

# Christian S. Ahart

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## Professional summary

I have recently passed my viva for a PhD in Condensed Matter and Materials Physics at University College London, under the supervision of Prof. Jochen Blumberger. The aim of my research was to better understand charge transport processes in materials through atomistic simulations.

## Publications

1. **Christian S. Ahart**, Kevin M. Rosso and Jochen Blumberger. Implementation and validation of constrained density functional theory forces in the CP2K package. *Accepted*, 2022.
2. **Christian S. Ahart**, Kevin M. Rosso and Jochen Blumberger. Electron and Hole Mobilities in Bulk Hematite from Spin-Constrained Density Functional Theory. *J. Am. Chem. Soc.* 144, 4623–4632, 2022.
3. **Christian S. Ahart**, Jochen Blumberger and Kevin M. Rosso. Polaronic structure of excess electrons and holes for a series of bulk iron oxides. *Phys. Chem. Chem. Phys.* 22, 10699–10709, 2020.

## Education

**2018 - 2022** University College London, UK  
PhD Condensed Matter and Materials Physics

### **Thesis: Charge transport in bulk hematite and at the hematite/water interface**

The mobility for excess electrons and electron holes in bulk hematite was calculated using spin-constrained and gap-optimised hybrid density functional theory, with comparison to calculations of charge transport at the hematite/water interface.

**2014 - 2018** University of Nottingham, UK  
MSc. Chemistry and Molecular Physics (First class Honours)

### **Modules include:**

- Scientific Computing
- Quantum Dynamics
- Solids, Interfaces and Surfaces
- Advanced Physical Chemistry

### **Master's project: Quantum mechanics of rotating electron nuclear spin systems**

This project involved research into, and application of, theoretical and computational techniques to model nuclear magnetic resonance with dynamic nuclear polarisation.

**2007 - 2014** William Howard School, Brampton, UK  
A Levels: Mathematics (A), Physics (A), Chemistry (A), Biology AS (A)  
GCSEs: 9 including Maths and English (A\*-B)

## Research/Teaching Experience

**2018-2021** University College London, UK  
*Postgraduate Teaching Assistant*

- Marked coursework for lecture courses and demonstrated in computer labs.
- Gained experience in a leadership role and working as part of a larger team.

- June - Aug 2017** Friedrich-Schiller-Universität Jena, Germany  
*Summer Research Student*
- Gained acceptance onto a competitive research program coordinated by the German Academic Exchange Service (DAAD).
  - Provided valuable contribution to a large team of established researchers.
  - Supported research into coupled electron-nuclear motion for attosecond time-resolved lasing experiments.
  - Provided input to a Fortran code base and independently wrote Python code for scientific analysis.
- June - Aug 2016** Johns Hopkins University Centre for Talented Youth, Pennsylvania, USA  
*Chemistry Teaching Assistant*
- Secured a position at a prestigious USA summer school for talented youths.
  - Supported the planning and delivery of lessons, workshops and laboratory work; progressed to leading all aspects.
- June - Aug 2015** Camp Marist, New Hampshire, USA  
*Camp Counsellor and Photographer*
- Taught photography and video editing skills to children aged 9-16; progressed to leading classes.
  - Produced photographs to a high standard which were used on the camp website and in the 2016 promotional literature.
- 8 - 10 July 2013** University of Exeter, Exeter, UK  
*Summer School*
- Attended lectures on latest research developments within the Physics and Astronomy Department.
  - Visited undergraduate and research laboratories and took part in demonstrations.
- 22 - 26 June 2013** University of Lancaster, Lancaster, UK  
*Academic work experience*
- Accepted onto a competitive, intensive work experience scheme.
  - Studied latest research developments within the Physics Department.
- Jan 2010 - Jan 2014** Bewcastle Scout Group, Bewcastle, UK  
*Young Leader*
- Assisted and led activities for children aged 6-14, with a focus on Cubs aged 8-10.
  - Responsible for supervising Cubs during activities, including overnight camps.
  - Gained the esteemed Chief Scout Platinum Award.

## Other Skills

- IT: Microsoft Office Suite, Adobe Creative Suite, LaTeX, LINUX.
- Programming: Fortran, Python, MATLAB.
- Bronze and Silver Duke of Edinburgh Awards.
- Full, clean driving licence (8 years).

## Interests

- eSports: captain of a 5-member team within the Nottingham Gaming Society competing in National tournaments.
- Homebrew: member of the London Amateur Brewers, participate in homebrew competitions.
- Rock climbing.