Viking Annual Report 2022/2023

HPC Management Committee

Introduction

In January 2018, University Executive Board authorised £2.5M for the purchase and support of a new central high-performance computing facility for the University of York, supplied by Dell and supported by Alces Flight. This aimed to accelerate research in the university across all of the faculties and to provide a focus for developing interdisciplinary activities across the University. On February 14th 2019, Viking went live, providing 7000 cores, 42 TB of memory, 2.5 PB of storage, free at the point of delivery, to staff, postgraduates, and undergraduates. This is a major university facility comparable to that provided by institutions much larger than York. This report describes the activity with Viking over the final year of its expected 5 year lifetime.

Summary

Despite being in its final year, Viking usage has continued to grow to 350 projects and 1500 registered users. The number of research outputs associated with Viking is 212, and Viking has supported upwards of £20M in funded research. Whilst still predominantly used by the Faculty of Sciences, it has been encouraging to see increased uptake in the Faculties of Social Sciences and Arts and Humanities.

With Viking now coming to end-of-life, focus has been the procurement of its successor, VIking2. Viking2 will be built and designed with a similar ethos, free at the point of use and with hardware that reflects the diversity of the research within the University. One major difference with Viking2 will be the move to a more sustainable data centre, EcoDatacentre in Falun, Sweden. This data centre has a negative carbon footprint, achieved with using sustainable building materials and also harnessing the heat produced by computer hardware to be used to dry wood pellets that are used to provide heating to businesses and homes. Viking2 is expected to come online in September 2023.

Thanks to support from several funding sources, we have expanded our capacity for GPU computing, allowing researchers to explore a technology that is rapidly growing in popularity. This capacity will be attached to Viking2 to offer researchers a seamless transition between traditional computing resources and the cutting edge.

The Viking support team has expanded, bringing broader knowledge and expertise. Lower resolution times on support cases are being delivered as a result, and we have further outreach to the University research community through Research Coding Club.

Statistics

- 1500 registered users across 382 projects, spanning 18 schools and departments
- At least £20 million in grant funding where Viking has contributed compared to an investment of £4.02 million (dedicated hardware, services and staff).

- 212 recorded research outputs
- 48 million CPU hours of work done over 4.4 million jobs
- Computing resources have been allocated to user jobs for 76% of the time in 2022
- 63% of Viking users are undergraduate/postgraduate taught students

Year Overview

Viking has continued to provide a valuable research facility for staff and students across the university. In addition to research, Viking is also used for three undergraduate modules, two based in the School of Physics, Engineering, and Technology (PET) and one based in Computer Science. We have seen an increased uptick in use and outputs from the Department of Biology, showing the growing need for computational resources in this area. In addition to this, the Viking team also branched into cloud, in conjunction with Alces and Azure and academics in the Department of Psychology. The project was a success which resulted in the team being shortlisted for an award at Supercomputing 2022, a large, international HPC conference. Viking was competing against Tier 1 and 2 facilities, which is a testament to innovative work continuing in the Viking team.

Whilst computing facilities of this nature tend to be science-focused, Viking has managed to capture a user base across 18 academic schools and departments.

Faculty of Sciences	Faculty of Social Sciences	Faculty of Arts and Humanities
Biology	**School for Business and Society**	**Archaeology**
Chemistry	**Economics and Related Studies**	**School of Arts and Creative Technologies**
Computer Science	**Education**	**Language and Linguistic Science**
Environment and Geography	**Centre for Health Economics**	**Philosophy**
Health Sciences		
Hull York Medical School		
Mathematics		
School of Natural Sciences		
School of Physics, Engineering and Technology		
Psychology		

Figure 1: Departments with registered Viking projects

The Department of Biology (80) has submitted the largest number of project applications on Viking, with a similar number in the School of Physics, Engineering and Technology (72), Chemistry (66) and Computer Science (58). We have seen some growth in the number of users from the Faculties of Arts and Humanities and Social Sciences (92 user applications) and we are working to further improve these figures.

Research Outputs

Using the University Research Database (Pure) and user surveys, we have recorded a total of 212 research outputs (papers, articles, datasets, software etc.) that have been produced using Viking. Another 37 research outputs are also in preparation. The split of outputs by department roughly reflects the departmental split of researchers on Viking.

