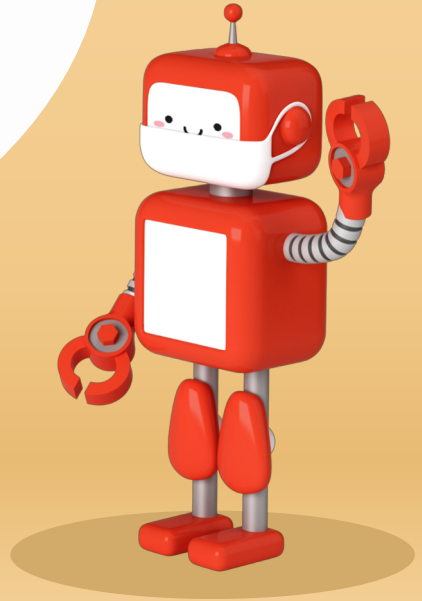
Defects and distortions in energy materials



Lucy Whalley
Vice Chancellor's Research Fellow
Northumbria University

About Me

Birmingham

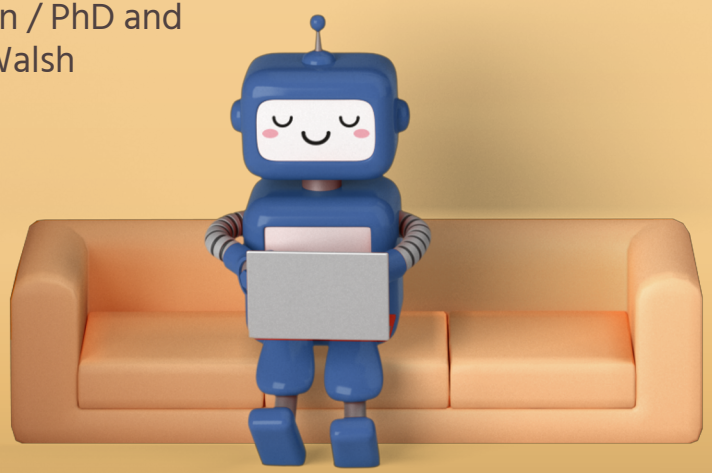
(2007-2011) University of Birmingham / Msci Theoretical Physics
(2011-2015) PGCE and Mathematics teacher

London

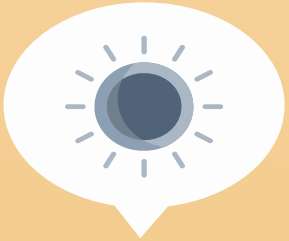
(2015-2020) Imperial College London / PhD and research assistant with Prof. Aron Walsh

Newcastle

(2020) Maternity leave
(2020-present) Northumbria University / Vice-chancellor's research fellow



Academic Interests



Energy materials

Photovoltaics
Battery cathodes

Atomistic modelling

Electronic structure
Solid state physics

Software engineering

Open source software development

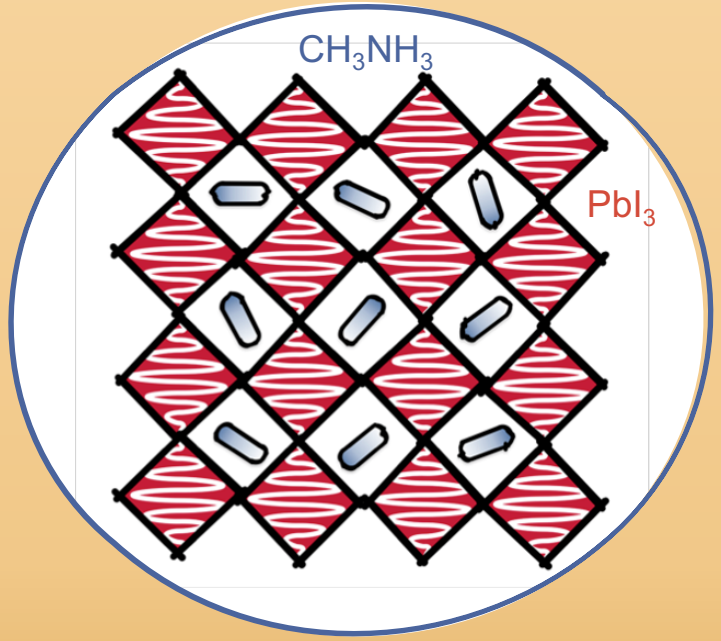
Teaching

Software Carpentry
CodeRefinery

"Theoretical materials science and technology has several levels, and also several roles. It provides a framework in which to organize empirical results. It can be used to scope a new field. It can be used to separate out the components of some complex system, where experiment alone still confuses. And one can imagine cases—especially for the shortest or the longest timescales—where theory can outreach experiment."

- Marshall Stoneham

Defects in semiconductors and oxides: where are the gaps in first principles theory?



