ANGELA HARPER

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I am a computational physicist passionate about leveraging machine learning to solve complex physical problems. As a postdoctoral fellow, I developed a workflow to predict high-quality spectroscopic properties from limited datasets and created computational tools for efficient data management and analysis. In my PhD, I combined ab-initio calculations with experimental spectroscopy data to enhance the accuracy of amorphous structure modelling. My expertise lies at the intersection of quantum-mechanical simulations and machine learning, with a focus on improving predictions in the physical sciences by incorporating experimental data. With strong communication and leadership skills, I thrive in interdisciplinary environments that value teamwork. I am looking for industry positions where I can improve my skills in machine learning and tackle new challenges in physics and chemistry.

EDUCATION

2018-2022 **PhD, Physics, University of Cambridge**

Thesis: "Extending first principles spectroscopy to disordered materials: a study on amorphous and crystalline aluminas" - Supervisors: Prof. Michael Payne, Prof. Andrew Morris

- Applied quantum mechanical methods to compute experimental NMR and XAS spectra, developing a workflow for their application to larger amorphous materials.
- Developed a method for incorporating vibrational properties into first principles calculations to improve their accuracy in comparison with ground-state DFT.
- Gained experience utilizing graph-based neural networks for ML interatomic potentials.

2017-2018 **MPhil, Physics, University of Cambridge**

Thesis: "Ab Initio Prediction of Metal Phosphide Anode Materials for Lithium and Beyond Lithium Batteries" – Supervisor: Prof. Andrew Morris

- Used high-throughput structure prediction methods including random structure searching and genetic algorithms to identify novel Li-ion battery materials.
- Gained proficiency with density-functional theory calculations including calculating phonon spectra, density of states, Li-ion battery capacity, and voltage profiles.
- Became proficient in using data visualization libraries, such as Matplotlib, seaborn, and pandas to communicate findings effectively.

2013-2017 **BS, Physics, Minor: CompSci/Math, Wake Forest University, USA**

- Graduated with honours, ranking first in the class with a 4.0 GPA.
- Developed an application using Java and Android Studio to trail mark in the Appalachians.
- Worked in a bioinformatics lab to develop an unsupervised learning protocol for protein structure-function identification.

RESEARCH EXPERIENCES

2022- **PostDoc, Computational Chemistry, Fritz Haber Institute of the MPG, DE**

Supervisors: Prof. Dr. Karsten Reuter, Dr. Christoph Scheurer

- Developed and implemented a workflow utilizing equivariant kernel-based methods to accurately predict Nuclear Magnetic Resonance (NMR) properties.
- Curated a comprehensive dataset of over 30k NMR tensors using a combination of DFT, AIMD, and statistical techniques for data filtering.
- Supervised two PhD students on individual projects in applying machine learning to predicting experimental observable properties

2016 **Research Intern, Computational Chemistry, Cornell University, USA**

Supervisor: Prof Paulette Clancy

- Employed Bayesian optimisation methods and LCAO DFT for understanding the solution processing of hybrid organic/inorganic perovskites.
- Utilized statistical sampling approaches to train an empirical potential for Fe atoms

COMPUTATIONAL SKILLS

Languages	Python, Fortran90, C++, Java	**Tools**	git, VisualStudio, Unix/Linux, vim
Packages	NumPy, matplotlib, scikit-learn, SciPy, pandas, pymatgen, ase, Tensorflow	**DFT**	CASTEP, VASP, Orca, Quantum Espresso, ONETEP, Fermions++
Spectra	NMR, XAS, XRD, Raman	**ML+Physics**	TENSOAP, GAP, SchNet, AENet

AWARDS AND SCHOLARSHIPS

2022	**Alexander von Humboldt PostDoctoral Fellowship, DE**
2018	**Gates Cambridge Scholarship, UK**
2018	**Winton Programme for the Physics of Sustainability Scholarship, UK**
2017	**Churchill Scholarship from the Churchill Foundation, USA**
2017	**LeRoy Apker Award from the American Physical Society, USA**

SKILLS

Project Management and Collaboration	• Orchestrated the collaborative writing, editing, and timely submission of a review article involving a team of 7 individuals for **Johnson Matthey Technology Review**. • Acted as the **Point of Contact for the HEC** Materials Chemistry Consortium, coordinating grant applications for 20+ scientists while following strict deadlines. • Lead communications for the **PostDoc Day Berlin** securing sponsorships from industry and academic partners and establishing effective platforms for engagement
Leadership and Mentoring	• **Physics 1A Senior Lab Instructor**, providing guidance to fellow PhD students on supervising the labs and supervising undergraduate students throughout the course • Led a team of 6 PhD students as part of the Cambridge University Science Policy Exchange, establishing **the Cambridgeshire Decarbonisation Fund** • Organised the **Electronic Structure Discussion Group** for 3 years during my PhD organising weekly seminars with international speakers.
Cooperation	• Contributed to public code repositories such as OptaDOS and matador by submitting pull requests, developing tests, and promptly addressing change requests. • Acted as the **Secretary of the Churchill College MCR**, effectively liaising with administrative and postgraduate members to address their respective needs

SELECTED PUBLICATIONS

Additional Publications available at ORCID: 0000-0002-0699-0450

Angela F. Harper, Simone Köcher, Karsten Reuter, and Christoph Scheurer. Towards *in silico* Spectroscopy: Machine learned electric field gradients using equivariant descriptors. *In Press,* 2023

Angela F. Harper, Steffen P Emge, Peter C M M Magusin, Clare P Grey, and Andrew J Morris. Modelling amorphous materials via a joint solid-state NMR and X-ray absorption spectroscopy and DFT approach: application to alumina. *Chemical Science*, 14:1155–1167, 2022 10.1039/D2SC04035B

Angela F. Harper, Bartomeu Monserrat, and Andrew J. Morris. Finite temperature effects on the X-ray absorption spectra of crystalline aluminas from first principles. *AIP Advances* 13, 055015, 2023 10.1063/5.0146033

Angela F. Harper, Matthew L Evans, and Andrew J Morris. Computational investigation of copper phosphides as conversion anodes for lithium-ion batteries. *Chemistry of Materials*, 32(15):6629–6639, 2020 10.1021/acs.chemmater.0c02054

Benjamin J Foley, Justin Girard, Blaire A Sorenson, Alexander Z Chen, J Scott Niezgoda, Matthew R Alpert, **Angela F. Harper**, Detlef-M Smilgies, Paulette Clancy, Wissam A Saidi, et al. Controlling nucleation, growth, and orientation of metal halide perovskite thin films with rationally selected additives. *Journal of Materials Chemistry A*, 5(1):113–123, 2017 10.1039/C6TA07671H

Angela F. Harper, Janelle B Leuthaeuser, Patricia C Babbitt, John H Morris, Thomas E Ferrin, Leslie B Poole, and Jacquelyn S Fetrow. An atlas of peroxiredoxins created using an active site profile-based approach to functionally relevant clustering of proteins. *PLoS computational biology*, 13(2):e1005284, 2017 10.1371/journal.pcbi.1005284