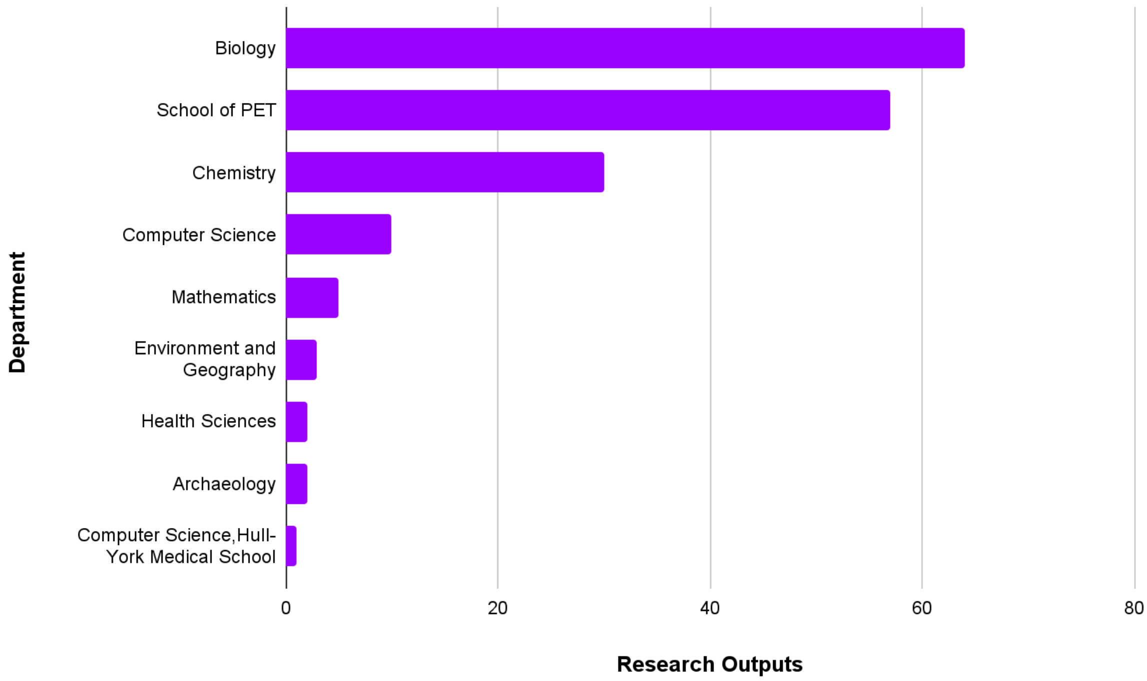


Figure 2: Research outputs which made use of Viking, counts by department. Data generated from Pure and user submissions.

This year Biology have significantly increased their outputs from 14 to 64. Although still STEM heavy we are seeing increased usage from other faculties however there is always a lag between usage and research outputs.

Case Studies

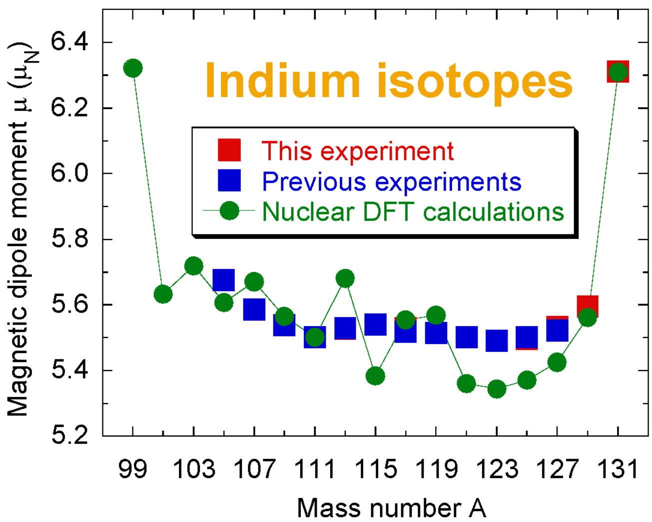
We have selected highlights of research completed on Viking. We present case studies from Physics, Atmospheric Chemistry, and Language & Linguistic Science.

Nuclear moments of indium isotopes reveal abrupt change at magic number 82

*A. R. Vernon et al. Nature **607**, 260 (2022).* [*https://doi.org/10.1038/s41586-022-04818-7*](https://doi.org/10.1038/s41586-022-04818-7)

In a famous experiment performed in 1820, Danish physicist and chemist Hans Christian Ørsted demonstrated that an electric current deflected a compass needle from magnetic north. As we understand it today, the electric current generates a magnetic field. In a similar way, a charged rotating body generates a magnetic field and acquires a so-called magnetic moment. Nuclear magnetic moments relate to the orbital and spin components. Experiments showed that the spin components were weaker than those of isolated protons and neutrons. So far, a common practice was to attenuate the spin components and employ a blanket common reduction factor called the effective g-factor.

