Adam R. **Symington**

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My research is multi-disciplinary, covers the fields of materials science, chemistry, computational materials science, and incorporates foundations of thermodynamics and theoretical chemistry. I focus on the development and application of computational techniques to study materials at the atomic scale. My research primarily focuses on the impact of structural defects - surfaces and grain boundaries, and chemical defects on the properties of materials.

Selected Publications

- **A. R. Symington***, M. Molinari, J. Statham, J. Wu & S. C. Parker*. *J. Phys. Energy*, **1**(4), 2005, 2019 – One of two papers focussing on transport properties using classical molecular dynamics simulations
- **A. R. Symington***, M. Molinari, S. Moxon, J. M. Flitcroft, D. C. Sayle & S. C. Parker*. *Accepted J. Phys. Chem. C*, 2019. Available on 10.26434/chemrxiv.9247709.v2 – Part of a collaboration across three universities, applying DFT and classical molecular dynamics to predict the morphology of nanoparticles.
- **A. R. Symington***, J. Tse, M. Molinari, A. Marmier & S. C. Parker. *J. Open Source Soft.*, **4**(34), 1210, 2019 – Development of reproducible analysis software that has been applied both in my own research and in within the wider community.

* Denotes corresponding authorship.

Research Experience

Postgraduate Research, Computational Chemistry (Prof Stephen C.Parker)

Bath, UK

PhD Project: "The Effect of Microstructure and Impurities on Transport in Actinide Oxide Films" *October 2016 - March 2019*

- PhD project supervised by Prof Steve Parker studying the effect of defects on the properties of materials
- Used classical molecular dynamics simulations to study oxygen transport in metal oxide grain boundaries. This has recently been expanded to study lithium transport in solid electrolyte materials.
- Used density functional theory to study the effect of dopants on the adsorption of atmospheric molecules on the surfaces of metal oxide materials. This included the development of new open source software dedicated to the analysis of DFT data.
- Used classical Monte Carlo simulations to study the distribution of defects in materials. This has been applied to metal oxide grain boundaries and solid electrolyte battery materials.
- Highly collaborative project, with academic collaborators at the Universities of Kent (Dean Sayle), Huddersfield (Marco Molinari), West of England (Arnaud Marmier) and Central Florida (Sudipta Seal), as well as industrial collaborators at AWE (Mark Storr and Robert Harker).
- Secured £31,000 of HPC time on the Archer supercomputer through membership of the MCC.

Post PhD Research

- Modelling the role of grain boundaries on Li diffusion in LLTO, NLTO and LLZO using hybrid Monte Carlo and molecular dynamics simulations.
- Modelling the interface between copper and cooper chloride - Collaboration with the Marken group at Bath.

Undergraduate Research, Computational Chemistry (Prof Stephen C.Parker)

Bath, UK

Masters Research Project: "Cerium Oxide Nanozymes - A computational Study" *October 2015 - June 2016*

- Part of an international collaboration between the University of Bath, Univeristy of Kent and the Univeristy of Central Florida.
- Resulted in a publication, Computer-Aided Design of Nanoceria as an Enzyme Mimetic Agent; a Prescription to Maximise its Activity, ACS Applied Bio Materials.
- This project and collaboration have continued into my PhD and a second publication is currently in preparation.

Collaborative Computational Projects 5 (CCP5) Summer Studentship

Bath, UK

Summer Studentship *June 2015 - October 2015*

- Undergraduate studentship funded by CCP5 investigating heavy metal adsorption at clay surfaces.
- The project was presented at the 2015 annual CCP5 conference.

Education

University of Bath

BATH, UK

PhD in Chemistry *SEPT. 2016 - Present*

- Undertook a PhD supervised by Prof. Stephen Parker
- PhD thesis is complete and currently being reviewed by my supervisor.

University of Bath

Bath, UK

MChem in Chemistry for Drug Discovery *SEPT. 2012 - JUN. 2016*

- Degree Classification: **II:I**

Awards

International

2018 **Winner**, Materials Science and Metalurgy Award - Plutonium Futures the Sciences 2018 *San Diego, USA*

Domestic

2019	**Winner**, Computational Chemistry Prize - Bolland Symposium	*Bath, UK*
2019	**Winner**, Best Presentation - High Performance Computing Symposium	*Bath, UK*
2018	**Winner**, Computational Chemistry Prize - Bolland Symposium	*Bath, UK*
2017	**Winner**, Material Horizons Award - SSCG	*Reading, UK*
2017	**Runner Up**, Presentation Award - Computational Collaborative Project 5 AGM	*Glasgow, UK*

Computational Skills

Programming fluency & Software familiarity

Expert Python, Git

Experienced FORTRAN90, HTML, CSS, Shell, Jupyer-Framework

Beginner Julia

Software development

surfinpy surfinpy is an open-source Python library to facilitate the analysis and visualisation of large scale ab initio calculation data. surfinpy has been published in the Journal of Open Source Software (Symington et al., J. Open. Source Soft. 4, 1210, 2019).

polypy polypy is an open-source Python library to designed to analyse molecular dynamics simulation data. polypy is built to read large datasets associated with molecular dynamics trajectories and from these produce insightful statistical information. polypy has been used in two pieces of published material science to data.

