Email: e.wolpert@imperial.ac.uk

## **CURRICULUM VITAE**

## **Emma Helen Wolpert**

Postdoctoral Research Associate Faculty of Natural Sciences Department of Chemistry Imperial College London London, United Kingdom

## ent of Chemistry

#### **Education**

Oct. 2017 — Mar. 2021**DPhil (Inorganic Chemistry), University of Oxford**Thesis title: Structural analogues of complex magnetic phases

Oct. 2013 — Sept. 2017 **MChem, University of Oxford, Chemistry (First Class)**Thesis title: Emergence of Polarisation in Disordered Systems

## Research experience

Mar. 2021 — present **Postdoctoral Research Associate, Imperial College London**Based in Prof. Kim Jelfs' group in the Department of Chemistry

Sept. — Dec. 2019 **Researcher, Chimie Paris Tech, PSL Research University (Paris, France)**I spent four months in Paris as part of my DPhil to learn DFT calculations and *ab initio* molecular dynamics simulations.

June — Aug. 2015 **Summer project student, University of Oxford**Based in Prof. Andrew Goodwin's group in the Inorganic Chemistry Department

## **Awards and Honours**

- RSC Researcher Development and Travel Grant £500 (April 2023)
- Awarded over 18,000 compute hours, worth £3780
- MaThCryst IUCr travel award €300 (2019)
- Poster prize—Physical Crystallography Group & Structural Condensed Matter Physics (2018)
- Hertford College Graduate Scholarship (2017—2020)
- Part II Thesis Prize (Inorganic Chemistry)—Best thesis (2017)
- New College Academic Scholarship (2015—2017)

#### **Journal Publications** (¥ = equal contribution, \* = corresponding author)

- 11. The effect of [n]-helicene length on crystal packing
- JA Schmidt<sup>¥</sup>, **EH Wolpert**<sup>¥</sup>, GM Sparrow, ER Johnson, KE Jelfs Under first revision at *Cryst. Growth & Des.* (2023) Link to article
- 10. Systematic exploration of accessible topologies of cage molecules via minimalistic models A Tarzia, **EH Wolpert**, KE Jelfs, GM Pavan, Accepted at *Chem. Sci.* (2023) Link to article
- 9. On the polytypism of layered MX2 materials
- EH Wolpert, SJ Cassidy, AL Goodwin, Phys. Rev. Mater. 7, 093605 (2023). Link to article
- 8. The effect of disorder in multicomponent covalent organic frameworks
- EH Wolpert\*, A. Tarzia, KE Jelfs\* Chem. Commun. 59, 6909-6912 (2023). Link to article
- 7. Observation of Rare Tri6Di9 Imine Cages Using Highly Fluorinated Building Blocks T Fleck-Kunde, **EH Wolpert**, L zur Horst, R Oestreich, C Janiak, KE Jelfs, BM Schmidt *Organic Materials* **4**, 255-260 (2022). Link to article
- 6. Coarse-grained modelling for predicting the packing of porous organic cages **EH Wolpert\*** and KE Jelfs\* *Chem. Sci.* **13**, 13588-13599 (2022). Link to article
- 5. Modelling the effect of defects and disorder in amorphous metal-organic frameworks I Bechis, AF Sapnik, A Tarzia, **EH Wolpert**, MA Addicoat, DA Keen, TD Bennett, KE. Jelfs, *Chem. Mater.* **34**, 9042-9054 (2022). Link to article
- 4. Into the unknown: how computation can help explore uncharted materials space AM Mroz, V Posligua, A Tarzia, **EH Wolpert**, KE Jelfs *J. Am. Chem. Soc.* **144**, 18730-18743 (2022). Link to article
- 3. Controlling anisotropic properties by manipulating the orientation of chiral small molecules

- J Wade, F Salerno, RC Kilbride, DK Kim, JA Schmidt, JA Smith, L LeBlanc, EH Wolpert, A Adeleke, ER Johnson, J Nelson, T Mori, KE Jelfs, S Heutz, MJ Fuchter Nature Chem. 14, 1383-1389 (2022). Link to article
- 2. Function from configurational degeneracy in disordered framework materials EM Reynolds, **EH Wolpert**, AR Overy, L Mizzi, A Simonov, JN Grima, S Kaskel, AL Goodwin Faraday Discuss. 225, 241-254 (2021). Link to article
- 1. Hybrid local-order mechanism for inversion symmetry breaking EH Wolpert, AR Overy, PMM. Thygesen, A Simonov, MS Senn, AL Goodwin Phys. Rev. B 97, 134106 (2018). Link to article

