Andrew R. **McCluskey**

Data Scientist · 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(UBath)/Diamond Light Source(DLS)

BATH/HARWELL-OXFORD, UK

PhD in Chemistry — *SEPT. 2015 - MAR. 2019*

- 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, reflectometry, 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.
- Participated in small angle scattering and reflectometry at Diamond Light Source and ISIS Neutron and Muon Source.

University of Edinburgh

EDINBURGH, UK

MChem in Materials Chemistry with a Year in Industry — *SEPT. 2010 - JUN. 2015*

- Degree Classification: **First Class**
- Spent one year learning practical soft matter chemistry/physics skills in industry at Cytec Industries.
- 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 (First Joint Meeting of the Scottish Microscopy Group & Microscopy Society of Ireland) 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 Intern — *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

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 intermolecular forces, 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*

- 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, 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 fundemental 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 - MAR. 2018*

- Contributed a series of practical workshop designed to introduce PhD student from through-out the university of Unix and programming.
- Included leading a "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 — *VARIOUS, UK*

Demonstrator — *MAR. 2017 - PRESENT*

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

Python in Chemistry — *BATH, UK*

Contributor — *NOV. 2017 - PRESENT*

- Actively contributing to the Python in Chemistry blog developed by the University of Bath.
- 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

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.

Software

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.

pylj An open source Python package to aid in the teaching of molecular dynamics simulations to both undergradute and postgraduate students, within the interface of a Jupyter notebook.

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 a heavy user of and occasional contributor to this open source package.

Awards

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

2017/04/11 **Research Student Travel Grant**, Armourers & Brasiers' Gauntlet Trust

Program Committees

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

Publications

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. Comparing simulation-derived and traditional analysis method for monolayer reflectometry. Journal of Applied Crystallography (*In Preparation*)
3. McCluskey, A. R., Grant, J., Parker, S. C., & Edler, K. J., 2018. falass: a Python library for neutron and X-ray reflectometry from molecular simulation. Journal of Open Research Software (*In Preparation*)
2. Sanchez-Fernandez, A., McCluskey, A. R., Edler, K. J., Jackson, A. J., Campbell, R. A., & Arnold, T., 2018. Structure of phospholipid monolayers at the interface between air and a deep eutectic solvent. Phys. Chem. Chem. Phys. (*In Preparation*)
1. McCluskey, A. R., & Edler, K. J., 2017. Model-dependent small-angle scattering for the study of complex organic materials. *Current Organic Chemistry*, 22(8), 750-757. 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

2018/02/09 **Probabilistic analysis of reflectometry data: Phospholipids at the DES-air interface**, Neutrons and Global Challenges II: Health and Healthcare *LONDON, UK*

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

2018/04/26	UK Neutron and Muon Science and User Meeting	*WARWICK, UK*
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*