

# Andrew R. McCluskey

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## Education

### University of Bath(UBath)/Diamond Light Source(DLS)

BATH/HARWELL-OXFORD, UK

PHD IN CHEMISTRY

SEPT. 2015 - MAR. 2019

- PhD supervised by Prof. Karen Edler (UBath), Prof. Stephen Parker (UBath), Dr Andrew Smith (DLS) and Dr Jonathan Rawle (DLS)
- Developing computational methodologies and software to improve the analysis of small angle scattering, reflectometry, and grazing incidence small angle scattering
- Applying classical atomistic and coarse-grained simulations to the study of soft matter systems

### University of Edinburgh

EDINBURGH, UK

MCHEM IN MATERIALS CHEMISTRY WITH A YEAR IN INDUSTRY

SEPT. 2010 - JUN. 2015

- Degree Classification: **First Class**

## Research Experience

### The Nudelman Group, University of Edinburgh

EDINBURGH, UK

SUMMER RESEARCH & MASTER'S PROJECT STUDENT

JUN.; 2014 - APR. 2015

- Using cryogenic transmission electron microscopy to investigate self-assembly of collagen

### Cyttec Industries

STAMFORD, USA

TEMPORARY RESEARCH INTERN

JUN. 2013 - JUN. 2014

- Researching on the functionalisation and application of polyelectrolyte emulsions

## Teaching Experience

### University of Bath

BATH, UK

PHYSICAL CHEMISTRY TUTOR

SEPT. 2015 - PRESENT

- Running physical chemistry tutorials for first year natural sciences undergraduate students
- Pioneered the use of Jupyter Notebooks in tutorials to both aid in the students understanding

COMPUTATIONAL LABORATORY DEMONSTRATOR

JAN. 2016 - PRESENT

- Demonstrated first and second year undergraduate computational chemistry laboratory exercises, particularly focussing on introducing Python programming
- Helped to develop laboratory exercises to develop skills in Microsoft Excel, an understanding of classical molecular dynamics simulations, and to introduce Python programming for data analysis

MATHEMATICS FOR CHEMISTRY LECTURER

SEPT. 2016 - MAR. 2017

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

X-RAY & NEUTRON TECHNIQUES FOR CHEMISTS LECTURER

JAN. 2016 - PRESENT

- Delivery of workshops devoted to the analysis of small angle scattering and reflectometry as a component of a final year undergraduate course

INTRODUCTION TO UNIX & PROGRAMMING LECTURER AND DEMONSTRATOR

FEB. 2018 - DEC. 2018

- Twice assisted in the delivery of a practical workshop designed to introduce PhD student from through-out the university of Unix and programming
- Included leading the "Introduction of Python" workshop, based on Software Carpentry materials

### ISIS Neutron Training Course

HARWELL-OXFORD, UK

LECTURER

MAR. 2017 - PRESENT

- Twice invited to lecture at the ISIS Neutron Training Course
- Developed and delivered a one hour lecture introducing classical molecular dynamics simulations and showing how they can be applied to neutron scattering
- Further prepared in interactive tutorial presenting how molecular dynamics simulation could be applied to the analysis of neutron reflectometry data

## SASSIE Training Course

DEMONSTRATOR

VARIOUS, UK

MAR. 2017 - PRESENT

- Aided in the demonstration of the SASSIE biological small angle scattering package at training events for PhD students and Postdocs

## pythoninchemistry.org

CONTRIBUTOR

BATH, UK

NOV. 2017 - PRESENT

- Webmaster and contributor to the pythoninchemistry web resource
- Resource designed to introduce chemistry students to aspects of programming, using Python and Jupyter Notebooks
- Developing teaching resources that introduce my basic concepts from programming, such as functions, loops, and plotting

## Memberships & Committees

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### RSC/IOP Neutron Scattering Group Committee

PHD REPRESENTATIVE

JUN. 2017 - PRESENT

- Served as a member of the NSG Committee offering the insight of student members

### UK Research Software Engineer Association

MEMBER

JUN. 2017 - PRESENT

- A member of UKRSE, a community and awareness organisation for the UK's Research Software Engineers

### Royal Society of Chemistry

ASSOCIATE MEMBER (POSTGRADUATE)

SEPT. 2010 - PRESENT

- Member of the RSC since start of undergraduate
- Took part in a young member focus group for the RSC Scottish Regional Steering Group

## Funding Awarded

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- 2018/08/28 **Travel Fund to Attend VICEPHEC18**, University of Bath Travel Fund for Teaching Development – £135
- 2018/08/28 **Group Bursary to Attend VICEPHEC18**, Royal Society of Chemistry Tertiary Education Group Bursary – £70
- 2017/04/11 **Research Student Travel Grant**, Armourers & Brasiers' Gauntlet Trust – £900

## Prizes

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- 2018/10/12 **IUCr Journals Prize for the Best Student Lecture**, SAS2018
- 2018/06/14 **The Computational Prize – Best Oral Presentation**, University of Bath Bolland Symposium
- 2018/05/17 **Nominated for Faculty Teaching Assistant Award**, University of Bath Faculty of Science
- 2017/06/12 **Best Talk Award – Sponsored by Santander**, University of Bath Faculty of Science Graduate School Research Afternoon

## Publications

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5. McCluskey, A. R., Symington, A. R., Grant, J., Morgan, B. J., Parker, S. C., & Edler, K. J., 2018. Introducing classical molecular dynamics simulation to users of scattering. *(In Preparation)*
4. McCluskey, A. R., Grant, J., Smith, A. J., Rawle, J. L., Barlow, D. J., Lawrence, M. J., Parker, S. C., & Edler, K. J., 2018. Applying molecular simulation to the analysis of lipid monolayer reflectometry. *(In Preparation)*
3. McCluskey, A. R., Sanchez-Fernandez, A., Edler, K. J., Parker, S. C., Jackson, A. J., Campbell, R. A., & Arnold, T., 2018. Bayesian determination of the effect of a deep eutectic solvent on the structure of lipid monolayers. *(Submitted)*. arXiv:1810.07616
2. McCluskey, A. R., Morgan, B. J., Edler, K. J., & Parker, S. C., 2018. pylj: A teaching tool for classical atomistic simulation. *J. Open Source Educ.*, 1(2), 19. DOI: 10.21105/jose.00019
1. McCluskey, A. R., & Edler, K. J., 2018. Model-dependent small-angle scattering for the study of complex organic materials. *Curr. Org. Chem.*, 22(8), 750-757. DOI: 10.2174/1875692115666170612104439