Christian S. Ahart

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Research Interests

My research focuses on developing first-principles electronic structure, molecular dynamics, and machine learning methods to understand charge carrier transport and electrochemical processes in transition metal oxides.

More broadly, my research spans several key areas:

- Electronic structure of solids and interfaces.
- Density functional theory molecular dynamics and neural network potentials.
- Method development.

Publications

1. Jan Wilhelm, Anna Hehn, Hossam Elgabarty, Beliz Sertcan Gökmen, Maximilian Graml, Stepan Marek, Ritaj Tyagi, Frederick Stein, Johann V. Potoschnig, Augustin Bussy, **Christian S. Ahart**, *et al.* CP2K: An Electronic Structure and Molecular Dynamics Software Package – Dynamics, Transport, and Spectroscopic Response, *under review*, arXiv:2607.22916, 2026.
2. **Christian S. Ahart**, Denan Li, Jochen Blumberger and Shi Liu. Polaron Dynamics in TiO_2 from Machine Learning Molecular Dynamics, *under review*, arXiv:2606.01763, 2026.
3. Denan Li, **Christian S. Ahart** and Shi Liu. Disentangling the discrepancy between theoretical and experimental Curie temperatures in ferroelectric $PbTiO_3$, *MRS Commun.* 2026.
4. **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.* 20, 6772–6780, 2024.
5. 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.
6. **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.
7. **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.
8. **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
Postdoctoral Researcher in Multiscale Materials Modelling
Dr. Shi Liu

- Developed DeepPolaron, a machine learning framework for first-principles simulation of adiabatic polaron transport and applied it to quantify the anisotropic polaron mobility in TiO_2.
- Awarded a competitive Fugaku Small-Scale Junior Researchers Project to extend DeepPolaron to polaron transport at oxide/water interfaces.
- Supervised and mentored PhD and Master's students.

2022–2024 Imperial College London, UK
Postdoctoral Researcher in Computational Nano-Electrochemistry
Dr. Clotilde S. Cucinotta

- Developed the CP2K+SMEAGOL interface, enabling ab-initio molecular dynamics simulations of electrochemical systems under applied bias potential.
- Supervised and mentored PhD and Master's students.
- Delivered lectures and led computational laboratory sessions.
- Collaborated with experimental scientists, providing 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

Developed spin-constrained and optimally tuned hybrid DFT approaches to investigate electron and hole transport in hematite and hematite/water interfaces.

2014–2018 University of Nottingham, UK
MSci Chemistry and Molecular Physics, First Class Honours
(Four-year integrated undergraduate Master's degree)

Modules include:

- Scientific Computing
- Quantum Dynamics
- Solids, Interfaces and Surfaces

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

Conducted research into theoretical and computational methods for modelling nuclear magnetic resonance enhanced by dynamic nuclear polarisation.

Skills

- Programming: Python, Fortran.
- Electronic Structure: CP2K, SIESTA.
- Machine Learning: DeePMD-kit (PyTorch).

Languages

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

Interests

Homebrewing, Badminton.

References

Dr. Shi Liu
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Relationship: Current supervisor

Dr. Clotilde S. Cucinotta
Imperial College London, UK
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Relationship: Post-doctoral supervisor

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