# Matthew Evans

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

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- 2016 **PhD Physics**, 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 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 Supervisor: Part IB Electromagnetism, Dynamics and Thermodynamics, (Selwyn College).
- 2016 Volunteer: Key Stage 2 Code Club (Ridgefield Primary School, Cambridge).
- 2016–2017 Demonstrator: Part IB Computational Physics (C++), (Cavendish Laboratory).
  - 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 (UK), Darwin (Cambridge)
Software vim, ETFX, Inkscape, GIMP Utilities git, shell scripting, 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, University of Oxford
- 2017 CASTEP Developer Workshop, 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, 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