Dr Andrew R. **McCluskey**

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Developing an international research and leadership profile in applied data science for analytical chemistry and physics 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.

Employment

University of Bristol   BRISTOL, GB
LECTURER IN CHEMISTRY   AUG. 2023 - ONGOING

- Leading the statistical chemical analysis methods research group at the University of Bristol (SCAMs@bristol)
- Teaching on the MSc Scientific Computing with Data Science program, focusing on training physical and life scientists in computational skills

European Spallation Source ERIC   KØBENHAVN, DK & LUND, SE
INSTRUMENT DATA SCIENTIST FOR NEUTRON REFLECTOMETRY   JAN. 2021 - AUG. 2023

- Leading data reduction and analysis development for reflectometry instruments at the European Spallation Source Data Management and Software Centre
- Interfacing between the software development and instrument groups to ensure data-centric aspects of instrumentation are ready for beam on target
- Independent research focusing on improving experimental analysis approaches using Bayesian methodologies
- Work package leader for the PaNOSC (photon and neutron open science cloud) subproject on User Training and e-Learning

Diamond Light Source   HARWELL-OXFORD, GB
DATA ANALYSIS SCIENTIST – REFLECTIVITY   APR. 2019 - DEC. 2020

- 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
- Supporting reflectometry users through local contacting on the I07 beamline; including instrument set-up, data collection, data reduction and analysis

Education

University of Bristol   BRISTOL, GB
POSTGRADUATE CERTIFICATE IN ACADEMIC PRACTICE   JAN. 2024 - JUL. 2025

University of Bath & Diamond Light Source   BATH & HARWELL-OXFORD, GB
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
- 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, GB
MCHEM IN MATERIALS CHEMISTRY WITH A YEAR IN INDUSTRY   SEPT. 2010 - JUN. 2015

- Degree Classification: **First Class**
- Year in Industry at Cytec Industries in Stamford, US

Invited Positions

Diamond Light Source   HARWELL-DIDCOT, GB
VISITING SCIENTIST   MAR. 2024 - ONGOING

European Spallation Source ERIC   KØBENHAVN, DK & LUND, SE
VISITING SCIENTIST   SEPT. 2023 - SEPT. 2024

University of Bath   *BATH, GB*

VISITING LECTURER   *SEPT. 2019 - SEPT. 2022*

– 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
– Successfully transferred this module to a completely online learning module in 2020

ISIS Neutron Training Course   *HARWELL-OXFORD, GB*

LECTURER   *MAR. 2017 - MAR. 2018*

Funding Secured

– **Royal Society of Chemistry Solid State Chemistry Group** – Support for the Solid Data Summer School (£10 000)
– **Biotechnology and Biological Sciences Research Council** – Co-investigator for "A unique cutting-edge Atomic Force Microscopy platform to converge frontier biosciences with engineering, environmental and physical sciences" (£1 000 000)
– **Carlsberg Fondet** – Conference grant for DMSC Summer School (60 000 DKK)
– **DanScatt** – Sponsorship of DMSC Summer School (25 000 DKK)
– **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

2024/04/11 **B.T.M. Willis Prize**, UK Neutron Scattering Group
2023/12/19 **Materials Advances Computational Science Prize**, Royal Society of Chemistry Solid State Chemistry Group Christmas Meeting
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

Software Projects

kinisi   A robust methodology for uncertainty quantification in *in-silico* diffusion, implemented in an open-source Python package and published in the Journal of Open Source Software with the methodology published in the Journal of Chemical Theory and Computation.

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. Published in the Journal of Open Source Software.

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.

