

Lucy Whalley

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Objective

To design and optimise materials for energy generation and storage using computational modelling and solid-state physics

Education

Imperial College London PhD in Materials Science	London, UK Exp. Sep. 2019
Birmingham City University PGCE in Post-Compulsory Education	Birmingham, UK Jul. 2012
University of Birmingham MSci in Theoretical Physics, 1st class Hons.	Birmingham, UK Jul. 2011

Research Experience

Imperial College London PhD student	London, UK Sep. 2015–present
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- Investigating the impact of point defects and anharmonicity in thin-film photovoltaic materials
- Using Density Functional Theory and High Performance Computing to calculate electronic structure
- Writing post-processing programmes using Python and the SciPy eco-system
- Reviewer for Journal of Chemical Physics, The Journal of Open Source Software and Nature Communications
- Member of the Imperial College Research Software Engineering Committee

University of Birmingham MSci student	Birmingham, UK Sep. 2010–Jul. 2011
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- Solved the Boltzmann transport equation to calculate the transverse magneto-resistance of a quasi 2-dimensional metal
- Used analytical methods, the Abrikosov-Chambers method, and numerical integration routines

University of Birmingham Summer intern	Birmingham, UK Jul. 2010–Sep. 2010
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- Used Bayesian inference to analyse gravitational wave data from the Laser Interferometer Gravitational-Wave Observatory

Teaching Experience

Software Carpentry Foundation Volunteer Instructor	London, UK Jan. 2018–present
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- Teaching basic computing skills (Git, Bash and Python) to academic researchers
- Designing workshops based upon the Software Carpentry scheme of work

Imperial College London Tutor	London, UK Sep. 2017–Jul. 2018
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- Tutored mathematics to first year students on the Materials Science degree programme
- Curriculum included calculus, complex numbers, matrices and ordinary differential equations

Arden Primary School
Mathematics teacher

Birmingham, UK
Jan. 2013–Jul. 2015

- Taught national curriculum mathematics to Year 5 and Year 6 students in a state funded inner-city school
- Designed and delivered training to teaching assistants and trainee teachers

Her Majesty's Prison Birmingham
Trainee teacher

Birmingham, UK
Sep. 2011–Jul. 2012

- Taught mathematics at GCSE level to adult male prisoners

Computer Skills

- **Operating systems:** Mac OS, Linux and Windows
- **Languages and protocols:** Python (incl. SciPy, NumPy, Pandas, Matplotlib), Julia, Git, LaTeX, Bash, HTML

Achievements

- Teaching judged as Outstanding by Ofsted, 2013
- Qualified Teaching and Learning Status awarded from the Institute for Learning, 2013
- SWJ Smith prize for graduating with the highest average, 2011
- Department of physics prize for highest average in 3rd year, 2010

Selected Talks and Outreach

- "*Breaking periodicity: vibrations of defects in photovoltaic materials*", CECAM anharmonicity and thermal properties of solids, Paris, January 2018
- "*Anharmonic lattice vibrations in halide perovskites: heat transport, vacancy formation, and non-radiative recombination*", International conference on perovskite solar cells and optoelectronics, Oxford, September 2017
- [Public talk] "*Saving the world with quantum mechanics*", The Gunmaker's Arms, Birmingham, July 2017

Selected Publications

- 1) L. D. Whalley, "effmass: An effective mass package," *The Journal of Open Source Software*, 2018.
- 2) L. D. Whalley, R. Crespo-Otero, and A. Walsh, "H-centre and V-centre defects in hybrid halide perovskites," *ACS Energy Letters*, vol. 2, 2017.
- 3) L. D. Whalley, J. M. Frost, Y.-K. Jung, and A. Walsh, "Perspective: Theory and simulation of hybrid halide perovskites," *The Journal of Chemical Physics*, vol. 146, 2017.
- 4) L. D. Whalley, J. M. Skelton, J. M. Frost, and A. Walsh, "Phonon anharmonicity, lifetimes, and thermal transport in $\text{CH}_3\text{NH}_3\text{PbI}_3$ from many-body perturbation theory," *Physical Review B*, vol. 94, 2016.

References

Available on request