This simplistic approach to magnetic moments abruptly ended with a breakthrough experiment performed on heavy indium isotopes. An international team of scientists showed that the almost constant value of nuclear magnetic moments measured in the past in the indium isotopes with neutron numbers from N=64 to 78 is continued till N=80, but then jumps to a much larger value at N=82.



Such a jump is a surprise and does not support the earlier assumptions of an effective g-factor but, rather, calls for invoking specific nuclear-structure effects. Advanced calculations, performed on Viking by Bonnard and Dobaczewski showed that the magnetic moments of the indium isotopes (proton number Z=49) are generated not only by the single odd-proton hole in the magic proton closed-shell corresponding to Z=50 but also by self-consistently polarised states of the entire Z=50 core.

In a mature domain of physics such as nuclear physics, it is not often that one has a chance to rewrite the textbooks written by the giants of the field. New ideas and breakthrough understanding come from combining the most advanced experimental and theoretical capabilities. A new chapter appears to be opening in the story of nuclear magnetic moments, for which the HPC calculations are, and will be of paramount importance.

The Nuclear-DFT calculations are particularly voracious in the consumption of processor time. They are typically performed in an embarrassingly parallel mode, whereupon a single self-consistent solution is determined within about 12h-24h of CPU time but has to be obtained for many different nuclei, configurations, deformations, etc. In addition, reliable estimates of various observables (nuclear moments in particular) require symmetry restoration, which multiplies the CPU times by factors anywhere between a few and a million. It is clear that progress in this domain of theoretical physics will be tightly governed by the availability of advanced computation capabilities.

Improving the Modelling of Atmospheric Volatile Organic Compounds

M. Rowlinson, M. Evans

Volatile organic compounds (VOCs) play an important role in regulating atmospheric chemistry and can lead to the formation of ozone, a greenhouse gas and air pollutant. Two of the most important VOCs are ethane and propane, but we don't understand where these chemicals are coming from in the atmosphere. We use the GEOS-Chem chemical transport model (www.geos-chem.org) on Viking to simulate the chemistry of the atmosphere and understand the sources of these molecules. GEOS-Chem is a well used open-source community atmospheric chemistry model used by groups around the world (Harvard, MIT, CalTech, NASA, Edinburgh, UCL, Peking University etc) to understand the composition of the atmosphere.

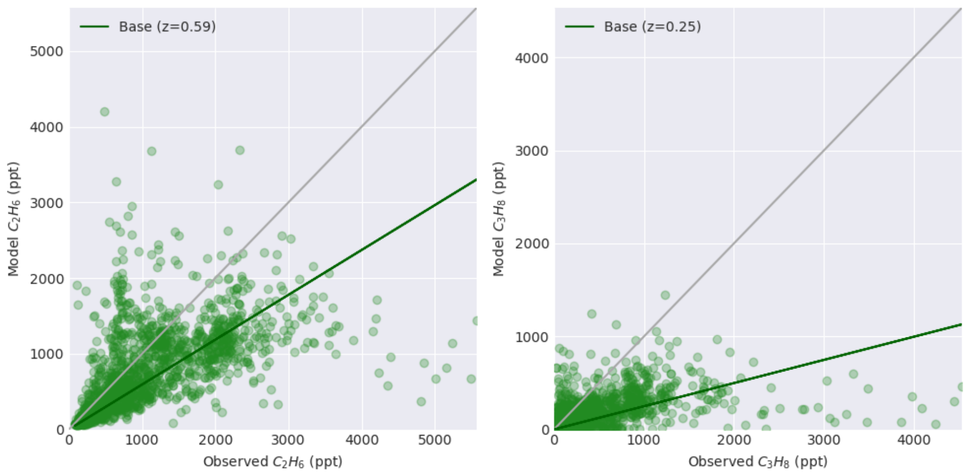
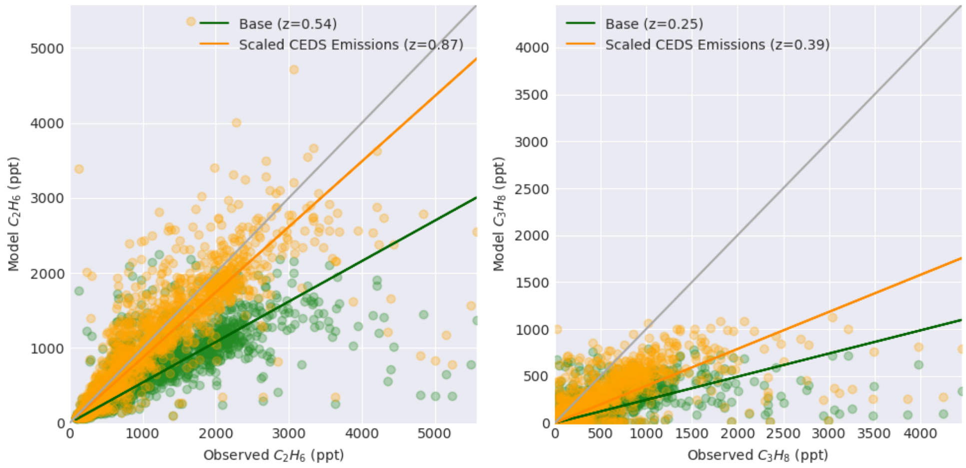


