Matthew Evans

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ml-evs

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

(TEACHING + SERVICE)

2016– Active member of TCM `sysadmin` team, Cavendish Laboratory

2018– Reviewed manuscripts for *Scientific Reports*

2018– Organiser of fortnightly computational physics talk series, CDT for Computational Materials Science

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

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.

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.

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

2015– Presented posters and talks at 20 conferences and workshops both nationally and internationally. Selected works can be found on my personal website.

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

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.

Invited talk: *`matador`: databases and crystal structure prediction* (slides), CECAM Workshop, Open Databases Integration for Materials Design, 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 Invited talk: *Crystal structure prediction for next-generation battery anodes* (slides), Solid State Seminar Series, University of Cambridge

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.

Last modified: January 28, 2019