#### PHD · DATA SCIENTIST · PROGRAMMER

□ 07460367765 | **☑** ars44@bath.ac.uk | **☆** ars44.github.io | **□** symmy596

# **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.

# 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 insghtful statistical information. polypy has been used in two pieces of published material science to data.