

Matthew Evans

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energy storage · ab initio calculations
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/University of Birmingham*)
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	Python , Fortran, C++, <i>Rust</i>	Databases	MongoDB , <i>SQL</i>
DFT	CASTEP , Quantum Espresso, GPAW	Packages	NumPy , <i>spglib</i> , <i>scikit-learn</i>
Platforms	Linux , <i>*nix</i>	Practices	Test-driven development , <i>CI</i>
Data viz	matplotlib , Bokeh, <i>d3.js</i>	Tools	git , <i>vim</i> , Docker

(TEACHING + SERVICE)

- 2018– Organiser of fortnightly computational physics talk series, (*CDT for Computational Materials Science*).
- 2018– Reviewed manuscripts of *Scientific Reports*.
- 2016– Active member of TCM sysadmin team, (*Cavendish Laboratory*).
- 2018 Demonstrator: Graduate-level Atomistic Modelling of Materials, (*Cavendish Laboratory*).
- 2016–2018 Supervisor: Part IB Electromagnetism, Dynamics and Thermodynamics, (*Selwyn College*).
- 2016–2018 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

4. **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).
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.* (2018). DOI:[10.1021/acs.chemmater.8b02803](https://doi.org/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](https://doi.org/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](https://doi.org/10.1103/PhysRevFluids.1.044502). arXiv:[1603.04313](https://arxiv.org/abs/1603.04313).

PROFESSIONAL ACTIVITIES

- 2015–2018 Presented posters and talks at 20 conferences and workshops both nationally and internationally. Selected works can be found on my [personal website](#).
- 2018 *Sn-P anodes for potassium-ion batteries: insights from crystal structure prediction*, Contributed Talk, SMARTER6, Ljubljana, Slovenia
- 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

References available on request.