Figure 1.

Simulated concentrations from our model are compared to measured values from around the world in Figure 1. This shows the model underestimates both ethane and propane. Comparing the default emissions inventory to regional emissions estimates for Europe, USA and China, it was found that ethane and propane emissions were substantially lower in the global database than in the regional. We then adapted the emissions of VOCs in the model, to match each of the regional estimates.

We run the model again on Viking with the new emissions, and compare the change in model performance in Figure 2. When using the adapted emissions the concentrations of ethane now compare much better with measurements, and there is also a smaller improvement for propane. Viking was vital for this study as it allowed us to run large simulations very efficiently, whilst also providing computing resources for the processing and analysis of the model output.



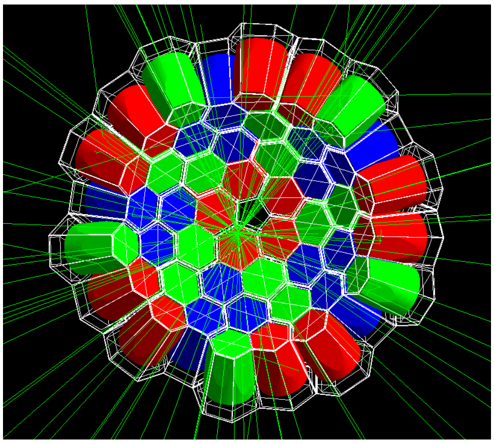
Base (z=0.54)
Scaled CEDS Emissions (z=0.87)
Model C_2H_6 (ppt)
Observed C_2H_6 (ppt)
Base (z=0.25)
Scaled CEDS Emissions (z=0.39)
Model C_3H_8 (ppt)
Observed C_3H_8 (ppt)

Figure 2.

Self-Calibration for γ-ray tracking array

S. Chen, S. Paschalis, M. Petri, M. Bentley, M. Labiche, F. Holloway and S. Heil

High precision γ-ray spectroscopy is one of the most powerful tools to study nuclear structures. In the last decades, the frontier of γ-ray spectroscopy was moved to the development of γ-ray tracking arrays based on highly segmented High Purity Germanium (HPGe) detectors, that allow for a better determination of the incoming γ-ray direction and the full deposited energy. The most advanced implementation of such a technique is in two arrays: the AGATA (Advanced Gamma Tracking Array) in Europe and the GRETA (Gamma Ray Energy Tracking Array) in the US. The tracking ability of these arrays very much relies on the precise determination of the interaction positions within the detector volume, which is realised by comparing the experimental signals against a pre-generated library of signals (signal basis) that maps the detector response at different interaction positions. A novel method, called Self-Calibration, is proposed to generate a reliable signal basis from a large experimental data set. Starting from the assumption of segment-sized position resolution for all signals, and using an iterative minimization procedure based on the Compton scattering formula, this method improves the position assignment for signals and converges to their real positions after a few iterations.



The simulation of AGATA with 45 detectors (3 types with different geometries in red, green and blue). Every detector is segmented by 6 sectors x 6 slices (36 segments). A radioactive source is placed at the centre of the array, emitting γ-rays (green lines) in 4π. Only Compton scattering events are saved for analysis. For every detector, signals are read from all segments as well as the core, which give 37 channels in total. Signal shape from each channel is recorded with 60 sampling points, leading to 37x60=2220 data points per detector per event.

