Dr Andrew R. **McCluskey**

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Developing an international research and leadership profile in neutron and X-ray reflectometry through fundamental research and collaborations. Interested in developing sophisticated analytical techniques and improving instrumentation through the use of data-driven methods. Driven by a collaborative approach to research and a founding member of the Open Reflectometry Standards Organisation. Experienced educator and developer of open educational resources, passionate about engaging others in scientific research and practice.

Selected Publications

- **A. R. McCluskey***, T. Arnold, J. F. K. Cooper, & T. Snow. *Mach. Learn.: Sci. Technol.*, **1**(3), 035002, 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. Doutch, 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

Employment

Diamond Light Source

HARWELL-OXFORD, UK

Data Analysis Scientist – Reflectivity

APR. 2019 - ONGOING

- A collaborative project between Diamond Light Source, ISIS Neutron and Muon Source and the Ada Lovelace Centre to increase automation in neutron and X-ray reflectometry reduction and analysis
- Working closely with instrument scientists from both Diamond Light Source and ISIS Neutron and Muon Source to develop cross-facility reduction and analysis solutions
- Supporting reflectometry users through local contacting on the I07 beamline; including instrument set-up, data collection, data reduction and analysis
- Assisting both neutron and X-ray reflectometry users with data analysis; developing batch time-resolved analysis methodologies
- Co-founded the Open Reflectometry Standards Organisation; a collaborative group of reflectometry instrument scientists focused on improving experimental and analytical standardisation, and elected as chair of the Reproducibility Working Group
- Developing an independent research profile using data-driven analysis for the interpretation of neutron and X-ray reflectometry data from biological membrane systems, in collaboration with staff from ISIS Neutron and Muon Source, European Spallation Source and Diamond Light Source

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 to improve the analysis of neutron and X-ray reflectometry
- Implemented high-performance optimisation & sampling algorithms to rationalise experimental scattering data
- Participated in many reflectometry and small-angle scattering experiments at Diamond Light Source and ISIS Neutron and Muon Source.
- 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**

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

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

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

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)

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, Docker

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

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

Software development

uravu An open-source Bayesian data analysis Python package. This gives access to powerful Bayesian inference libraries through a simple interface for model-dependent data analysis. Published in the Journal of Open Source Software.

islatu A open-source, documented package enabling reproducible and automated X-ray reflectometry reduction for data collected at the I07 beamline.

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 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. Published in the Journal of Open-Source Education.

Service/Community

American Chemical Society/Open Journals

Peer Reviewer

MAY 2020 - PRESENT

- Carried out peer review for Journal of Physical Chemistry & Journal of Open Source Software

Open Reflectivity Standards Organisation

Member

OCT. 2019 - PRESENT

- A founding member of an international collaborative organisation aiming to standardise reflectivity measurements
- Organised two workshops, bringing together experts in reflectometry to collaborate on open standards
- Chair of the Reproducibility working group

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
- Responsible for the organisation of Early Career Meetings for the group and acting as *de-facto* webmaster

M4 Colloids

Organising Committee Member

JUL. 2016

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

Royal Society of Chemistry

Member *SEPT. 2010 - PRESENT*

- Associated member of the RSC since start of undergraduate
- Full member since August 2020

Publications

8. A. R. McCluskey, K. S. W. Hung, B. Marzec, J. O. Sindt, N. A. J. M. Sommordijk, P. J. Camp, & F. Nudelman*. Disordered Filaments Mediate the Fibrillogenesis of Type-I Collagen in Solution, *Biomacromolecules,* **21**(9), 3631-3643, 2020. DOI: 10.1021/acs.biomac.0c00667
7. A. R. McCluskey*, T. Arnold, J. F. K. Cooper, & T. Snow. A general approach to maximise information density in neutron reflectometry analysis, *Mach. Learn.: Sci. Technol.,* **1**(3), 035002, 2020. DOI: 10.1088/2632-2153/ab94c4.
6. A. R. McCluskey*, & T. Snow. uravu: making Bayesian data analysis easy(er), *J. Open Source Softw.,* **5**(50), 2214, 2020. DOI: 10.21105/joss.02214.
5. A. R. McCluskey*, J. Grant, A. J. Smith, J. L. Rawle, D. J. Barlow, M. J. Lawrence, S. C. Parker, & K. 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. A. R. McCluskey*, J. Grant, A. R. Symington, T. Snow, J. Doutch, B. J. Morgan*, S. C. Parker, & K. 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. A. R. McCluskey*, A. Sanchez-Fernandez, K. J. Edler, S. C. Parker, A. J. Jackson, R. A. Campbell, & T. 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. A. R. McCluskey*, B. J. Morgan, K. J. Edler, & S. 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. A. R. McCluskey, & K. 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-grained 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 modelling**, 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*