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

- **Andrew R. McCluskey***, Tom Arnold, Joshaniel F. K. Cooper, & Tim 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
- **Andrew R. McCluskey***, Adrian Sanchez-Fernandez, Karen J. Edler, Stephen C. Parker, Andrew J. Jackson, Richard A. Campbell, & Tom Arnold*. *Phys. Chem. Chem. Phys.*, **21**(11), 6133-6141, 2019 – Highly collaborative work, developed a novel analysis methodology for application to expertimental X-ray reflectometry
- **Andrew R. McCluskey***, James Grant, Adam R. Symington, Tim Snow, James Doutch, Benjamin J. Morgan*, Stephen C. Parker, & Karen 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 Teriary 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 fundemental 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 enable 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.

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).

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 Doutch, 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	**Reflectometry and data science**, #theLightStuff Webinars (youtu.be/PHBLK_3sfi8)	*ONLINE*
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

2019/07/12	**Automating reflectometry reduction and analysis at Diamond Light Source**, M4 COLLOIDS	*BATH, UK*
2019/05/07	**Bayesian determination of the effect of a deep eutectic solvent on the structure of lipid monolayers**, BAYES@LUND 2019	*LUND, SWEDEN*
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*