Andrew R. **McCluskey**

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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 & sampling algorithms to rationalise experimental scattering data.
- Collaborative project co-funded by Diamond Light Source and the University of Bath.
- Participated in many small-angle scattering and reflectometry experiments 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 & Summer Research Student — *SEPT. 2014 - APR. 2015*

- Using cryogenic transmission electron microscopy to investigate self-assembly of collagen.

Cytec Industries

STAMFORD, USA

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

- Conducted research on the functionalisation and application of polyelectrolyte emulsions.

Teaching Experience

University of Bath

BATH, UK

Physical Chemistry Tutor — *SEPT. 2015 - PRESENT*

- Running physical chemistry tutorials for first year natural sciences undergraduate students.
- 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*

- Helped in the running and development of first and second year undergraduate laboratory exercises, with a focus on the teaching of basic programming skills in Python and classical molecular dynamics.

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 - DEC. 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 and interactive tutorial introducing classical molecular dynamics simulations and showing how they can be applied to neutron scattering.

Python in Chemistry

BATH, UK

CONTRIBUTOR

NOV. 2017 - PRESENT

- Actively contributing to the pythoninchemistry project developed by the University of Bath.
- Developing teaching resources that introduce my basic concepts from programming, such as functions, loops, and plotting.
- Lead the development of an open educational resource focussed on the introduction of classical simulation to users of small-angle scattering.

Computational Skills

PROGRAMMING FLUENCY & SOFTWARE FAMILIARITY

Beginner	FORTRAN90, SQL, Julia
Expeienced	C, C++, OpenMP, MPI, Qt, HTML, CSS, BinderHub, AWS, Google Cloud, Docker
Expert	Python, Git, Jupyter-Framework

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. This project is currently led by Andrew Nelson (ANSTO).

Memberships & Committees

RSC/IOP Neutron Scattering Group Committee

EARLY CAREER REPRESENTATIVE

JUN. 2017 - PRESENT

- Currently serve as a member of the NSG Committee offering the insight of student and early career 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.

Prizes & Funding

2018/10/12 **IUCr Journals Prize for the Best Student Lecture**, SAS2018
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
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
2017/04/11 **Research Student Travel Grant**, Armourers & Brasiers' Gauntlet Trust – £900

Publications

5. Andrew R. McCluskey, James Grant, Adam R. Symington, Tim Snow, James Doutch, Benjamin J. Morgan, Stephen C. Parker, & Karen J. Edler., 2019. Introducing classical molecular dynamics simulation to users of scattering. *(Submitted)*. Preprint available on arXiv: 1902.01324.
4. Andrew R. McCluskey, James Grant, Andrew J. Smith, Jonathan L. Rawle, David J. Barlow, M. Jayne Lawrence, Stephen C. Parker, & Karen J. Edler., 2019. Applying molecular simulation to the analysis of lipid monolayer reflectometry. *(Submitted)*. Preprint available on arXiv: 1901.05514.
3. Andrew R. McCluskey, Adrian Sanchez-Fernandez, Karen J. Edler, Stephen C. Parker, Andrew J. Jackson, Richard A. Campbell, & Tom Arnold., 2019. Bayesian determination of the effect of a deep eutectic solvent on the structure of lipid monolayers. *(Submitted)*. Preprint available on arXiv: 1810.07616.
2. Andrew R. McCluskey, Benjamin J. Morgan, Karen J. Edler, & Stephen C. Parker., 2018. pylj: A teaching tool for classical atomistic simulation. *J. Open Source Educ.*, 1(2), 19. DOI: 10.21105/jose.00019.

1. Andrew R. McCluskey, & Karen J. Edler., 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

2018/12/17	Solid State Chemistry Group Christmas Meeting 2018	*LONDON, UK*
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*