Matthew Evans

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ab initio calculations • *energy storage crystal structure databases* • *software development*

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2016-	PhD Phy	ysics, Universi	y of Cambridge,	, Expected	graduation	2019.
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- 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 energy storage applications

with Dr Andrew Morris

Discovery and computational characterisation of novel high-capacity anode materials for Li and Na-ion batteries, using *ab initio* random structure searching (AIRSS) and related approaches.

MPhil High-throughput ab initio materials discovery

with Dr Andrew Morris

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 of graphene superlattices

with Prof Francisco Guinea

Nearly-free electron model of graphene/h-BN superlattices with arbitrary defects included via Green's function methods. Awarded Tessella Prize for development of a high-performance Python code to perform the computation and analysis.

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 Experience

- 2016-2018 Supervisor: Part IB Electromagnetism, Dynamics and Thermodynamics, (Selwyn College).
- 2016–2018 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

Computation CASTEP, Quantum Espresso Packages NumPy, spglib, Jupyter

Platforms Linux, *nix HPC Facilities ARCHER, Thomas, BNL, Darwin

Software vim, LTEX, Inkscape, GIMP Utilities git, Docker, GNU toolchain

Data viz **matplotlib**, Bokeh, d3.js, seaborn Web JavaScript, HTML, CSS

Conferences & Presentations

2017 Second conference of Research Software Engineers, Volunteer, University of Manchester

2017 CASTEP Developer Workshop, Demonstrator and Poster Presentation, University of Oxford

2017 13th RSC Conference in Materials Chemistry, Poster Presentation, University of Liverpool

2017 STFC Annual Battery Meeting, Attendee, Abingdon

2017 CCP9 Young Researchers Event, Poster Presentation, University of Cambridge

2016 High Performance Computing Autumn Academy, Presenter, University of Cambridge

2016 SMARTER5, Poster Presentation, University of Bayreuth, Germany

2016 CASTEP Workshop, Demonstrator and Poster Presentation, University of Oxford

2016 CCP9 Young Researchers Event, Poster Presentation, University of York

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

2015 CASTEP Workshop, Attendee, University of Oxford

Publications

[1] T. Zhu, **M. L. Evans**, R. A. Brown, P. M. Walmsley, and A. I. Golov. Interactions between unidirectional quantized vortex rings. *Phys. Rev. Fluids*, 1:044502, Aug 2016.

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