

# Dr Andrew R. McCluskey

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Currently developing an international research profile in the application of computational statistics to synchrotron- and neutron-based measurements. Interested in utilising data-driven methods, including Bayesian inference, machine learning and applied information theory, for the analysis of physically-relevant measurements. Driven by collaborative research and focused on helping experimentists take advantage of tools developed within data science. Experienced educator and developer of open education resources, passionate on improving familiarity with mathematical and computational tools.

## Selected Publications

- **A. R. McCluskey\***, T. Arnold, J. F. K. Cooper, & T. Snow. *Mach. Learn.: Sci. Technol.*, Accepted, 2020 – Independent research publication, making use of Bayesian model selection to improve understanding of the analysis of neutron reflectometry measurements
- **A. R. McCluskey\***, A. Sanchez-Fernandez, K. J. Edler, S. C. Parker, A. J. Jackson, R. A. Campbell, & T. Arnold\*. *Phys. Chem. Chem. Phys.*, **21**(11), 6133-6141, 2019 – Highly collaborative work, developed a novel analysis methodology for application to experimental X-ray reflectometry
- **A. R. McCluskey\***, J. Grant, A. R. Symington, T. Snow, J. Douth, B. J. Morgan\*, S. C. Parker, & K. J. Edler. *J. Appl. Crystallogr.*, **52**(3), 665-668, 2019 – An education-focused publication, discussing an open education resource to introduce users of diffraction techniques to classical simulation methods

## Funding Secured

- **Diamond Light Source Year in Industry Studentship 2020/2021** – Development of a Bayesian regularisation framework for the analysis of reflectometry (~£20 000)
- **Royal Society of Chemistry Higher Education Group Kickstart Scheme** – pythoninchemistry Hackathon (£300)
- **University of Bath Travel Fund for Teaching Development** – VICEPHEC18 Travel Grant (£135)
- **Royal Society of Chemistry Tertiary Education Group** – VICEPHEC18 Group Bursary (£70)
- **Armourers & Brasiers' Gauntlet Trust** – Research Student Travel Grant (£900)

## Teaching Experience

### University of Bath

BATH, UK

#### VISITING LECTURER

SEPT. 2019 - ONGOING

- Co-organisation and delivery of final year Chemistry course (CH40208), focused on introducing Python programming and applications of programming to computational chemistry
- Developed and delivered twenty-one hours of lecture-workshop hybrid classes to a cohort of seventy students

#### 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

#### X-RAY & NEUTRON TECHNIQUES FOR CHEMISTS LECTURER

JAN. 2016 - MAY 2018

- Delivery of workshops devoted to the analysis of small-angle scattering and reflectometry as a component of a final year undergraduate course

#### MATHEMATICS FOR CHEMISTRY LECTURER

SEPT. 2016 - MAR. 2017

- Delivery of workshops in fundamental mathematical concepts for chemists, ensuring that all chemistry first year students had a consistent mathematical background

#### COMPUTATIONAL LABORATORY DEMONSTRATOR

JAN. 2016 - MAY 2018

- 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

#### PHYSICAL CHEMISTRY TUTOR

SEPT. 2015 - MAY 2018

- Running physical chemistry tutorials for first year natural sciences undergraduate students
- Pioneered the use of Jupyter Notebooks in tutorials to aid in the students understanding of the physical chemistry while introducing programming concepts

### Python in Chemistry

BATH, UK

#### CONTRIBUTOR

NOV. 2017 - PRESENT

- Lead developer of the open source "An Introduction to Python for Chemists" textbook; providing programming and data science skills to chemistry students
- Responsible for the development of an open educational resource focussed on the introduction of classical simulation to users of small-angle scattering
- Co-investigator for the pythoninchemistry Hackathon event, funded by the Royal Society of Chemistry Higher Education Group Kickstart Scheme

## ISIS Neutron Training Course

HARWELL-OXFORD, UK

### LECTURER

MAR. 2017 - MAR. 2018

- 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

## Research Experience

### Diamond Light Source

HARWELL-OXFORD, UK

#### DATA ANALYSIS SCIENTIST – REFLECTIVITY

APR. 2019 - ONGOING

- Ada Lovelace Centre project to increase automation in X-ray and neutron reflectometry reduction and analysis
- Local contacting on the I07 reflectometry beamline to support soft matter users
- Assisting both X-ray and neutron reflectometry users with data analysis, leveraging automation
- Developing independent research on the application of Bayesian and Machine Learning methodologies for the analysis of X-ray and neutron data

