Andrew R. **McCluskey**

Educator · Data Scientist · Neutron/X-ray Scatterer

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

(+44) 7873906296 | a.r.mccluskey@bath.ac.uk | andrew.mccluskey@diamond.ac.uk | arm61.github.io | 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.
- Implementing high performance optimisation algorithms to rationalise experimental scattering data.
- 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.

Computational Skills

Programming fluency

Basic	FORTRAN90, SQL, Julia
Intermediate	C, C++, OpenMP, MPI, Qt, Git
Expert	Python

Software development

pylj pylj is an open-source Python library to facilitate student interaction with classical atomistic simulation. It is designed to operate within the Jupyter notebook framework, making it easy to implement in the classroom, or computer lab. pylj has been published in the Journal of Open-Source Education.

refnx refnx is a python package for the fitting of neutron and X-ray reflectometry data. I am a power-user of this software and an have recently worked to contribute the analysis of molecular simulation input. this project is currently led by Andrew Nelson (ANSTO).

Funding Awarded

2018/08/28 **Travel Fund to Attend VICEPHEC18**, University of Bath Travel Fund for Teaching Development – £135
2018/08/28 **Group Bursary to Attend VICEPHEC18**, Royal Society of Chemistry Teriary Education Group Bursary – £70
2017/04/11 **Research Student Travel Grant**, Armourers & Brasiers' Gauntlet Trust – £900

Prizes

2018/10/12 **IUCr Journals Prize for the Best Student Lecture**, SAS2018
2018/06/14 **The Computational Prize – Best Oral Presentation**, University of Bath Bolland Symposium
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

Program Committees

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

Publications

5. McCluskey, A. R., Symington, A. R., Grant, J., Morgan, B. J., Parker, S. C., & Edler, K. J., 2018. Introducing classical molecular dynamics simulation to users of scattering. *(In Preparation)*
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. Applying molecular simulation to the analysis of lipid monolayer reflectometry. *(In Preparation)*
3. McCluskey, A. R., Sanchez-Fernandez, A., Edler, K. J., Parker, S. C., Jackson, A. J., Campbell, R. A., & Arnold, T., 2018. Bayesian determination of the effect of a deep eutectic solvent on the structure of lipid monolayers. *(Submitted)*. arXiv:1810.07616
2. McCluskey, A. R., Morgan, B. J., Edler, K. J., & Parker, S. C., 2018. pylj: A teaching tool for classical atomistic simulation. *J. Open Source Educ.*, 1(2), 19. DOI: 10.21105/jose.00019
1. McCluskey, A. R., & Edler, K. J., 2018. Model-dependent small-angle scattering for the study of complex organic materials. *Curr. Org. Chem.*, 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

2018/10/30	**Comparing coarse-grainged simulation-derived and traditional analysis method for monolayer reflectometry**, TRENDS AND PERSPECTIVES IN NEUTRON INSTRUMENTATION	*TUTZING, GERMANY*
2018/10/12	**Using high-performance computing and molecular dynamics to rationalise micelle structure from small angle scattering**, SAS2018	*TRAVERSE CITY, USA*
2018/10/09	**pylj: an open-source Python library for teaching the interaction between molecular simulation and scattering**, SAS2018 – **Best Student Lecture Prize**	*TRAVERSE CITY, USA*
2018/09/16	**Introducing programming to undergraduate chemists: and the tools we've developed to help them**, PYCON UK	*CARDIFF, UK*
2018/08/23	**Introducing programming to undergraduate chemists: and the tools we've developed to help them**, VICEPHEC18	*SHEFFIELD, UK*
2018/06/14	**Using markov chain monte-carlo to estimate uncertainties in x-ray reflectometry modeling**, University of Bath Bolland Symposium	*BATH, UK*
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*