

# Lucy Whalley

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## Objective

To design and optimise renewable energy materials using solid-state physics and computational modelling

## Education

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

## Research Experience

<b>Imperial College London</b> PhD student	London, UK Sep. 2015–present
<ul style="list-style-type: none"><li>• Investigating the impact of point defects and anharmonicity in thin-film photovoltaic materials</li><li>• Using Density Functional Theory and High Performance Computing to calculate electronic structure</li><li>• Writing post-processing software using Python and the SciPy eco-system</li><li>• Reviewer for Journal of Chemical Physics</li><li>• Member of the Imperial College Research Software Engineering Committee</li></ul>	
<b>University of Birmingham</b> MSci student	Birmingham, UK Sep. 2010–Jul. 2011
<ul style="list-style-type: none"><li>• Solved the Boltzmann transport equation to calculate the transverse magneto-resistance of a quasi 2-dimensional metal</li><li>• Used analytical methods, the Abrikosov-Chambers method, and numerical integration routines</li></ul>	
<b>University of Birmingham</b> Summer intern	Birmingham, UK Jul. 2010–Sep. 2010
<ul style="list-style-type: none"><li>• Used Bayesian inference to analyse gravitational wave data from the Laser Interferometer Gravitational-Wave Observatory</li></ul>	

## Teaching Experience

<b>Software Carpentry Foundation</b> Volunteer Instructor	London, UK Jan. 2018–present
<ul style="list-style-type: none"><li>• Teaching basic computing skills (Git, Bash and Python) to academic researchers</li><li>• Designing workshops based upon the Software Carpentry scheme of work</li></ul>	
<b>Imperial College London</b> Tutor	London, UK Sep. 2017–Jul. 2018
<ul style="list-style-type: none"><li>• Tutored mathematics to first year students on the Materials Science degree programme</li><li>• Curriculum included calculus, complex numbers, matrices and ordinary differential equations</li></ul>	
<b>Arden Primary School</b> Mathematics teacher	Birmingham, UK Jan. 2013–Jul. 2015

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

#### **Her Majesty's Prison Birmingham**

Trainee teacher

Birmingham, UK

Sep. 2011–Jul. 2012

- Taught basic skills mathematics to adult male prisoners
- Lessons supported students' vocational training in, for example, plumbing or barbering

#### **Computer Skills**

- **Operating systems:** Mac OS, Linux and Windows
- **Languages and protocols:** Python (incl. SciPy, NumPy, Pandas, Matplotlib), 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 upon request