## Education

### University of Bath/Diamond Light Source

BATH/HARWELL-OXFORD, UK

#### PHD IN CHEMISTRY

SEPT. 2015 - APR. 2019

- Undertook a PhD supervised by Prof. Karen Edler, Prof. Stephen Parker, Dr Andrew Smith and Dr Jonathan Rawle
- Developed computational methodologies and software to improve the analysis of small-angle scattering and reflectometry
- Implemented high-performance optimisation & sampling algorithms to rationalise experimental scattering data
- Developed open educational resources to introduce classical simulation methods, including the pylj Python package and an introduction to classical simulation for users of small-angle scattering

### University of Edinburgh

EDINBURGH, UK

#### MCHEM IN MATERIALS CHEMISTRY WITH A YEAR IN INDUSTRY

SEPT. 2010 - JUN. 2015

- Degree Classification: **First Class**

## Awards

- 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

## Computational Skills

### PROGRAMMING FLUENCY & SOFTWARE FAMILIARITY

**Beginner** FORTRAN90, C++, SQL, Julia, Docker

**Experienced** C, Java, OpenMP, MPI, Qt, HTML, CSS, TensorFlow, Keras, PyMC3, BinderHub, AWS, Google Cloud

**Expert** Python, Git, Jupyter-Framework, emcee, dynesty

### SOFTWARE DEVELOPMENT

**uravu** a Bayesian data analysis package writing in Python and open-source. This package gives access to the powerful Bayesian inference Python packages through a simple interface to enable the application of these methods to model-dependent data analysis. uravu has been published in the Journal of Open Source Software.

**kinisi** a Python library that offers uncertainty determination and propagation from diffusion in molecular dynamics simulations. This enables the use of Bayesian inference to study diffusion in battery materials.

**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.

## Service/Community

### American Chemical Society

#### PEER REVIEWER

MAY 2020 - PRESENT

- Carried out peer review for Journal of Physical Chemistry

### Open Reflectivity Standards Organisation

#### MEMBER

OCT. 2019 - PRESENT

- A founding member of a collaborative organisation aiming to standardise reflectivity measurements
- Chair of the Reproducibility working group

## ISIS/Diamond Light Source Reflectivity Developers Workshop

ORGANISING COMMITTEE MEMBER

OCT. 2019

- Co-organisation of a workshop to develop data analysis and formats for neutron and X-ray reflectometry methods
- Served as co-chair during introductory and round up sessions

## 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

## M4 Colloids

ORGANISING COMMITTEE MEMBER

JUL. 2016

- Organisation of the student-led M4 Colloids conference at the University of Bath

## Royal Society of Chemistry

ASSOCIATE MEMBER

SEPT. 2010 - PRESENT

- Member of the RSC since start of undergraduate

## Publications

9. Andrew R. McCluskey\*, Samuel W. Coles, & Benjamin J. Morgan\* Uncertainty quantification and model comparison for diffusion in materials, *In Preparation*, 2020.
8. Andrew R. McCluskey\*, Samuel W. Coles, & Benjamin J. Morgan kinisi: Accurate uncertainties and model selection for simulation of diffusion in atomistic materials, *In Preparation*, 2020.
7. Andrew R. McCluskey\*, Tom Arnold, Joshaniel F. K. Cooper, & Tim Snow. A general approach to maximise information density in neutron reflectometry analysis, *Mach. Learn.: Sci. Technol.*, Accepted 2020. DOI: 10.1088/2632-2153/ab94c4.
6. Andrew R. McCluskey\*, & Tim Snow uravu: making Bayesian data analysis easy(er), *J. Open Source Softw.*, **5**(50), 2214, 2020. DOI: 10.21105/joss.02214.
5. Andrew R. McCluskey\*, James Grant, Andrew J. Smith, Jonathan L. Rawle, David J. Barlow, M. Jayne Lawrence, Stephen C. Parker, & Karen J. Edler\*. Assessing molecular simulation for the analysis of lipid monolayer reflectometry, *J. Phys. Comm.*, **3**(7), 075001, 2019. DOI: 10.1088/2399-6528/ab12a9.
4. Andrew R. McCluskey\*, James Grant, Adam R. Symington, Tim Snow, James Douth, Benjamin J. Morgan\*, Stephen C. Parker, & Karen J. Edler. An introduction to classical molecular dynamics simulation for experimental scattering users, *J. Appl. Crystallogr.*, **52**(3), 665-668, 2019. DOI: 10.1107/S1600576719004333.
3. Andrew R. McCluskey\*, Adrian Sanchez-Fernandez, Karen J. Edler, Stephen C. Parker, Andrew J. Jackson, Richard A. Campbell, & Tom Arnold\*. Bayesian determination of the effect of a deep eutectic solvent on the structure of lipid monolayers, *Phys. Chem. Chem. Phys.*, **21**(11), 6133-6141, 2019. DOI: 10.1039/C9CP00203K.
2. Andrew R. McCluskey\*, Benjamin J. Morgan, Karen J. Edler, & Stephen C. Parker. pylj: A teaching tool for classical atomistic simulation, *J. Open Source Educ.*, **1**(2), 19-21, 2018. DOI: 10.21105/jose.00019.
1. Andrew R. McCluskey, & Karen J. Edler\*. Model-dependent Small-angle Scattering for the Study of Complex Organic Materials, *Curr. Org. Chem.*, **22**(8), 750-757, 2018. DOI: 10.2174/1875692115666170612104439.

