

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

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.

- 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

SOFTWARE FAMILIARITY

Basic Mantid, Igor Pro

Intermediate Dawn, BornAgain, EPSR, Gudrun, SasView

Expert DL_POLY, DL_FIELD, GROMACS, Microsoft Office, iWork, \LaTeX

PROGRAMMING FLUENCY

Basic FORTRAN90

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

Expert Python

SOFTWARE DEVELOPMENT

falassGUI

A graphical application for the determination of neutron and X-ray reflectometry profiles from molecular dynamics simulation. This is available open source on GitHub, with executables for all major platforms to follow soon. This application 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