Christian S. Ahart

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Professional summary

I have recently joined the group of Dr. Clotilde Cucinotta at Imperial College London as a Research Associate (postdoctoral researcher), working to enable the dynamical modelling of electrochemical systems under applied potential by interfacing the DFT code CP2K with the NEGF code SMEAGOL.

Publications

1. **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.
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.

Research Experience

2022-2024 Imperial College London, UK
Research Associate

- Working to enable the dynamical modelling of electrochemical systems under applied potential by.
- Responsible for supporting PhD and Masters students with their research.

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)

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 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.

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's Awards.
- Full, clean driving licence (10 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, badminton.