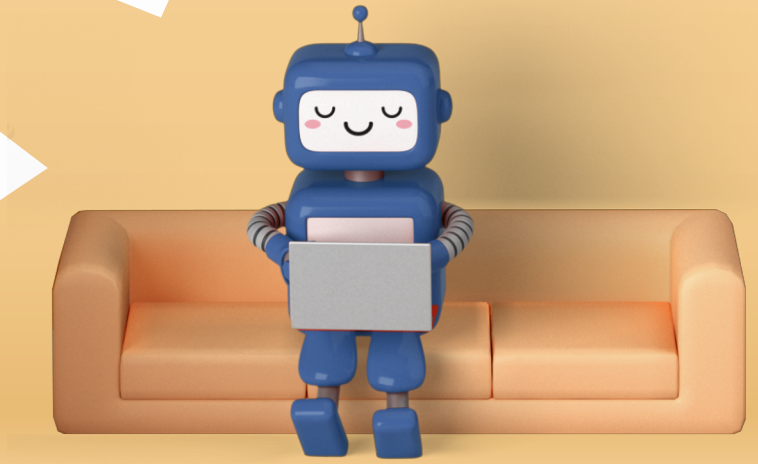
Hybrid halide perovskites

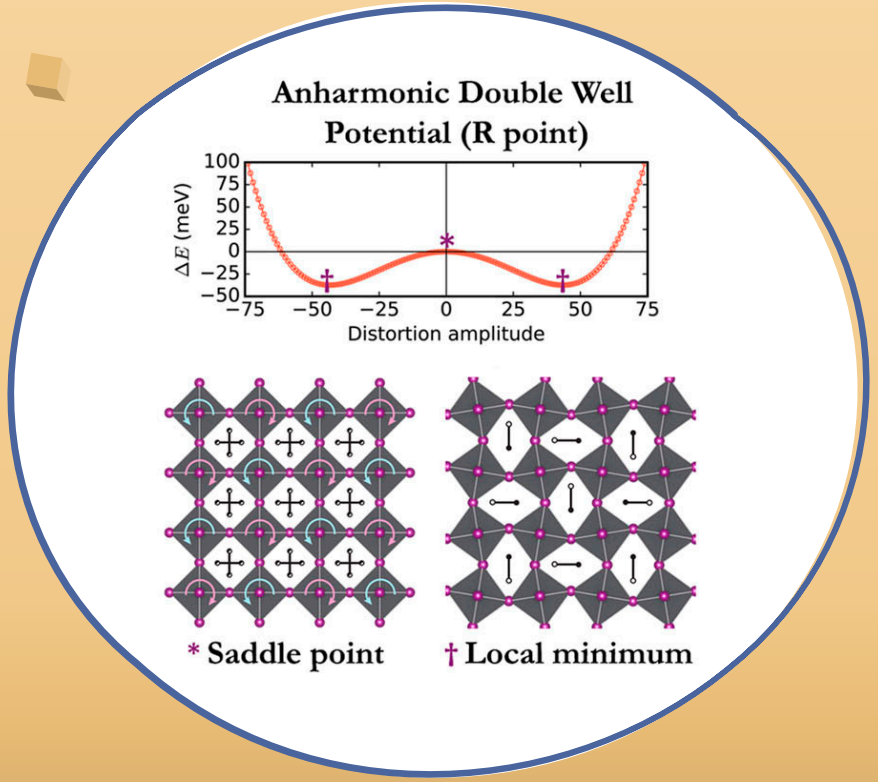
A challenge for computational modelling:

- Large anharmonic tilting
- Strong electron-phonon coupling
- Spin-orbit effects
- Halide segregation
- High defect densities
- Mobile ions
- ….

Research interests

Lattice distortions and **carrier capture**





Anharmonic lattice distortions

Hybrid halide perovskites are highly anharmonic and these distortions lead to:

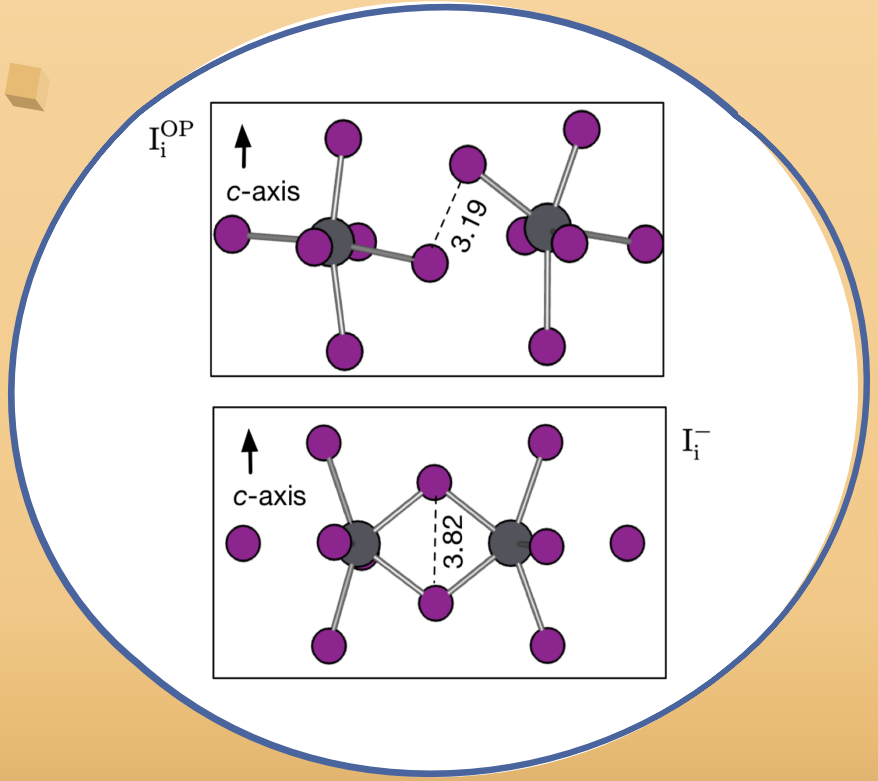
- Band gap broadening (30meV at RT)
- Ultra-low thermal conductivity (0.05 $Wm^{-1}K^{-1}$)
- Slow cooling of hot polarons (100's ps)

