PHD · DATA SCIENTIST · PROGRAMMER

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Education

University of Bath

PhD - Chemistry

Bath, England

• Undertaking a PhD in computational chemistry / materials science, supervised by Prof. Stephen C.Parker

- Collaborative project funded by AWE and the University of Bath
- Research collaboration with the University of Huddersfield, University of Kent and the University of Central Florida

MChem - Chemistry with Drug Discovery

Bath, England

October. 2016 - March 2020

University of Bath October 2012 - June 2016

- Degree Classification: II:I
- Masters project Cerium Oxide Nanozymes A computational study

Experience _

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

Bath, England

PHD PROJECT: "THE EFFECT OF MICROSTRUCTURE AND IMPURITIES ON TRANSPORT IN ACTINIDE OXIDE FILMS"

October 2016 - March 2019

- Computational chemistry project Applications Nuclear Waste Remediation, Energy Materials, Environmental Chemistry
- During this project I ran large scale simulations on currently used and new materials in order to generate data that I used to make predictions about the behaviour and properties of these materials.
- This has required the development of bespoke software designed for the specific needs of the project. Full details can be found on my github account (symmy596)

University of Bath Chemistry Department

Bath, England

POSTGRADUATE TEACHING ASSISTANT

October 2016 - Present

- Throughout the duration of my PhD I have taught undergraduate chemists how to program, specifically focusing on high level programming in **Python** and low level programming in **fortran**.
- I developed a new masters level course focusing on using **Python** programming to better understand and make predictions about the behaviour of materials.
- Part of an ongoing project to develop a new masters course focusing on teaching students how to use **Python** in data analysis.

MATHS FOR CHEMISTS LECTURER

October 2016 - Present

Delivery of workshops in fundamental mathematical concepts for chemists, ensuring that all chemistry first year students had a consistent mathematical background.

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

Bath, England

MASTERS RESEARCH PROJECT: "CERIUM OXIDE NANOZYMES - A COMPUTATIONAL STUDY"

October 2015 - June 2016

· Part of an international collaboration between the University of Bath, University of Kent and the University of Central Florida

Collaborative Computational Projects 5 (CCP5) Summer Studentship

Bath, England

SUMMER STUDENTSHIP

June 2015 - October 2015

• Undergraduate studentship funded by CCP5.

Skills ____

PROGRAMMING FLUENCY

Basic Ruby, SQL, HTML/CSS **Intermediate** Python, Git, Fortran, Shell

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.

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

| 2019 | A R. Symington, J Tse, M Molinari, S C. Parker. surfinpy - A python module for the analysis of solid state simulation data | | |
|------|--|--|--|
| 2019 | A R. McCluskey, A R. Symington, J Grant, B J. Morgan, S C. Parker, K J. Edler. <i>Introducing classical molecular dynamics</i> | | |
| 2019 | simulation to users of scattering | | |
| 2019 | M. Molinari, A. Symington D. Sayle, T. Sakthivel, S. Seal, S. Parker. Computer-Aided Design of Nanoceria as an Enzyme | | |
| 2019 | Mimetic Agent; a Prescription to Maximise its Activity | | |
| 2019 | J. Flitcroft, A R. Symington, M. Molinari, N. Brincat, and S. Parker. A Stable Oxygen Defect Cluster in Uranium Oxide at low | | |
| 2019 | Excess Oxygen Concentration from ab initio Calculations | | |
| 2019 | A. Symington, N.Brincat, N.Williams, M.Molinari, S.Parker. Fission Products and Oxygen Vacancy Segregation Facilitate | | |
| 2019 | Oxygen Transport at UO2 Grain Boundaries | | |
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Awards _____

2019

2019

INTERNATIONAL

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

A. Symington, M.Molinari, S.Parker. Carbonate Formation at Low Index Cerium Oxide Surfaces

San Diego, USA

DOMESTIC

| 2018 | Winner , Computational Chemistry Prize - Bolland Symposium | Bath, England |
|------|---|-------------------|
| 2017 | Winner, Material Horizons Award - Solid State Chemistry Group | Reading, England |
| 2017 | Runner Up, Computational Collaborative Project 5 AGM - Presentation Award | Glasgow, Scotland |

A. Symington, J.Flitcroft, M.Molinari, S.Parker. Water Adsorption at Cerium Oxide Surfaces Altered by Trivalent Dopants

Committees and Organisations

Chemistry Postgraduate Exec Committee

Bath, England

2017/18

SECRETAR

- Committee responsible for organising events within the chemistry department
- Organised the annual Bolland symposium.
- Responsible for organising external speakers and securing funding.

University of Bath Cricket Club

Bath, England

SECRETARY

2013/14

• Committee responsible for organising games, training and social events.

Extracurricular Activity _____

Senior Golf Caddy

Newcastle, N.I

ROYAL COUNTRY DOWN GOLF CLUB

June 2009 - October 2016

- Annual summer job during my high school and university career.
- This job involved quickly building a strong working relationship with a international clients in order to provide advice and knowledge on the course.
- I have also been a playing member of the club from 2012 Present and I play to a handicap of 16

Cricket Player / Coach

Newcastle / Bath

DUNDRUM CC | UNIVERSITY OF BATH CC | ROYAL OAK CC | SOUTHSTOKE CC

2000 - PRESENT

- I have played cricket as a member of several clubs since the age of 8.
- I played at Dundrum CC between the ages of 12 -24 and captained the first XI during the 2014-2016 seasons.
- I coached the U15/U13/U11 teams at Dundrum for 6 years.

Cycling

I am a keen cyclist in my spare time and in 2018 I participated in a charity cycle between Lands end and Bristol, raising £4000 for the MS society.