\* Denotes corresponding authorship.

## Presentations

### INVITED TALKS

2020/04/03	<b>Reflectometry and data science</b> , #theLightStuff Webinars (youtu.be/PHBLK_3sfi8)	ONLINE
2017/06/19	<b>Surfactants and Molecular Dynamics</b> , CCP-SAS Joint Meeting, Cardiff University	CARDIFF, UK
2017/06/12	<b>Putting computers to work for large experiments</b> , Faculty of Science Graduate School Research Afternoon, Bath University – <b>Best Talk Award</b>	BATH, UK
2016/05/23	<b>SAS, Sims and Soft Matter Self-Assembly</b> , CCP-SAS Joint Meeting, NIST	GAITHERSBURG, USA

## CONTRIBUTED TALKS

2019/07/12	<b>Automating reflectometry reduction and analysis at Diamond Light Source</b> , M4 COLLOIDS	BATH, UK
2019/05/07	<b>Bayesian determination of the effect of a deep eutectic solvent on the structure of lipid monolayers</b> , BAYES@LUND 2019	LUND, SWEDEN
2018/10/30	<b>Comparing coarse-grained simulation-derived and traditional analysis method for monolayer reflectometry</b> , TRENDS AND PERSPECTIVES IN NEUTRON INSTRUMENTATION	TUTZING, GERMANY
2018/10/12	<b>Using high-performance computing and molecular dynamics to rationalise micelle structure from small-angle scattering</b> , SAS2018	TRAVERSE CITY, USA
2018/10/09	<b>pylj: an open-source Python library for teaching the interaction between molecular simulation and scattering</b> , SAS2018 – Best Student Lecture Prize	TRAVERSE CITY, USA
2018/09/16	<b>Introducing programming to undergraduate chemists: and the tools we've developed to help them</b> , PYCON UK	CARDIFF, UK
2018/08/23	<b>Introducing programming to undergraduate chemists: and the tools we've developed to help them</b> , VICEPHEC18	SHEFFIELD, UK
2018/06/14	<b>Using markov chain monte-carlo to estimate uncertainties in x-ray reflectometry modeling</b> , University of Bath Bolland Symposium	BATH, UK
2018/02/09	<b>Probabilistic analysis of reflectometry data: Phospholipids at the DES-air interface</b> , Neutrons and Global Challenges II: Health and Healthcare	LONDON, UK
2017/09/12	<b>Simulations to understand reflectivity: How coarse can we go?</b> , CCP5 AGM	GLASGOW, UK
2017/04/13	<b>Simulations to understand reflectivity: How coarse can we go?</b> , Faraday Joint Interest Group Conference	WARWICK, UK
2017/03/23	<b>Coarse graining and reflectivity: a love story?</b> , CompChem Seminar, University of Bath	BATH, UK
2017/02/28	<b>Reflectivity: from simulation to experiment</b> , International Soft Matter Workshop	HELFDORF, UK
2016/06/23	<b>Smart analysis of soft matter</b> , Bombannes Summer School	BOMBANNES, FRANCE
2016/01/28	<b>Nanodisc models for calculation of small-angle scattering patterns</b> , SMALP Meeting 2016	BIRMINGHAM, UK