

Dr Andrew R. McCluskey

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An international research leader at the interface between statistics, applied mathematics, and the physical sciences to improve neutron scattering and computational simulation methods through fundamental research and collaborations. Driven by a collaborative approach to research, a commitment to open science, and a passion for excellent mentorship. Experienced educator and developer of open educational resources, passionate about engaging others in scientific research and practice.

Employment

University of Bristol

BRISTOL, GB

SENIOR LECTURER IN CHEMISTRY

FEB. 2026 - ONGOING

LECTURER IN CHEMISTRY

AUG. 2023 - JAN. 2026

European Spallation Source ERIC

KØBENHAVN, DK & LUND, SE

INSTRUMENT DATA SCIENTIST FOR NEUTRON REFLECTOMETRY

JAN. 2021 - AUG. 2023

Diamond Light Source

HARWELL-OXFORD, GB

DATA ANALYSIS SCIENTIST – REFLECTIVITY

APR. 2019 - DEC. 2020

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 – SUPERVISORS: PROF. KAREN EDLER, PROF. STEPHEN PARKER, DR ANDREW SMITH AND DR JONATHAN RAWLE

SEPT. 2015 - APR. 2019

University of Edinburgh

EDINBURGH, GB

MCHEM IN MATERIALS CHEMISTRY WITH A YEAR IN INDUSTRY – FIRST CLASS

SEPT. 2010 - JUN. 2015

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

ISIS Neutron Training Course

HARWELL-OXFORD, GB

LECTURER

MAR. 2017 - MAR. 2018

Funding Secured

- 2025/12 **Digital engineering biology - Accelerating digital biology from models to innovation**, University of Bristol, Faculty of Science and Engineering Strategic Research Accelerator – £134 000 (Co-investigator)
- 2025/06 **Support for the Solid Data Summer School**, Royal Society of Chemistry Solid State Chemistry Group – £10 000 (Co-organiser)
- 2024/08 **A unique cutting-edge Atomic Force Microscopy platform to converge frontier biosciences with engineering, environmental and physical sciences**, Biotechnology and Biological Sciences Research Council (BBSRC) ALERT – £1 000 000 (Co-investigator)
- 2023/07 **Conference grant for DMSC Summer School**, Carlsberg Fondet – 60 000 DKK (Project lead)
- 2023/07 **Sponsorship of DMSC Summer School**, DanScat – 25 000 DKK (Project lead)
- 2020/08 **Development of a Bayesian regularisation framework for the analysis of reflectometry**, Diamond Light Source Year in Industry Studentship 2020/2021 – £20 000 (Project lead)
- 2019/11 **pythoninchemistry Hackathon**, Royal Society of Chemistry Higher Education Group Kickstart Scheme – £300 (Co-investigator)

Awards/Memberships

- 2025/11/05 **Springboard Award**, ISIS Neutron and Muon Source
- 2025/07/25 **Fellow of the Higher Education Academy (FHEA)**, Advance HE
- 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

Service/Community

Journal of Open Source Education

TOPIC EDITOR (COMPUTATIONAL CHEMISTRY & PHYSICS)

OCT 2022 - PRESENT

Open Reflectivity Standards Organisation

FOUNDING MEMBER

OCT. 2019 - JUN. 2025

RSC/IOP Neutron Scattering Group Committee

TREASURER

OCT. 2024 - PRESENT

ORDINARY COMMITTEE MEMBER

JUN. 2023 - SEPT. 2024

EARLY CAREER REPRESENTATIVE

JUN. 2017 - JUN. 2023

Royal Society of Chemistry

MEMBER

SEPT. 2010 - PRESENT

Language Fluency

Mother tongue English

CEFR-level B2 Danish (Prøve i Dansk 3)

Publications

26. **A. R. McCluskey***, S. W. Coles, B. J. Morgan*. Bayesian Methods for the Investigation of Temperature-Dependence in Conductivity, *Submitted*, 2025. Available on arXiv: 2512.17792.
25. B. J. Morgan* & **A. R. McCluskey***. Uncertainty in MD-Derived Diffusion Coefficients Depends on Analysis Protocol, Not Just Simulation Data, *Submitted*, 2025. Available on ChemRxiv: 10.26434/chemrxiv-2025-9dbv9-v3.
24. B. A. Humphreys*, P. Gutfreund, **A. R. McCluskey**, T. Arnold, J. Vind, & T. Nylander. Following the structural changes of triolein films during lipolysis, *Soft Matter*, **22**(2), 343-354, 2026. DOI: 10.1039/D5SM00820D.
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. Soman, 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

2026/01/16	A Case for Good Simulation To Complement Neutron Scattering: A p-QENS Example , Neutron Scattering Group Early Career Meeting	BRISTOL, UK
2026/01/15	Accurate Diffusion Estimation From Simulation and the Impacts on Temperature Dependent Modelling , University of Bristol, School of Mathematics, Fluids and Materials Seminar	BRISTOL, UK
2025/06/03	Accurate Estimation of Self- and Collective-Motion from Molecular Dynamics Simulation , PAQ-MAN	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_3sf18)	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 (VILIGEN, CH)
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	HELPFORD, GB
2016/06/23	Smart analysis of soft matter , Bombannes Summer School	BOMBANNES, FR