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. 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**. FitBenchmarking: 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

2025/01/16	**A Case for Good Simulation To Complement Neutron Scattering: A p-QENS Example**, Neutron Scattering Group Early Career Meeting	*BRISTOL, UK*
2025/01/15	**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**, 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)*
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*