2016 **MPhil Scientific Computing**, University of Cambridge, *Distinction*.  
2011–2015 **MPhys Physics with Theoretical Physics**, University of Manchester, *First Class (Hons)*.

## (RESEARCH INTERESTS + EXPERIENCE)

- PhD Crystal structure prediction for next-generation energy storage applications**  
with Dr Andrew Morris (*University of Cambridge*)  
Discovery and computational characterisation of novel high-capacity anode materials for Li-, Na- and K-ion batteries, using *ab initio* random structure searching (AIRSS) and evolutionary approaches, implemented in the open-source [ilustrado](#) package. PhD research undertaken as a member of the EPSRC CDT for Computational Methods in Materials Science.
- MPhil High-throughput *ab initio* materials discovery**  
with Dr Andrew Morris (*University of Cambridge*)  
Database approaches to materials design; developed an open-source software package, [matador](#), to aggregate and analyse the results of first-principles calculations.
- MPhys Electronic structure of defects in graphene superlattices**  
with Prof Francisco Guinea (*University of Manchester*)  
Nearly-free electron model of graphene/h-BN superlattices with arbitrary defects included via Green's function methods. Awarded Tessella Prize for software development.
- UG Interactions of quantised vortices in superfluid helium**  
with Dr Paul Walmsley & Prof Andrei Golov (*University of Manchester*)  
Spent two summers developing [vfmcpp](#), a C++/OpenMP implementation of the vortex filament model of superfluid helium, to study microscopic vortex dynamics and reconnection events [1].
- UG Hard sphere packing of nanotube-encapsulated fullerenes**  
with Dr Ho-Kei Chan & Prof Elena Besley (*University of Nottingham*)

## COMPUTING

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

Languages	<b>Python</b> , Fortran, C++, <i>Rust</i>	Databases	<b>MongoDB</b> , <i>SQL</i>
DFT	<b>CASTEP</b> , Quantum Espresso	Packages	<b>NumPy</b> , <i>spglib</i> , <i>scikit-learn</i>
Platforms	<b>Linux</b> , <i>*nix</i>	Practices	<b>Test-driven development</b> , <i>CI</i>
Data viz	<b>matplotlib</b> , Bokeh, d3.js, seaborn	Toolset	<b>git</b> , <i>vim</i> , Docker

## (TEACHING + SERVICE)

- 2018– Organiser of fortnightly computational physics talk series, (*CDT for Computational Materials Science*).
- 2016– Active member of TCM syadmin team, (*Cavendish Laboratory*).
- 2016– Supervisor: Part IB Electromagnetism, Dynamics and Thermodynamics, (*Selwyn College*).
- 2016– Demonstrator: Part IB Computational Physics (C++), (*Cavendish Laboratory*).
- 2016– Demonstrator: 3x 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*).
- 2016 Demonstrator: Graduate-level Electronic Structure, (*Cavendish Laboratory*).
- 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.

## PUBLICATIONS

Status: in preparation, [preprint](#), published.

3. **Evans, M. L.**, Griffith, K. J. & Morris, A. J. Sn-P anodes for K-ion batteries: insights from *ab initio* structure prediction. (*in preparation*), (2018).
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](#).

## PROFESSIONAL ACTIVITIES

- Upcoming *Sn-P anodes for potassium-ion batteries: insights from crystal structure prediction*, Contributed Talk, SMARTER 6, Kemijski Institut, Slovenia
- 2015–2018 Presented posters and talks at nearly 20 conferences and workshops both nationally and internationally. Selected works can be found on my [personal website](#).
- 2018 *matador: databases and crystal structure prediction* ([slides](#)), Invited Talk, OPTiMaDe workshop, CECAM@EPFL, Switzerland
  - HPC Midlands+ Substantial Project: awarded 1.3 MCPUh for *High-throughput materials discovery for energy applications*, M. L. Evans and A. J. Morris.
- 2017 *Crystal structure prediction for next-generation battery anodes* ([slides](#)), Invited Talk, Solid State Seminar Series, University of Cambridge
  - Tier-2 Resource Allocation: awarded 4 MCPUh for *Ab initio structure prediction for next-generation battery materials*, B. Karasulu, M. L. Evans and A. J. Morris.
  - 13th RSC Conference in Materials Chemistry, Poster Presentation ([link](#)), University of Liverpool

## REFEREES

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

Prof Francisco Guinea, University of Manchester; [paco.guinea@icm.csic.es](mailto:paco.guinea@icm.csic.es)

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