Christian S. Ahart

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Research Interests

I am a researcher interested in gaining a fundamental understanding of important physical and chemical and processes in materials through computer simulations.

My research spans several key areas:

- Electronic structure of solids and interfaces.
- Density functional theory molecular dynamics and machine learning interatomic potentials.
- Method development.

Publications

1. **Christian S. Ahart**, Sergey Chulkov and Clotilde Cucinotta. Enabling Ab-Initio Molecular Dynamics under Bias: The CP2K+SMEAGOL Interface for Integrating Density Functional Theory and Non-Equilibrium Green Functions. *J. Chem. Theory Comput.* 2024.
2. Hannah Nerl, **Christian S. Ahart**, Alberto Eljarrat, Christoph Koch, Clotilde Cucinotta, Milivoj. Plodinec. Transitional surface Pt carbide formation during carbon nanotube growth. *Carbon*, 228, 119399, 2024.
3. **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.
4. **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.
5. **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

2024-2026 Westlake University, Hangzhou, China
Research Assistant Professor in Multiscale Materials Modelling
Dr. Shi Liu

- Combining machine learning molecular dynamics with electronic structure theory to provide fundamental insight into charge transfer dynamics in TiO_2.
- Supporting and supervising PhD and Master's students.

2022-2024 Imperial College London, UK
Research Associate in Computational Nano-Electrochemistry
Dr. Clotilde S. Cucinotta

- Developing and applying 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 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.

Skills

- Programming: Python, Fortran.
- Machine Learning: DeePMD-kit (PyTorch).
- Density Functional Theory: CP2K, SIESTA.
- IT: Microsoft Office Suite, Adobe Creative Suite.

Languages

English (native), Mandarin (basic), French (basic).

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.
- Badminton.

References

Dr. Shi Liu Westlake University, Hangzhou, China
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Relationship: Current supervisor

Prof. Jochen Blumberger
University College London, UK
j.blumberger@ucl.ac.uk
Relationship: Doctoral supervisor