Matthew Evans

energy storage · ab initio calculations crystal structure databases · software development

EDUCATION

2016– **PhD Physics**, Theory of Condensed Matter Group, University of Cambridge.

2015–2016 MPhil Scientific Computing, University of Cambridge, Distinction.

2011–2015 MPhys Physics with Theoretical Physics, University of Manchester, First Class (Hons).

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.

Internship Scientific Software Developer

Enthought Inc., Cambridge

Worked on the open source, Horizon 2020 funded FORCE project, with a focus on adding functionality to the workflow manager for multi-criteria optimisations, including developing a Bayesian optimisation plugin. Helped develop Cython bindings for the ACADO toolkit.

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)

UG Interactions of quantised vortices in superfluid helium

with Dr Paul Walmsley & Prof Andrei Golov (University of Manchester)

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, Cython, C++ Databases MongoDB, SQL

DFT **CASTEP**, Quantum Espresso Packages **NumPy, SciPy, spglib**, scikit-learn

Platforms Linux, *nix Practices Test-driven development, CI

Data viz matplotlib, Bokeh, d3.js Tools git, vim, Docker

(TEACHING + SERVICE)

- 2018- Reviewed manuscripts for Scientific Reports
- 2016 Active member of TCM sysadmin team, Cavendish Laboratory
- 2019 Demonstrator: Part II Computational Physics, Cavendish Laboratory
 - Demonstrated scientific Python to beginners in weekly labs.
 - 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
 - Small group teaching, providing detailed feedback on assigned problems.
- 2016–2018 Demonstrator: Part IB Introduction to Computing (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.

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
 - Invited talk: matador: databases and crystal structure prediction (slides), CECAM Workshop, Open Databases Integration for Materials Design, EPFL, Switzerland
- 2017 Invited talk: Crystal structure prediction for next-generation battery anodes (slides), Solid State Seminar Series, University of Cambridge
 - Poster Presentation: 13th RSC Conference in Materials Chemistry (poster), University of Liverpool
- 2016 Poster Presentation: SMARTER5 Conference, University of Bayreuth, Germany

(AWARDS + HONOURS)

- 2018 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.
 - HPC Midlands+ Substantial Project: awarded 1.3 MCPUh for *High-throughput materials discovery for energy applications*, **M. L. Evans** and A. J. Morris.
- 2017 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.
- 2015 Tesella Prize for Software, University of Manchester, for the most effective use of software in a final year physics project.
- 2013, 2014 Undergraduate research bursary for two summers as an undergraduate, totalling £4200.
- 2011–2015 Means-tested and merit based scholarship to study at the University of Manchester, worth £12,000.

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.

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

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