ANGELA F. HARPER

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

harpaf13.github.io | harper@fhi.mpg.de | @ScienceAnge

EDUCATION

PhD in Theoretical Condensed Matter Physics — September 2018 – October 2022

University of Cambridge, Cambridge UK

"Extending first principles spectroscopy to disordered materials: a study on amorphous and crystalline aluminas"

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

"Ab Initio Prediction of Metal Phosphide Anode Materials for Lithium and Beyond Lithium Batteries"

Churchill Scholarship

Supervisor Prof. Andrew J. Morris

B.S. with Honors in Physics — August 2013 – June 2017

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

Theory 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 National Science Foundation of the USA.

PUBLICATIONS

12. **Angela F. Harper**, Simone Köcher, Karsten Reuter, and Christoph Scheurer. A data-driven approach to machine learning tensors in quantum chemistry. *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- **Scientific Consultant** for Anqalab, LTD a quantum chemistry and AI start-up
2023- **Battery Journal Club** organizer of the bi-weekly seminar series
2023- **Application Reviewer** for the Physical Sciences applications of the 2024 Churchill Scholars
2023- **CECAM Workshop Co-Organiser** securing funding through Psi-K, DFG, and CECAM for a workshop of 75 people on "ML for Experimental Observables"
2023 **Girls' Day Volunteer** helping with the technical organisation of the "Crystal Math" program teaching young girls about quantum chemistry

2022-23	**PostDoc Day Berlin Co-Organizer** 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
2014-17	**Girls in STEM** developed a mentorship program between middle-school girls and undergraduate women in STEM at Wake Forest University

MEDIA

2022	**Interview –** "Cavendish Inspiring Womxn – Angela Harper"
2021	**Presentation –** "Cambridgeshire Business Decarbonisation Contribution Plan"
2021	**CoSeC Press Release –** "Coding, Collaborating and Communicating to keep energy materials discovery and development flowing"
2020	**Interview –** "Churchill College student on a rowing adventure at Cambridge University Women's Boat Club that STEMs from a musical passion"
2020	**Interview –** "Women in STEM: Angela Harper"
2019	**LeRoy Apker Press Release –** "2017 LeRoy Apker Recipient"

CONFERENCES & PRESENTATIONS

October 2023	**Poster** – The e-conversion Conference 2023, Tutzing, DE
September 2023	**Flash Talk** – The Inaugural Lennard Jones Centre Meeting, Cambridge UK
June 2023	**Invited Talk** – Seminar Series of Prof. Dr. Bittl, Freie Universität Berlin, DE
June 2023	**Poster** – CECAM-Psi-K Research Conference, Zuse Institut Berlin, DE
March 2023	**Presentation** – German Physical Society (DPG) Spring Meeting
March 2023	**Twitter Poster -** #RSCPoster
February 2023	**Presentation** – Multiscale Modelling in Materials Energy & Catalysis
September 2022	**Presentation** – German Physical Society (DPG) Spring Meeting
August 2022	**Presentation** – Psi-K Conference 2022, Lausanne, CH
May 2021	**Presentation** – Climate Exp0 Pre-COP26 UN Meeting
March 2021	**Presentation** – American Physical Society (APS) Online March Meeting
June 2020	**Invited Talk** – University of Bath Seminar Series of Kit McColl
June 2020	**Invited Talk** – University of Oxford Seminar Series of Rebecca Nicholls
March 2019	**Presentation** – German Physical Society (DPG) Spring Meeting
March 2018	**Invited Talk** – APS March Meeting LeRoy Apker Award Presentation

ACADEMIC ASSOCIATIONS

2023-	**American Physical Society (APS)** Early Career Member
2023-	**Royal Society of Chemistry (RSC)** Affiliate Member
2023-	**PyLadies'** Member
2019-	**Deutsche Physikalische Gesellschaft (DPG)** Member
2017-2022	**American Physical Society (APS)** Student Member

COMPUTATIONAL SKILLS

Languages	Python, Fortran90, C++, Java
Packages	NumPy, matplotlib, scikit-learn, SciPy, pandas, pymatgen, ase
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