

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

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.

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

PROGRAMMING FLUENCY

Basic FORTRAN90

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

Expert Python

SOFTWARE DEVELOPMENT

falassGUI 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

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

2016/07/20 **Co-organiser**, M4 Colloids

BATH, UK

Publications

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

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