# **Matthew Evans**

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++ Databases **MongoDB**, SQL

DFT CASTEP, Quantum Espresso, ASE, Packages NumPy, spglib, scikit-learn

**GPAW** 

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
- 2019 Demonstrator: Part II Computational Physics, Cavendish Laboratory
  - Wrote and delivered a tutorial on the basics of version control with Git.
- 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 *αb 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.

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