Language Fluency

Mother tongue   English
CEFR-level B2   Danish (Prøve i Dansk 3)

Service/Community

Journal of Open Source Education

TOPIC EDITOR   *OCT 2022 - PRESENT*

– Served as a topic editor for the Journal of Open Source Education (Open Journals), focusing on computational chemistry and physics

Various Academic Journals

PEER REVIEWER   *MAY 2020 - PRESENT*

– Carried out peer review for Journal of Physical Chemistry, Journal of Chemical Education (American Chemical Society), Journal of Open Source Software (Open Journals), Journal of Applied Crystallography (International Union of Crystallography) & Journal of Statistics and Data Science Education (Taylor & Francis)

Open Reflectivity Standards Organisation

MEMBER   *OCT. 2019 - JUN. 2025*

– 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

TREASURER/ORDINARY COMMITTEE MEMBER/EARLY CAREER REPRESENTATIVE   *JUN. 2017 - PRESENT*

– Currently serve as the treasurer of the NSG Committee (since 2024) and the RSC Materials Chemistry Community Representative (since 2023), previously served as Eary Career Representative and an Ordinary Committee Member
– Responsible for the organisation of Early Career Meetings for the group and acting as *de-facto* webmaster

Royal Society of Chemistry

MEMBER   *SEPT. 2010 - PRESENT*

– Member of the RSC since start of undergraduate
– Full member since August 2020

Publications

24. B. A. Humphreys*, P. Gutfreund, **A. R. McCluskey**, T. Arnold, J. Vind, & T. Nylander.   Following the structural changes of triolein films during lipolysis *Submitted,* 2025.

23. H. Richardson, J. Dunn*, & **A. R. McCluskey*** On the Estimation of Centre of Mass in Periodic Systems, *J. Chem. Phys.,* **162**(20), 204103, 2025. DOI: 10.1063/5.0260928.

22. **A. R. McCluskey***, S. W. Coles, & B J. Morgan*.   Accurate Estimation of Diffusion Coefficients and their Uncertainties from Computer Simulation, *J. Chem. Theory Comput.,* **21**(1), 79-87, 2025. DOI: 10.1021/acs.jctc.4c01249.

21. N. Shiaelis*, L. A. Clifton, & **A. R. McCluskey***.   Investigating model influence on the analytical resolution of neutron reflectometry, *Preprint,* 2024. Available on arXiv: 2403.13566.

20. **A. R. McCluskey***, M. Rivera*, & A. S. J. S. Mey*.   Digital Skills in Chemical Education, *Nat. Chem.,* **16**(9), 1383-1384, 2024. DOI: 10.1038/s41557-024-01613-x.

19. J. Dunn, J. M. Crossley-Lewis, **A. R. McCluskey**, F. Jackson, C. Buda, G. Sunley, A. J. Mulholland, N. L. Allan.* Diffusion Mechanisms and Preferential Dynamics of Promoter Molecules in ZSM-5 Zeolite, *Catal. Sci. Technol.,* **14**(13), 3674-3681, 2024. DOI: 10.1039/D4CY00506F.

18. **A. R. McCluskey***, P. Aulin, F. Bolmsten, M. Bertelsen, C. M. C. Lobley, J. Lewis, M. Novelli, C. Somani, A. Stefanov, M. Trajanovski, N. Vaytet, P. K. Willendrup, J.-L. Wynen, S. Yoo, T. H. Rod*.   The First European Spallation Source Data Management and Software Centre Summer School, *Neutron News,* **35**(1), 1-3, 2024. DOI: 10.1080/10448632.2024.2331387.

17. **A. R. McCluskey***, A. G. Squires, J. Dunn, S. W. Coles, & B. J. Morgan*.   kinisi: Bayesian analysis of mass transport from molecular dynamics simulations, *J. Open Source Softw.,* **9**(94), 5984, 2024. DOI: 10.21105/joss.05984.

16. **A. R. McCluskey***.   Is there still a place for linearization in the chemistry curriculum?, *J. Chem. Educ.,* **100**(11), 4174-4176, 2023.   DOI: 10.1021/acs.jchemed.3c00466.

