Samuel J. Hall, Ph.D.

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Personal Profile

Chemistry doctoral graduate, who specialised in electronic structure calculations for core-level x-ray spectroscopy simulations of metal-organic interfaces. Looking into using machine learning techniques to predict core-level spectra.

Employment

2022 – 2023 **Postdoctoral Research Fellow** Maurer Group, Department of Chemistry, University of Warwick, United Kingdom.

Education

2018 – 2022 **Ph.D., University of Warwick** in Analytical Science (*MAS CDT*)
Thesis title: *Computational Prediction of Core-Level Spectroscopy of Metal-Organic Interfaces to Reveal Chemical Interactions, Bonding and Behaviours* - Prof. Reinhard J. Maurer

2017 – 2018 **M.Sc., University of Warwick** in Analytical Science (*MAS CDT*)

2012 – 2016 **MChem., University of Leicester** in Chemistry
Year abroad at Oklahoma State University (2014 – 2015)

Key Research Publications

1. **Hall**, **S. J.**, Klein, B. P., & Maurer, R. J. (2022, October 4). Characterizing molecule-metal surface chemistry with ab-initio simulation of x-ray absorption and photoemission spectra. doi:10.48550/arXiv.2210.02187
2. Chaudhuri, S., **Hall**, **S. J.**, Klein, B. P., Walker, M., Logsdail, A. J., Macpherson, J. V., & Maurer, R. J. (2022). Coexistence of carbonyl and ether groups on oxygen-terminated (110)-oriented diamond surfaces. *Communications Materials*, *3*(1), 6. doi:10.1038/s43246-022-00228-4
3. **Hall**, **S. J.**, Klein, B. P., & Maurer, R. J. (2021, December 1). Self-interaction error induces spurious charge transfer artefacts in core-level simulations of x-ray photoemission and absorption spectroscopy of metal-organic interfaces. doi:10.48550/arXiv.2112.00876
4. Klein, B., **Hall**, **S. J.**, & Maurer, R. (2021). The nuts and bolts of core-hole constrained ab-initio simulation for k-shell x-ray photoemission and adsorption spectra. *Journal of Physics: Condensed Matter*, *33*(15), 154005. doi:10.1088/1361-648x/abdf00
5. Klein, B. P., Ruppenthal, L., **Hall**, **S. J.**, Sattler, L. E., Weber, S. M., Herritsch, J., … Gottfried, J. M. (2021). Topology effects in molecular organic electronic materials: Pyrene and azupyrene. *ChemPhysChem*, *22*(11), 1065–1073. doi:10.1002/cphc.202100222
6. Klein, B. P., Harman, S. E., Ruppenthal, L., Ruehl, G. M., **Hall**, **S. J.**, Carey, S. J., … Gottfried, J. M. (2020). Enhanced bonding of pentagon–heptagon defects in graphene to metal surfaces: Insights from the adsorption of azulene and naphthalene to pt(111). *Chemistry of Materials*, *32*(3), 1041–1053. doi:10.1021/acs.chemmater.9b03744

For a full list of publications see ORCID or Google Scholar pages linked above.

Conferences

DPG Spring Meeting - September 2022 *X-ray Spectroscopic Fingerprints of Chemical Bonding at Molecule-Metal Interfaces Revealed by First-Principles Core-Level Simulation*

Psi-k Conference - August 2022 *Spurious Charge Transfer Artefacts in Core-Level Constrained X-ray Spectroscopy Simulations of Metal-Organic Interfaces*

ACS Spring - March 2022 *Revealing a Self-Interaction Error from Spurious Charge Transfer Artefacts in Core-Level X-Ray Spectroscopy of Metal-Organic Interfaces*

Faraday Discussions - February 2022 *Spurious Charge Transfer Artefacts in Core-Level Constrained X-ray Spectroscopy Simulations of Metal-Organic Interfaces*

CONEXS Conference - February 2021 *First-Principles Simulation of Core-Level Spectroscopy to Reveal the Nature of Chemical Bonding at Metal-Organic Interfaces*

CONEXS Conference - February 2020 *Disentangling Core-Level Spectroscopy Signals of Chemical Interaction at Metal-Organic Interfaces*

DPG Spring Meeting - April 2019 *Revealing Spectroscopic Signatures of Molecule-Metal Interaction: A Computational Core-Level Spectroscopy Study*

Skills

General	X-ray spectroscopy, Density Functional Theory, Software development, Data processing and analysis
Coding	Python, Fortran, Bash, Git
I.T	Unix command line, Slurm,
DFT	CASTEP, FHI-aims
Software	ASE, IgorPro, Origin, GNUplot, Inkscape, PyMol, Balsac, VMD

Miscellaneous

Memberships

2018 – present	Institute of Physics
2022 – present	American Chemical Society

Group Responsibilities

2018 – present	Maurer Group Webpage Admin
2018	Creation of Maurer Group Logo

References

Prof. Reinhard Maurer
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Prof. Steven Brown
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