Matthew Evans

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ml-evs

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

EDUCATION

2016– **PhD Physics**, *Theory of Condensed Matter Group*, University of Cambridge, *Expected graduation 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 `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; wrote a 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 C_{60} molecules.

TEACHING

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**, Intermittant, *Occasional*.

Languages	**Python**, Fortran, C++, *Rust*	Databases	**MongoDB**, *SQL*
DFT	**CASTEP**, Quantum Espresso	Packages	**NumPy, spglib, scikit-learn**
Platforms	**Linux**, **nix*	HPC Facilities	ARCHER, CSD3, BNL
Software	**vim**, LaTeX, Inkscape, GIMP	Utilities	**git**, Docker, GNU toolchain
Data viz	**matplotlib**, Bokeh, d3.js, seaborn	Web	*JavaScript, HTML, CSS*

(CONFERENCES + PRESENTATIONS)

2018 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

2015 High Performance Computing Autumn Academy, Attendee, University of Cambridge

CASTEP Workshop, Attendee, University of Oxford

PUBLICATIONS

3. **M. L. Evans**, Griffith, K. J. & Morris, A. J. Sn-P anodes for K-ion batteries: insights from *ab initio* structure prediction. *(in preparation),* (2018).
2. Marbella, L. E. *et al.* (De)Sodiation via Helical Phosphorus Intermediates in High Capacity Anodes for Sodium-ion Batteries. *(submitted),* (2018).
1. Zhu, T., **M. L. Evans**, 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; ajm255@cam.ac.uk

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

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

Last modified: March 15, 2018