15. G. Krenzer, J. Klarbring, K. Tolborg, H. Rossignal, **A. R. McCluskey**, B. J. Morgan*, & A. Walsh*.   Nature of the Superionic Transition of Lithium Nitride from Machine Learning Force Fields, *Chem. Mater.,* **35**(15), 6133-6140, 2023. DOI: 10.1021/acs.chemmater.3c01271.

14. **A. R. McCluskey***, A. J. Caruana*, C. J. Kinane, A. J. Armstrong, T. Arnold, J. F. K. Cooper, D. L. Cortie, A. V. Hughes, J.-F. Moulin, A. R. J. Nelson, W. Potrzebowski, & V. Starostin.   Advice on describing Bayesian analysis of neutron and X-ray reflectometry, *J. Appl. Crystallogr.,* **56**(1), 12-17, 2023. DOI: 10.1107/S1600576722011426.

13. R. Brearton*, **A. R. McCluskey**, & T. Snow. islatu: A Python package for the reduction of reflectometry data, *J. Open Source Softw.,* **7**(77), 4397, 2022. DOI: 10.21105/joss.04397.

12. T. Arnold*, A. Terry, E. Blackburn, U. Hejral, Z. Heyles, **A. R. McCluskey**, T. Nylander, & M. Wolff. The 16th International Conference on Surface X-ray and Neutron Scattering (SXNS16), *Neuton News,* **33**(2), 2, 2022. DOI: 10.1080/10448632.2022.2050633.

11. T. Arnold*, B. Murphy, **A. R. McCluskey**, J. Stahn, & M. W. A. Skoda. A Report on the Third Meeting of the Open Reflectivity Standards Organisation (ORSO), *Neuton News,* **33**(1), 2, 2022. DOI: 10.1080/10448632.2021.2005422.

10. J. M. Dean, S. W. Coles*, W. R. Saunders, **A. R. McCluskey**, M. J. Wolf, A. B. Walker, & B. J. Morgan*. Overscreening and Underscreening in Solid-Electrolyte Grain Boundary Space-Charge Layers, *Phys. Rev. Lett.,* **127**(13), 135502, 2021. DOI: 10.1103/PhysRevLett.127.135502.

9. A. Markvardsen*, T. Rees, M. Wathen, A. Lister, P. Odagiu, A. Anuchitanukul, T. Farmer, A. Lim, F. Montesino, T. Snow, & **A. McCluskey**. Fit-Benchmarking: an open source Python package comparing data fitting software, *J. Open Source Softw.,* **6**(62), 3127, 2021. DOI: 10.21105/joss.03127.

8. **A. R. McCluskey**, K. S. W. Hung, B. Marzec, J. O. Sindt, N. A. J. M. Sommerdijk, 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

2025/06/03	**Accurate Estimation of Self- and Collective-Motion from Molecular Dynamics Simulation**, PAQMAN	*STAVANGER, NO*
2025/05/01	**Accurate Diffusion Estimation From Simulation and the Impacts on Temperature Dependent Modelling**, DAMTP BioLunch	*CAMBRIDGE, UK*
2025/04/16	**Accurate Diffusion Estimation From Simulation**, Digital Chemistry Festival – **Plenary Speaker**	*BRISTOL, UK*
2025/02/20	**Accurate Diffusion Estimation From Simulation: Can We Improve QENS Analysis?**, ISIS Research Seminar	*HARWELL, UK*
2025/01/19	**Accurate Diffusion Estimation From Simulation**, Bragg Exchange 2025	*LEEDS, UK*
2024/11/27	**Accurate Diffusion Estimation From Simulation and Propagation to Temperature Dependent Modelling**, University of Warwick Computational Chemistry Seminar	*WARWICK, UK*
2024/06/26	**A Short History of Trying To Make Computational Research More Reproducible**, Reproducibility By Design Workshop	*BRISTOL, UK*
2024/06/05	**Accurate Diffusion Estimation From Simulation and Propagation to Temperature Dependent Modelling**, University of Birmingham Research Seminar	*BIRMINGHAM, UK*
2024/04/11	**How To Care About Data in Neutron Scattering: A Biased Perspective**, UK Neutron and Muon Science User Meeting 2024 – **B.T.M. Willis Prize Lecture**	*WARWICK, GB*
2024/03/12	**Introduction to Reflectometry: With a Focus on Analysis**, French-Swedish Academy for Scattering Experiments and Modelling for Life Science	*LUND, SE*
2022/07/05	**Developing and sharing an undergraduate chemistry course for Python**, 2022 RACI National Congress, Physical and Computational Chemistry Education Symposium – **Keynote Speaker**	*HYBRID (BRISBANE, AU)*
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, GB*
2017/06/12	**Putting computers to work for large experiments**, Faculty of Science Graduate School Research Afternoon, Bath University – **Best Talk Award**	*BATH, GB*
2016/05/23	**SAS, Sims and Soft Matter Self-Assembly**, CCP-SAS Joint Meeting, NIST	*GAITHERSBURG, US*

