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)*

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

(TEACHING + SERVICE)

2018–	Organiser of fortnightly computational physics talk series, *(CDT for Computational Materials Science)*.
2016–	Active member of TCM `sysadmin` 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

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.

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

2018	*Sn-P anodes for potassium-ion batteries: insights from crystal structure prediction*, Contributed Talk, SMARTER6, Ljubljana, 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`

Prof Mike Payne, University of Cambridge; `mcp1@cam.ac.uk`

Dr Paul Walmsley, University of Manchester; `paul.walmsley@manchester.ac.uk`