

# Andrew R. McCluskey

COMPUTATIONAL SCIENTIST · DATA ANALYST · NEUTRON/X-RAY SCATTERER

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## Education

### University of Bath

BATH, UK

PHD IN CHEMISTRY

Sept. 2015 - PRESENT

- Undertaking a 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, reflectivity, and grazing incidence small angle scattering.
- Applying classical atomistic and coarse-grained simulations to the study of soft matter systems.
- Collaborative project co-funded by Diamond Light Source and the University of Bath.

### University of Edinburgh

EDINBURGH, UK

MCHEM IN MATERIALS CHEMISTRY WITH A YEAR IN INDUSTRY

Sept. 2010 - June 2015

- Degree Classification: **First Class**
- Gained a broad introduction to many areas of chemistry.
- Spent one year learning practical soft matter chemistry/physics skills in industry
- Masters research project: Collagen self-assembly using cryo-TEM.

## Research Experience

### The Nudelman Group, University of Edinburgh

EDINBURGH, UK

MASTER'S PROJECT STUDENT

SEPT. 2014 - APR. 2015

- Continued work from summer, investigating collagen self-assembly.
- Significant independent use of the cryogenic transmission electron microscope.
- Presented work at a national conference as well as regularly at group meetings.

SUMMER RESEARCH STUDENT

JUL. 2014 - SEPT. 2014

- Using cryogenic transmission electron microscopy to investigate self-assembly of collagen.
- Gained an appreciation of basic concepts from biochemistry and biophysics.
- Lead to work that continued during Master's project.

### Cyttec Industries

STAMFORD, USA

TEMPORARY RESEARCH INTERM

JUN. 2013 - JUN. 2014

- Spent fourth year of Master's course in the Alumina group at Cyttec Industries.
- Conducted research on the functionalisation and application of polyelectrolyte emulsions.
- Gained an understanding of common soft matter concepts, including colloid theory, and surfactant science.
- Developed skills related to statistical analysis, including significance testing and design of experiments.
- Presented work at group meeting and wrote monthly reports to keep group members updated on progress.

## Teaching Experience

### Python in Chemistry

BATH, UK

CONTRIBUTOR

NOV. 2017 - PRESENT

- I have actively contributed to the Python in Chemistry blog developed by the University of Bath.
- This is a resource designed to introduce chemistry students to aspects of programming, using Python and Jupyter Notebooks
- This has involved developing teaching resources that introduce my basic concepts from programming; such as functions, loops, and plotting.

### ISIS Neutron Training Course

HARWELL-OXFORD, UK

LECTURER

MAR 2017

- Developed and delivered a one hour lecture introducing classical molecular dynamics simulations and showing how they can be applied to neutron scattering.

## University of Bath

BATH, UK

### PHYSICAL CHEMISTRY TUTOR

SEPT. 2015 - PRESENT

- Running physical chemistry tutorials for first year natural sciences undergraduate students.
- Covering topics including gas theory, kinetics, spectroscopy, and thermodynamics.
- Pioneered the use of Jupyter Notebooks in tutorials to both aid in the students understanding of the physical chemistry while introducing programming concepts.

### COMPUTATIONAL LABORATORY DEMONSTRATOR

JAN. 2016 - PRESENT

- Involved in helping first and second year undergraduate students as they undertake the laboratory exercises, with a focus on the teaching of basic programming skills in Python.
- Helped to develop laboratory exercises to develop skills in Microsoft Excel and an understanding of classical molecular dynamics simulations.

## 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)

Sep. 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.

## Software

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### PROGRAMMING FLUENCY

**Basic** FORTRAN90, SQL, Julia

**Intermediate** C, C++, OpenMP, MPI, Qt, Git

**Expert** Python

### SOFTWARE DEVELOPMENT

#### falass

A pure python library for the calculation of neutron and X-ray reflectometry data from molecular simulation. This is an open source package available on GitHub. This library was developed as part of my PhD studies.

#### refnx

A python package dedicated to the application of the Abelès matrix formalism to the analysis of reflectometry measurements. This also enables detailed statistical analysis of the resulting models by using Markov-Chain Monte-Carlo to enable Bayesian inference. I have recently been actively contributing to this open source package.

## Awards

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2017/06/12

**Best Talk Award – Sponsored by Santander**, University of Bath Faculty of Science Graduate School Research Afternoon

2017/04/11

**Research Student Travel Grant**, Armourers & Brasiers' Gauntlet Trust

## Program Committees

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2016/07/20

**Co-organiser**, M4 Colloids

BATH, UK

## Publications

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1.

**Model-dependent small-angle scattering for the study of complex organic materials**, Current Organic Chemistry, (E-pub Ahead of Print) DOI: 10.2174/1875692115666170612104439

# Presentations

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## INVITED TALKS

- 2017/06/19 **Surfactants and Molecular Dynamics**, CCP-SAS Joint Meeting, Cardiff University *CARDIFF, UK*
- 2017/06/12 **Putting computers to work for large experiments**, Faculty of Science Graduate School  
Research Afternoon, Bath University – **Best Talk Award** *BATH, UK*
- 2016/05/23 **SAS, Sims and Soft Matter Self-Assembly**, CCP-SAS Joint Meeting, NIST *GAITHERSBURG, USA*

## CONTRIBUTED TALKS

- 2017/09/12 **Simulations to understand reflectivity: How coarse can we go?**, CCP5 AGM *GLASGOW, UK*
- 2017/04/13 **Simulations to understand reflectivity: How coarse can we go?**, Faraday Joint Interest  
Group Conference *WARWICK, UK*
- 2017/03/23 **Coarse graining and reflectivity: a love story?**, CompChem Seminar, University of Bath *BATH, UK*
- 2017/02/28 **Reflectivity: from simulation to experiment**, International Soft Matter Workshop *HELFORD, UK*
- 2016/06/23 **Smart analysis of soft matter**, Bombannes Summer School *BOMBANNES, FRANCE*
- 2016/01/28 **Nanodisc models for calculation of small angle scattering patterns**, SMALP Meeting  
2016 *BIRMINGHAM, UK*

## POSTER PRESENTATIONS

- 2017/06/28 UK Neutron and Muon Science and User Meeting *WARWICK, UK*
- 2017/06/06 canSAS-IX *BERKELEY, USA*
- 2017/02/07 ESRF User Meeting *GRENOBLE, FRANCE*
- 2016/11/21 BornAgain Workshop *MUNICH, GERMANY*
- 2016/11/16 GISAXS2016 *HAMBURG, GERMANY*
- 2016/11/07 ISIS Student Meeting *ABINGDON, UK*
- 2016/07/27 UK Neutron and Muon Science and User Meeting *WARWICK, UK*
- 2016/07/20 M4 Colloids *BATH, UK*
- 2016/06/13 Molecular Simulation @ Bristol *BRISTOL, UK*
- 2016/06/06 Diamond Science Away Day *OXFORD, UK*
- 2016/05/23 CCP-SAS Joint Meeting, NIST *GAITHERSBURG, USA*
- 2016-04-13 2nd Conference on Multiscale Modelling of Condensed Phase and Biological Systems *MANCHESTER, UK*
- 2016-04-04 Solutions in the Spring *CAMBRIDGE, UK*
- 2014/11/27 First Joint Meeting of the Scottish Microscopy Group & Microscopy Society of Ireland *GLASGOW, UK*