Publications

9. A. R. Symington*, M. Molinari, & S. C. Parker. Controlling Cerium Oxide Nanoparticle Morphology Using Carbonate Species, *Submitted J. Phys. Chem. C,* 2019.
8. S. Moxon, A. R. Symington, J. M. Flitcroft, S. C. Parker, D. J. Cooke, M. Molinari*. The interaction of CO2 with Surfaces of PuO_2: an ab initio investigation, *Submitted J. Mat. Chem. A,* 2019.
7. A. R. Symington*, M. Molinari, S. Moxon, J. M. Flitcroft, D. C. Sayle, & S. C. Parker. Strongly Bound Surface Water Affects the Shape Evolution of Cerium Oxide Nanoparticles, *Accepted J. Phys. Chem. C* 2019. Available at - DOI: 10.26434/chemrxiv.9247709.v2.
6. A. R. Symington, M. Molinari, M. Molinari, N. A. Brincat, N. R. Williams & S. C. Parker*. Defect segregation facilitates oxygen transport at fluorite UO_2 grain boundaries, *Phil. Tans. A,* **377**(2152), 20190026, 2019. DOI: 10.1098/rsta.2019.0026.
5. A. R. Symington*, M. Molinari, J. Statham, J. Wu & S. C. Parker. The role of dopant segregation on the oxygen vacancy distribution and oxygen diffusion in CeO_2 grain boundaries, *J. Phys. Energy,* **1**(4), 2005, 2019. DOI: 10.1088/2515-7655/ab28b5.
4. A. R. McCluskey*, J. Grant, A. R. Symington, T. Snow, J. Doutch, B. J. Morgan*, S. C. Parker, & K. J. Edler. An introduction to classical molecular dynamics simulation for experimental scattering users, *J. Appl. Crystallogr.,* **52**(3), 665-668, 2019. DOI: 10.1107/S1600576719004333.
3. J. M. Flitcroft, A. R. Symington, M. Molinari, N. A. Brincat, N. R. Williams & S. C. Parker. Impact of Hydrogen on the Intermediate Oxygen Clusters and Diffusion in Fluorite Structured UO_{2+x}, *Inorganic Chemistry,* **58**(6), 3774-3779, 2019. DOI: 10.1021/acs.inorgchem.8b03317.
2. A. R. Symington*, J. Tse, M. Molinari, A. Marmier & S. C. Parker. surfinpy: A Surface Phase Diagram Generator, *J. Open Source Soft,* **4**(34), 1210, 2019. DOI: 10.21105/joss.01210.
1. M. Molinari*, A. R. Symington, D. C. Sayle, T. S. Sakthivel, S. Seal & S. C. Parker*. Computer-Aided Design of Nanoceria Structures as Enzyme Mimetic Agents: The Role of Bodily Electrolytes on Maximising Their Activity, *ACS Appl. Mater. Interfaces,* **2**(3), 1098-1106, 2019. DOI: 10.1021/acsabm.8b00709.

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Presentations

Invited Talks

2019/06/17	**Developing Software to Aid Your Research**, MCC Surfin Group Meeting, University of Huddersfield	*Huddersfield, UK*
2019/05/21	**Modelling Complex Interfaces in Uranium Oxide**, Materials Modelling Symposium	*Aldermaston, UK*

Contributed Talks

2019/08/20	**Modelling the mineral-water interface of polycrystalline surfaces**, Goldschmidt 2019	*Barcelona, SPAIN*
2019/06/21	**Studying Dopants at Interfaces**, CompChem Seminar, University of Bath	*Bath, UK*
2019/06/19	**Predicting Cerium Oxide Nanoparticle Morphology: The Role of Surface Water**, University of Bath Bolland Symposium	*Bath, UK*
2019/05/21	**Understanding Defects in Uranium Oxide**, AWE Modelling Workshop	*Aldermaston, UK*
2018/07/21	**Modelling the Interfaces of Fluorite Structured Oxides**, South Western Computational Chemistry Group Meeting	*Bath, UK*
2018/06/21	**Against the Grain: The Effect of Grain Boundaries on the Diffusion Properties of Fluorite Oxides**, CompChem Seminar, University of Bath	*Bath, UK*

Teaching Experience

Computational Laboratory Demonstrator *OCT. 2016 - PRESENT*

- Developed a third year computational chemistry teaching lab, designed to get students to use basic programming skills to run and analyse molecular dynamics simulations within the context of solid state chemistry.
- Helped in the running and development of first, second and fourth year undergraduate laboratory exercises, with a focus on the teaching of basic programming skills in Python and classical molecular dynamics

Introduction to Unix & Programming Lecturer and Demonstrator *APR. 2019 - OCT. 2019*

- Contributed a series of practical workshops designed to introduce PhD students from throughout the university to Unix and programming

Mathematics for Chemistry Lecturer *SEPT. 2016 - MAR. 2017*

- Delivery of workshops in fundemental mathematical concepts for chemists, ensuring that all chemistry first year students had consistent mathematical background