

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 submission 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*)
Application of a novel hard sphere packing regime to study CNT-encapsulated fullerenes.

(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*).

- 2016–2017 Volunteer: Key Stage 2 Code Club (*Ridgefield Primary School, Cambridge*).
- 2016 Demonstrator: Graduate-level Electronic Structure, (*Cavendish Laboratory*).
- 2016 Demonstrator: CASTEP Workshop (*Oxford*) (x2), HPC Autumn Academy (*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.

COMPUTING

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

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

PUBLICATIONS

- 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](#).
- 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](#).

(CONFERENCES + PRESENTATIONS)

- 2018 *matador: databases and crystal structure prediction (slides)*, Invited Talk, OPTiMaDe workshop, CECAM@EPFL, Switzerland
- Total Energy and Force Methods, Poster Presentation, University of Cambridge
- 2017 *Crystal structure prediction for next-generation battery anodes (slides)*, Invited Talk, Solid State Seminar Series, University of Cambridge
- Second conference of Research Software Engineers, Volunteer, University of Manchester
- CASTEP Developer Workshop, Demonstrator and Poster Presentation, University of Oxford
- 13th RSC Conference in Materials Chemistry, Poster Presentation ([link](#)), University of Liverpool
- STFC Annual Battery Meeting, Attendee, Abingdon
- CCP9 Young Researchers Event, Poster Presentation, University of Cambridge
- Scientific Computing Day, Poster Presentation, University of Cambridge
- 2016 High Performance Computing Autumn Academy, Presenter, University of Cambridge
- SMARTER5, Poster Presentation, University of Bayreuth, Germany
- CASTEP Workshop, Demonstrator and Poster Presentation, University of Oxford
- CCP9 Young Researchers Event, Poster Presentation, University of York

REFEREES

Dr Andrew Morris, University of Birmingham; a.j.morris.1@bham.ac.uk

Prof Francisco Guinea, University of Manchester; paco.guinea@icm.csic.es

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