

# 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 – 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

15. **Angela F. Harper**, Tabea Huss, Simone Köcher, Christoph Scheurer. Tracking Li atoms in real-time with ultra-fast NMR simulations. *Submitted to Faraday Disc.* 2024 [10.26434/chemrxiv-2024-k4fbw](https://doi.org/10.26434/chemrxiv-2024-k4fbw)

14. Javier Valenzuela Reina, Federico Civaia, **Angela F. Harper**, Christoph Scheurer, Simone Köcher, The EFG Rosetta Stone: Translating between DFT calculations and solid state NMR experiment. *Submitted to Faraday Disc.* 2024

13. James P. Darby, **Angela F. Harper**, Joseph R. Nelson, Andrew J. Morris. Structure prediction of stable sodium germanides at 0 and 10 GPa. *ArXiv*, 2024 [arxiv.org/abs/2402.15299](https://arxiv.org/abs/2402.15299)

12. **Angela F. Harper**, Simone Köcher, Karsten Reuter, and Christoph Scheurer. A data-driven approach to machine learning tensors in quantum chemistry. *Submitted*, 2023

11. **Angela F. Harper**, K. Iwanowski, M. C. Payne, M. Simoncelli. Vibrational and thermal properties of amorphous alumina from first principles. *Phys. Rev. Mat.* 10, 1103, 2024 [10.1103/PRM.8.043601](https://doi.org/10.1103/PRM.8.043601)

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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/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](https://doi.org/10.1002/pro.3112).

## INTERNATIONAL AWARDS

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- 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

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- 2018-22 **Churchill College Supervisor** leading weekly supervisions for 3<sup>rd</sup> 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

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2023-	<b>Scientific Consultant</b> for Anqalab, LTD a quantum chemistry and AI start-up
2023-	<b>Battery Journal Club</b> organizer of the bi-weekly seminar series
2023-	<b>Application Reviewer</b> for the Physical Sciences applications of the 2024 Churchill Scholars
2023-	<b>CECAM Workshop Co-Organiser</b> securing funding through Psi-K, DFG, and CECAM for a workshop of 75 people on “ML for Experimental Observables”
2023	<b>Girls’ Day Volunteer</b> helping with the technical organisation of the “Crystal Math” program teaching young girls about quantum chemistry
2022-23	<b>PostDoc Day Berlin Co-Organizer</b> for the two-day conference with over 250 PostDocs across disciplines in Berlin alongside a team of 5 other PostDocs
2019-22	<b>Grant Submission</b> for the <a href="#">HEC Materials Chemistry Consortium</a> , managing the submission of grants for compute time worth over 20M CPUh every 6 months
2020-21	<b>Consultant for the Cambridgeshire County Council</b> as part of the Cambridge Uni. Science Policy Exchange to design a <a href="#">Cambridgeshire Decarbonisation Fund</a>
2018-21	<b>Chair of the <a href="#">Electronic Structure Discussion Group</a></b> leading weekly talks from speakers both internal and external to Cambridge
2017-21	<b>Secretary of the Churchill College MCR</b> 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	<b>Girls in STEM</b> developed a mentorship program between middle-school girls and undergraduate women in STEM at Wake Forest University

## MEDIA

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2024	<b>Lindau Press Release</b> – “ <a href="#">Dr. Harper...selected for Lindau Nobel Laureate Meeting</a> ”
2022	<b>Interview</b> – “ <a href="#">Cavendish Inspiring Womxn – Angela Harper</a> ”
2021	<b>Presentation</b> – “ <a href="#">Cambridgeshire Business Decarbonisation Contribution Plan</a> ”
2021	<b>CoSeC Press Release</b> – “ <a href="#">Coding, Collaborating and Communicating to keep energy materials discovery and development flowing</a> ”
2020	<b>Interview</b> – “ <a href="#">Churchill College student on a rowing adventure at Cambridge University Women's Boat Club that STEMs from a musical passion</a> ”
2020	<b>Interview</b> – “ <a href="#">Women in STEM: Angela Harper</a> ”
2019	<b>LeRoy Apker Press Release</b> – “ <a href="#">2017 LeRoy Apker Recipient</a> ”

## CONFERENCES & PRESENTATIONS

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June 2024	<b>Invited Speaker</b> – <a href="#">ELECTRA Battery Symposium</a> , Jülich, DE
June 2024	<b>Invited Attendance</b> – The 2024 Lindau Nobel Prize Meeting, Lindau, DE
April 2024	<b>Presentation</b> – <a href="#">Multiscale Modelling in Materials Energy &amp; Catalysis</a>
March 2024	<b>Talk</b> – German Physical Society (DPG) Spring Meeting
February 2024	<b>Poster</b> – Batteries, Gordon Research Conference, Ventura, CA, USA
February 2024	<b>Invited Talk</b> – Batteries, Gordon Research Seminar, Ventura, CA, USA
October 2023	<b>Poster</b> – The <a href="#">e-conversion Conference</a> 2023, Tutzing, DE
September 2023	<b>Flash Talk</b> – The Inaugural <a href="#">Lennard Jones Centre Meeting</a> , Cambridge UK
June 2023	<b>Invited Talk</b> – Seminar Series of Prof. Dr. Bittl, Freie Universität Berlin, DE
June 2023	<b>Poster</b> – CECAM-Psi-K Research Conference, Zuse Institut Berlin, DE
March 2023	<b>Presentation</b> – German Physical Society (DPG) Spring Meeting
March 2023	<b>Twitter Poster</b> - <a href="#">#RSCPoster</a>
February 2023	<b>Presentation</b> – <a href="#">Multiscale Modelling in Materials Energy &amp; Catalysis</a>
September 2022	<b>Presentation</b> – German Physical Society (DPG) Spring Meeting
August 2022	<b>Presentation</b> – Psi-K Conference 2022, Lausanne, CH
May 2021	<b>Presentation</b> – <a href="#">Climate Exp0 Pre-COP26 UN Meeting</a>
March 2021	<b>Presentation</b> – American Physical Society (APS) Online March Meeting
June 2020	<b>Invited Talk</b> – University of Bath Seminar Series of Kit McColl
June 2020	<b>Invited Talk</b> – University of Oxford Seminar Series of Rebecca Nicholls
March 2019	<b>Presentation</b> – German Physical Society (DPG) Spring Meeting
March 2018	<b>Invited Talk</b> – APS March Meeting LeRoy Apker Award Presentation

## ACADEMIC ASSOCIATIONS

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

## COMPUTATIONAL SKILLS

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<b>Languages</b>	Python, Fortran90, C++, Java
<b>Packages</b>	NumPy, matplotlib, scikit-learn, SciPy, pandas, pymatgen, ase
<b>DFT</b>	CASTEP, VASP, Orca, Quantum Espresso, ONETEP, Fermions++
<b>ML Descriptors</b>	TENSOAP, GAP, e3nn
<b>Open Source</b>	<a href="#">Jupyter Notebook</a> example of structure prediction for copper phosphides Contributor to <a href="#">matador</a> the first principles high throughput computational tool Implemented chemical shifts for XANES in <a href="#">OPTADOS</a>