## Additional submitted papers

- 2. Structure and dynamics of the negative thermal expansion material Cd(CN)2 under pressure CS Coates, M Baise, JM Bulled, EH Wolpert, JW Makepeace, HC Walker, AS Gibbs, DA Fortes, B Slater, AL Goodwin DOI: 10.48550/arXiv.2302.09963 Link to article
- 1. Skyrmion lattices in chiral metal-organic frameworks

EH Wolpert, FX Coudert, AL Goodwin, DOI: 10.26434/chemrxiv.12515594.v1 Link to article

### **Oral Presentations**

•	British Crystallographic Association Spring Meeting (Nottingham) American Chemical Society Fall meeting (Chicago, USA)
Jul 2021 Aug 2021 Aug 2021 Aug 2022 July 2023	Correlated Disorder workshop (Herzberg, Switzerland) FEZA 2021 (Virtual) IUCr 2021 (Hybrid conference, Prague, Czech Republic) IUCr 2021 (Hybrid conference, Prague, Czech Republic) American Chemical Society Fall meeting (Chicago, USA) MC16 (Dublin, Ireland) CECAM Crystal structure prediction in materials discovery (Liverpool, UK)
National Nov 2017 Mar 2018 Jan 2020 Dec 2021 June 2022 Dec 2022	Physical Crystallography Group & Structural Condensed Matter Physics (Abingdon) British Crystallographic Association Spring Meeting (Warwick) Frontiers in Condensed Matter Physics Conference (Bristol) RSC Solid State Chemistry Christmas Meeting (Virtual) UKPormat (Glasgow) Molecular and Supramolecular Chemistry (MASC) (Nottingham) Recent appointees in Materials Science (RAMS) (Lincoln)
Apr 2023 Apr 2023	Imperial College London (UK) UC Riverside (USA) UC Berkeley (USA) Warwick University (UK)

#### Poster Presentations

Nov 2016	Physical Crystallography Group & Structural Condensed Matter Physics (Abingdon, England)
May 2018	European Doctoral Symposium on Metal-Organic Frameworks
	(Raitenhaslach, Germany)
Aug 2018	European Crystallography Meeting (Oviedo, Spain)
July 2018	Aperiodic 2018 (Des Moines, Iowa, USA)
Nov 2018	Physical Crystallography Group & Structural Condensed Matter Physics (Abingdon,
	England)
Apr 2019	Conference on Analysis of Diffraction Data in Real Space (Grenoble, France)
Aug 2019	European Crystallography Meeting (Vienna, Austria)
Oct 2019	CZ-UK Workshop on Nanomaterials (Prague, Czech Republic)

Jul 2021 FEZA 2021 (Virtual)

Aug 2021 IUCr 2021 (Hybrid conference, Prague, Czech Republic)

June 2022 GRC crystal engineering (Maine, USA)

Sept 2022 Design, synthesis and application of next-generation organic semiconductors (London, England)

Sept 2022 Leverhulme Research Centre Symposium (Liverpool, England)

## **Summer Schools**

July 2018	PCG Intensive School in Physical Crystallography
Aug 2018	Physics by the Lake Summer School (Windsor, UK)
Aug 2019	MaThCryst satellite meeting (Vienna, Austria)

# **Teaching Experience**

2019-

2023	Tutor in Inorganic Chemistry, Imperial College London	
2020	Non Stipendiary Lecturer in Inorganic chemistry, St. Catherine's College, University of Oxford	
2018-2019	<b>Non Stipendiary Lecturer</b> in maths for chemistry, St. Catherine's College, University of Oxford	
2018-2019	<b>Non Stipendiary Lecturer</b> in maths for chemistry, St. Anne's College, University of Oxford	
2018-2019	<b>Non Stipendiary Lecturer</b> in maths for chemistry, Oriel College, University of Oxford	
2018	<b>Graduate Teaching Assistant</b> physical chemistry, New College, University of Oxford	
2017-2018	Junior Demonstrator Inorganic Chemistry Laboratory, University of Oxford	
2017-2018	Graduate Tutor maths for chemistry, Jesus College, University of Oxford	
Professional Activities		

2022	Co-organised the "Design, synthesis and application of next-generation organic semiconductors" conference (London, England)
2022-	Reviewer for Journal of American Chemistry Society (2022-), Crystal Growth & Design (2022-), and Chemistry of Materials (2023-)
2022-	Member of the American Chemical Society
2021-	Member of the Royal Society of Chemistry
2019-2021	Committee Member of the Young Crystallographers' Group
2017-2021	Member of the British Crystallographic Association
2018-2021	Member of the European Crystallographic Association
2018-2020	I have conducted undergraduate interviews at three different colleges at the
	University of Oxford: (i) St. Anne's College (2018), (ii) Oriel College (2018), and (iii)
	Corpus Christi College (2019,2020)

Presently supervising 1 MRes, previously supervised 2 UROP students (2019,2023)

and 2 master students, (2020-2021 and 2021-2022)