Theory/Methods: Hybrid DFT, lattice dynamics, mode-mapping, Boltzmann transport, classical diffusion

Codes: ModeMap.py (Jonathan Skelton), PolaronMobility.jl (Jarvist Frost)

Publications: Phys. Rev. B 94 (22), 220301 // ACS Energy Lett. 2 (12), 2647-2652

Non-radiative carrier capture



There is fast electron capture at the H-centre (neutral iodine intersitial) in $CH_3NH_3PbI_3$.

- The electron capture coefficient is $10^{-10}cm^3s^{-1}$ (c.f. radiative: $10^{-13}cm^3s^{-1}$)
- Strong electron-phonon coupling: S_{HR}=350
- The process is irreversible

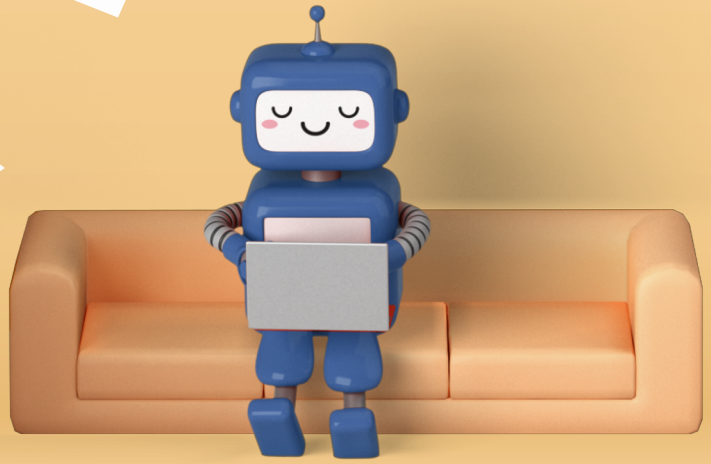
Theory/Methods: DFT, First-principles multiphonon carrier capture, lattice dynamics

Codes: CarrierCapture.jl (Walsh group), JuliaPhonons.jl (Jarvist Frost)

Publications: ACS Energy Lett. 2 (12), 2713-2714 //

Future plans

Battery cathode materials and **experimental collaborations**



Disorder in spinel cathode materials

Combining quantum chemical simulations (DFT) with statistical techniques (cluster expansion) to better understand the defect properties of battery electrodes **during the charge/discharge cycle**.

- Focus on spinel: $MgCr_2(S/Se)_4$ and $MgMn_2O_4$
- Link the effects of site disorder and point defects with battery performance
- Develop methods and tools for calculating the vibrational spectra of disordered materials (doi:10.3389/fenrg.2018.0082)
- A PhD project is available: *"Modelling disorder in Mg-ion battery cathode materials"* – ***bit.ly/renu_mg***

Experimental collaborations

Northumbria University has a strong track record in the synthesis and characterisation of PV materials

- Northumbria University Photovoltaics (NUPV)
- CDT-Renewable Energies North-east Universities (CDT-RENU)
- North East Centre for Energy Materials (NECEM)

Michael Jones

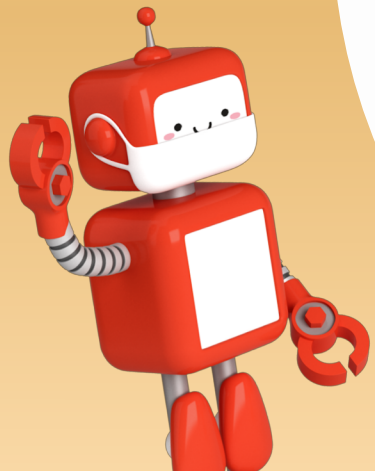
Back contact engineering of thin-film kesterite solar cells

Ewan Matheson

ZnO-based nanostructures for hydrogen storage

Thanks!!

PhD project available: bit.ly/renu_mg

Email: l.whalley@northumbria.ac.uk

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