ANGELA F. HARPER

Theoretical Chemistry Group, Fritz-Haber Institute, Max Planck Society, DE
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EDUCATION

PhD in Theoretical Condensed Matter Physics — September 2018 – September 2022
University of Cambridge, Cambridge UK
Gates Cambridge Fellowship
Winton Fellowship for the Physics of Sustainability
Supervisors Prof. Michael Payne and Prof. Andrew J. Morris

MPhil in Physics — September 2017 – September 2018
University of Cambridge, Cambridge UK
Churchill Scholarship
Supervisor Prof. Andrew J. Morris

B.S. with Honors in Physics — August 2013 – June 2018
Wake Forest University, Winston-Salem, NC, USA
4.0 GPA in Physics, Minors in Mathematics and Computer Science
LeRoy Apker Award from the American Physical Society (APS)
Awarded to 2 undergraduates in the USA per year for the best senior thesis in Physics.
Stamps Scholarship for Academic Excellence

RESEARCH EXPERIENCES

Theoretical Chemistry Group — September 2022 – Present
Fritz-Haber Institute of the Max Planck Society, Berlin, DE
Alexander von Humboldt Research Fellow – Faculty Host Prof. Dr. Karsten Reuter

Smith School of Chemical and Biomolecular Engineering — Summer 2016
Cornell University, Ithaca, NY, USA
REU in Computational Chemistry funded by the NSF

PUBLICATIONS

12. **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

11. **Angela F. Harper**, Kamil Iwanowski, Mike C. Payne, Michele Simoncelli. Vibrational and thermal properties of amorphous alumina from first principles. *Under Review in Phys. Rev. Mat.* 2023 arxiv.org/abs/2303.08637

10. **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

9. **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

8. **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

7. **Angela F. Harper**, Matthew L. Evans, James P. Darby, Bora Karasulu, Can P. Koçer, Joseph R. Nelson, and Andrew J. Morris. Ab initio structure prediction methods for battery materials. *Johnson Matthey Technology Review*, 2020. 10.1595/205651320X15742491027978.

6. **Angela F. Harper**, Peter J Diemer, and Oana D Jurchescu. Contact patterning by laser printing for flexible electronics on paper. *npj Flexible Electronics*, 3(1):1–6, 2019. 10.1038/s41528-019-0055-3.

5. 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

4. Peter J Diemer, **Angela F. Harper**, Muhammad R Niazi, Anthony J Petty, John E Anthony, Aram Amassian, and Oana D Jurchescu. Laser-printed organic thin-film transistors. *Advanced Materials Technologies*, 2(11):1700167, 2017. 10.1002/admt.201700167.

3. Janelle B Leuthaeuser, John H Morris, **Angela F. Harper**, Thomas E Ferrin, Patricia C Babbitt, and Jacquelyn S Fetrow. DASP3: identification of protein sequences belonging to functionally relevant groups. *BMC bioinformatics*, 17(1):458, 2016. 10.1186/s12859-016-1295-z.

2. **Angela F. Harper**, Janelle B Leuthaeuser, Patricia C Babbitt, John H Morris, Thomas 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

1. Stacy T Knutson, Brian M Westwood, Janelle B Leuthaeuser, Brandon E Turner, Don Nguyendac, Gabrielle Shea, Kiran Kumar, Julia D Hayden, **Angela F. Harper**, Shoshana D Brown, et al. An approach to functionally relevant clustering of the protein universe: Active site profile-based clustering of protein structures and sequences. *Protein Science*, 26(4):677–699, 2017. 10.1002/pro.3112.

INTERNATIONAL AWARDS

2022 Alexander von Humboldt Postdoctoral Fellowship, DE. Value: €60,000
2021 Computational Science Centre for Research Communities (CoSeC) Impact Award, UK.
2018 Gates Cambridge Scholarship, UK. Value: £70,000
2018 Winton Programme for the Physics of Sustainability Scholarship, UK. Value: £70,000
2017 National Science Foundation Graduate Research Fellowship *(Declined for Gates Cambridge)*
2017 Rhodes Scholar District 6 - *Finalist*
2017 Churchill Scholarship from the Churchill Foundation, USA. Value: £15,000
2017 LeRoy Apker Award from the American Physical Society, USA. Value: $10,000
2016 Goldwater Scholarship: Value: $10,000
2013 Stamps Scholarship for Academic Excellence, USA. Value: $180,000

TEACHING

2018-22 **Churchill College Supervisor** leading weekly supervisions for 3rd year physicists
2021 **Invited Lecturer** for the NanoDTC M.Sci. program, Cambridge University UK
2018-22 **Senior Lab Instructor** for the Physics 1A undergraduate lab course at Cambridge

2018-19 **Invited Tutor** for the CASTEP Workshop leading online tutorials for new PhDs
2017-19 **Pembroke College Supervisor** leading weekly maths supervisions for small-groups

PROFESSIONAL SERVICE

2023 **Consultant** for a Battery Materials Design start-up in their seed funding round
2023 **Grant Application Reviewer** for the Physical Sciences applications of the 2024 Churchill Scholars, reading between 25-35 applications
2023- **CECAM Workshop Organiser** securing funding through Psi-K, DFG, and CECAM for a workshop of 75 people on "ML for Experimental Observables"
2022-23 **PostDoc Day Berlin** **Communications Liason** for the two day conference with over 250 PostDocs across disciplines in Berlin alongside a team of 5 other PostDocs
2019-22 **Grant Submission** for the HEC Materials Chemistry Consortium, managing the submission of grants for compute time worth over 20M CPUh every 6 months
2020-21 **Consultant for the Cambridgeshire County Council** as part of the Cambridge Uni. Science Policy Exchange to design a Cambridgeshire Decarbonisation Fund
2018-21 **Chair of the Electronic Structure Discussion Group** leading weekly talks from speakers both internal and external to Cambridge
2017-21 **Secretary of the Churchill College MCR** acting as a communication for graduate students to administrators, I designed an "Active Bystander" program for all incoming students which is still used today

COMPUTATIONAL SKILLS

Languages	Python, Fortran90, C++, Java
Packages	NumPy, matplotlib, scikit-learn, SciPy, pandas, pymatgen, ase
Expt.	NMR, XAS, XRD, Raman
Tools	git, VisualStudio, Unix/Linux, vim
DFT	CASTEP, VASP, Orca, Quantum Espresso, ONETEP, Fermions++
ML Descriptors	TENSOAP**,** GAP, e3nn
Open Source	Jupyter Notebook example of structure prediction for copper phosphides Contributor to matador the first principles high throughput computational tool Implemented chemical shifts for XANES in OPTADOS