Christian S. Ahart

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Research Interests

I am a postdoctoral researcher interested in gaining a fundamental understanding of important chemical and physical processes in materials through computer simulations. My research spans several key areas:

- Electronic structure of solids and interfaces.
- Ab initio molecular dynamics.
- Charge transport.
- Method development.

Publications

1. Hannah C Nerl, **Christian S. Ahart**, Alberto Eljarrat, Christoph T Koch, Clotilde S Cucinotta, Milivoj Plodinec. Transitional surface Pt carbide formation during carbon nanotube growth. *submitted to Nat. Catal., 2023.*
2. **Christian S. Ahart**, Kevin M. Rosso and Jochen Blumberger. Implementation and Validation of Constrained Density Functional Theory Forces in the CP2K Package. *J. Chem. Theory Comput.* 18, 4438–4446, 2022.
3. **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.
4. **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.

Research Experience

2022-2024 Imperial College London, UK
Research Associate

- Developing methodologies to enable the dynamical modelling of electrochemical systems under applied potential.
- Supporting and supervising PhD and Master's students.
- Giving lectures and leading demonstrating sessions in computer labs.
- Collaborating with experimental scientists, contributing theoretical and computational expertise.

Education

2018 - 2022 University College London, UK
PhD Condensed Matter and Materials Physics
Prof. Jochen Blumberger

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.

Conferences and talks

1. Materials and Molecular Modelling Hub. UK, 2023. Poster presentation.
2. Psi-k. Switzerland, 2022. Poster presentation.
3. Supercomputer modelling of advanced materials at the Royal Society. UK, 2022. Poster presentation.
4. Research Group Seminar at Chicheley Hall. UK, 2022. Oral Presentation.
5. Computational Molecular Science. UK, 2019. Poster presentation.

Skills

- Programming: Fortran including MPI and OpenMP, Python, MATLAB.
- IT: Microsoft Office Suite, Adobe Creative Suite.
- Bronze and Silver Duke of Edinburgh's Awards.

Interests

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

Reference contacts

Dr. Clotilde S. Cucinotta
Imperial College London, UK
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Relationship: Supervisor

Dr. Sergey Chulkov
University of Lincoln, UK
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Relationship: Research collaborator

Prof. Jochen Blumberger
University College London, UK
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Relationship: PhD supervisor