Contributed Talks

2024/07/03	**Accurate Diffusion Estimation From Simulation and Propagation to Temperature Dependent Modelling**, Workshop on Synergies Between Mathematics, Data Science, and Molecular Simulations in Materials Science	*BIRMINGHAM, UK*
2023/09/22	**A perspective on probabilistic chemical models to complement quantum algorithms**, Scientific Applications of Quantum Computing: Materials, Chemistry and Biology	*LONDON, GB*
2022/09/21	**PaN-Training e-Learning: education and training for scientists and students**, NOBUGS (New Opportunities for Better User Group Software) 2022	*HYBRID (VILLIGEN, CH)*

Date	Title	Location
2022/08/22	**Using Bayesian inference as a tool to more completely understand neutron reflectometry**, International Conference on Neutron Scattering 2022	*BUENOS AIRES, AR*
2019/07/12	**Automating reflectometry reduction and analysis at Diamond Light Source**, M4 COLLOIDS	*BATH, GB*
2019/05/07	**Bayesian determination of the effect of a deep eutectic solvent on the structure of lipid monolayers**, BAYES@LUND 2019	*LUND, SE*
2018/10/30	**Comparing coarse-grained simulation-derived and traditional analysis method for monolayer reflectometry**, Trends and Perspectives in Neutron Instrumentation	*TUTZING, DE*
2018/10/12	**Using high-performance computing and molecular dynamics to rationalise micelle structure from small-angle scattering**, SAS2018	*TRAVERSE CITY, US*
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, US*
2018/09/16	**Introducing programming to undergraduate chemists: and the tools we've developed to help them**, PYCON UK	*CARDIFF, GB*
2018/08/23	**Introducing programming to undergraduate chemists: and the tools we've developed to help them**, VICEPHEC18	*SHEFFIELD, GB*
2018/06/14	**Using markov chain monte-carlo to estimate uncertainties in x-ray reflectometry modelling**, University of Bath Bolland Symposium	*BATH, GB*
2018/02/09	**Probabilistic analysis of reflectometry data: Phospholipids at the DES-air interface**, Neutrons and Global Challenges II: Health and Healthcare	*LONDON, GB*
2017/09/12	**Simulations to understand reflectivity: How coarse can we go?**, CCP5 AGM	*GLASGOW, GB*
2017/04/13	**Simulations to understand reflectivity: How coarse can we go?**, Faraday Joint Interest Group Conference	*WARWICK, GB*
2017/03/23	**Coarse graining and reflectivity: a love story?**, CompChem Seminar, University of Bath	*BATH, GB*
2017/02/28	**Reflectivity: from simulation to experiment**, International Soft Matter Workshop	*HELFORD, GB*
2016/06/23	**Smart analysis of soft matter**, Bombannes Summer School	*BOMBANNES, FR*