Andrew R. **McCluskey**

Computational Scientist · Data Analyst · Neutron/X-ray Scatterer

0.15 1S, Department of Chemistry, University of Bath, Claverton Down, Bath, BA2 7AY, UK

(+44) 7873906296 | arm61@bath.ac.uk | people.bath.ac.uk/arm61 | arm61

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.

Cytec Industries — *STAMFORD, USA*

Temporary Research Interm — *JUN. 2013 - JUN. 2014*

- Spent fourth year of Master's course in the Alumina group at Cytec 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.

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

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	**Simulation to understand reflectivity: How coarse can we go?**, UK Neutron and Muon Science and User Meeting	*WARWICK, UK*
2017/06/06	**Simulation to understand reflectivity: How coarse can we go?**, canSAS-IX	*BERKELEY, USA*
2017/02/07	**`falass`: for fast, intuitive, and open-source reflectivity from simulation**, ESRF User Meeting	*GRENOBLE, FRANCE*
2016/11/21	**`falass`: for fast, intuitive, and open-source reflectivity from simulation**, BornAgain Workshop	*MUNICH, GERMANY*
2016/11/16	**`falass`: for fast, intuitive, and open-source reflectivity from simulation**, GISAXS2016	*HAMBURG, GERMANY*
2016/11/07	**`falass`: for fast, intuitive, and open-source reflectivity from simulation**, ISIS Student Meeting	*ABINGDON, UK*
2016/07/27	**Coarse-graining of soft matter assemblies: For application to small angle scattering**, UK Neutron and Muon Science and User Meeting	*WARWICK, UK*
2016/07/20	**Coarse-graining of soft matter assemblies: For application to small angle scattering**, M4 Colloids	*BATH, UK*
2016/06/13	**Coarse-graining of soft matter assemblies: For application to small angle scattering**, Molecular Simulation @ Bristol	*BRISTOL, UK*
2016/06/06	**Coarse-graining of soft matter assemblies: For application to small angle scattering**, Diamond Science Away Day	*OXFORD, UK*
2016/05/23	**Coarse-graining of soft matter assemblies: For application to small angle scattering**, CCP-SAS Joint Meeting, NIST	*GAITHERSBURG, USA*
2016-04-13	**Coarse-graining of soft matter assemblies: For application to small angle scattering**, 2nd Conference on Multiscale Modelling of Condensed Phase and Biological Systems	*MANCHESTER, UK*
2016-04-04	**Coarse-graining of soft matter assemblies: For application to small angle scattering**, Solutions in the Spring	*CAMBRIDGE, UK*
2014/11/27	**Collagen self-assembly by cryoTEM: a time resolved study**, First Joint Meeting of the Scottish Microscopy Group & Microscopy Society of Ireland	*GLASGOW, UK*