

# 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

SENIOR LECTURER IN CHEMISTRY

BRISTOL, GB

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. Loble, 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), *Neutron 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), *Neutron 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. Douth, 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	<b>A Case for Good Simulation To Complement Neutron Scattering: A p-QENS Example</b> , Neutron Scattering Group Early Career Meeting	BRISTOL, UK
2026/01/15	<b>Accurate Diffusion Estimation From Simulation and the Impacts on Temperature Dependent Modelling</b> , University of Bristol, School of Mathematics, Fluids and Materials Seminar	BRISTOL, UK
2025/06/03	<b>Accurate Estimation of Self- and Collective-Motion from Molecular Dynamics Simulation</b> , PAQ-MAN	STAVANGER, NO
2025/05/01	<b>Accurate Diffusion Estimation From Simulation and the Impacts on Temperature Dependent Modelling</b> , DAMTP BioLunch	CAMBRIDGE, UK
2025/04/16	<b>Accurate Diffusion Estimation From Simulation</b> , Digital Chemistry Festival – Plenary Speaker	BRISTOL, UK
2025/02/20	<b>Accurate Diffusion Estimation From Simulation: Can We Improve QENS Analysis?</b> , ISIS Research Seminar	HARWELL, UK
2025/01/19	<b>Accurate Diffusion Estimation From Simulation</b> , Bragg Exchange 2025	LEEDS, UK
2024/11/27	<b>Accurate Diffusion Estimation From Simulation and Propagation to Temperature Dependent Modelling</b> , University of Warwick Computational Chemistry Seminar	WARWICK, UK
2024/06/26	<b>A Short History of Trying To Make Computational Research More Reproducible</b> , Reproducibility By Design Workshop	BRISTOL, UK
2024/06/05	<b>Accurate Diffusion Estimation From Simulation and Propagation to Temperature Dependent Modelling</b> , University of Birmingham Research Seminar	BIRMINGHAM, UK
2024/04/11	<b>How To Care About Data in Neutron Scattering: A Biased Perspective</b> , UK Neutron and Muon Science User Meeting 2024 – <b>B.T.M. Willis Prize Lecture</b>	WARWICK, GB
2024/03/12	<b>Introduction to Reflectometry: With a Focus on Analysis</b> , French-Swedish Academy for Scattering Experiments and Modelling for Life Science	LUND, SE

2022/07/05	<b>Developing and sharing an undergraduate chemistry course for Python</b> , 2022 RACI National Congress, Physical and Computational Chemistry Education Symposium – <b>Keynote Speaker</b>	<i>HYBRID (BRISBANE, AU)</i>
2020/04/03	<b>Reflectometry and data science</b> , #theLightStuff Webinars (youtu.be/PHBLK_3sf8)	<i>ONLINE</i>
2017/06/19	<b>Surfactants and Molecular Dynamics</b> , CCP-SAS Joint Meeting, Cardiff University	<i>CARDIFF, GB</i>
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>	<i>BATH, GB</i>
2016/05/23	<b>SAS, Sims and Soft Matter Self-Assembly</b> , CCP-SAS Joint Meeting, NIST	<i>GAITHERSBURG, US</i>

## CONTRIBUTED TALKS

2024/07/03	<b>Accurate Diffusion Estimation From Simulation and Propagation to Temperature Dependent Modelling</b> , Workshop on Synergies Between Mathematics, Data Science, and Molecular Simulations in Materials Science	<i>BIRMINGHAM, UK</i>
2023/09/22	<b>A perspective on probabilistic chemical models to complement quantum algorithms</b> , Scientific Applications of Quantum Computing: Materials, Chemistry and Biology	<i>LONDON, GB</i>
2022/09/21	<b>PaN-Training e-Learning: education and training for scientists and students</b> , NOBUGS (New Opportunities for Better User Group Software) 2022	<i>HYBRID (VILLIGEN, CH)</i>
2022/08/22	<b>Using Bayesian inference as a tool to more completely understand neutron reflectometry</b> , International Conference on Neutron Scattering 2022	<i>BUENOS AIRES, AR</i>
2019/07/12	<b>Automating reflectometry reduction and analysis at Diamond Light Source</b> , M4 COLLOIDS	<i>BATH, GB</i>
2019/05/07	<b>Bayesian determination of the effect of a deep eutectic solvent on the structure of lipid monolayers</b> , BAYES@LUND 2019	<i>LUND, SE</i>
2018/10/30	<b>Comparing coarse-grained simulation-derived and traditional analysis method for monolayer reflectometry</b> , Trends and Perspectives in Neutron Instrumentation	<i>TUTZING, DE</i>
2018/10/12	<b>Using high-performance computing and molecular dynamics to rationalise micelle structure from small-angle scattering</b> , SAS2018	<i>TRAVERSE CITY, US</i>
2018/10/09	<b>pylj: an open-source Python library for teaching the interaction between molecular simulation and scattering</b> , SAS2018 – <b>Best Student Lecture Prize</b>	<i>TRAVERSE CITY, US</i>
2018/09/16	<b>Introducing programming to undergraduate chemists: and the tools we've developed to help them</b> , PYCON UK	<i>CARDIFF, GB</i>
2018/08/23	<b>Introducing programming to undergraduate chemists: and the tools we've developed to help them</b> , VICEPHEC18	<i>SHEFFIELD, GB</i>
2018/06/14	<b>Using markov chain monte-carlo to estimate uncertainties in x-ray reflectometry modelling</b> , University of Bath Bolland Symposium	<i>BATH, GB</i>
2018/02/09	<b>Probabilistic analysis of reflectometry data: Phospholipids at the DES-air interface</b> , Neutrons and Global Challenges II: Health and Healthcare	<i>LONDON, GB</i>
2017/09/12	<b>Simulations to understand reflectivity: How coarse can we go?</b> , CCP5 AGM	<i>GLASGOW, GB</i>
2017/04/13	<b>Simulations to understand reflectivity: How coarse can we go?</b> , Faraday Joint Interest Group Conference	<i>WARWICK, GB</i>
2017/03/23	<b>Coarse graining and reflectivity: a love story?</b> , CompChem Seminar, University of Bath	<i>BATH, GB</i>
2017/02/28	<b>Reflectivity: from simulation to experiment</b> , International Soft Matter Workshop	<i>HELDFORD, GB</i>
2016/06/23	<b>Smart analysis of soft matter</b> , Bombannes Summer School	<i>BOMBANNES, FR</i>