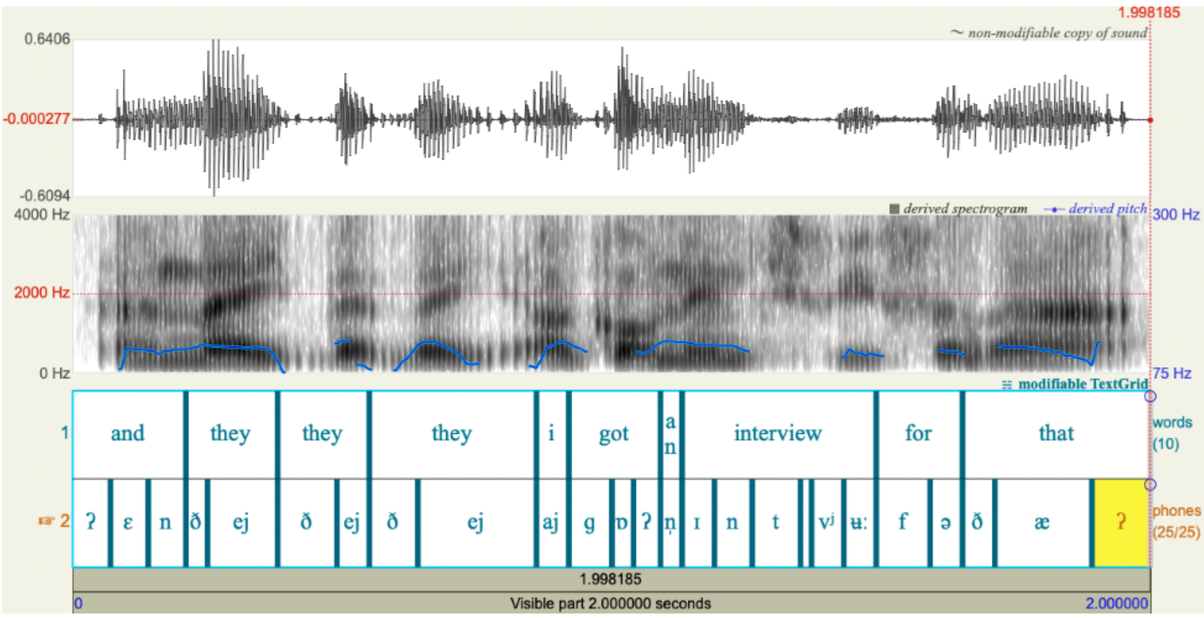
To achieve the converging condition and generate signal basis with enough density, the order of 10^8 Compton events need to be accumulated and analysed, which uses hundreds of GB of memory and thousands of hours of CPU time. The large number of CPUs and large size of memory in Viking allow us to process this work in a highly parallelized way - the program is developed with multi-threads and the analysis of each detector can be separated in parallel processes - eventually, hundreds of CPUs can be utilised simultaneously to make the program two orders of magnitude faster. With Viking, this method can be completed in a reasonable time scale, therefore, becoming really practical.

Forced-Alignment of Large Speech Corpora to Facilitate Forensic Speech Research

Harrison, P., Xu, C., Hughes, V., Foulkes, P., Welch, P., Wormald, J.

'Person-Specific Automatic Speaker Recognition (PASR): understanding the behaviour of individuals for applications of ASR' is a 3-year, £1 million ESRC funded project in the Department of Language and Linguistic Science in the Faculty of Arts and Humanities. The project is investigating the characteristics of people's voices that influence the performance of automatic speaker recognition systems used in forensic casework. To discover which characteristics are important to an ASR, the results of more traditional and interpretable phonetic analyses are being used to provide insights into the opaque statistical speaker models generated by ASR systems and identify groups and patterns within the results of automatic speaker comparison tests.

Many types of phonetic analysis require the timing location of different categories of speech sounds (e.g. vowels, consonants) within a recording to produce meaningful measurements. This segmentation process is often manual and very labour intensive. To ensure the findings are robust, large speech corpora containing thousands of speakers with diverse characteristics including age, regional/ethnic accent are being used but this makes the manual segmentation approach impossible. Instead, a process known as 'forced alignment' is used to automatically align a written transcript of a recording with the audio signal at the level of individual speech sounds, (i.e. individual vowels and consonants).



Word and segment (phone) level segmentation (bottom half) of a short section of a speech recording generated from a written transcript using the Montreal Forced Aligner. The amplitude waveform and spectrogram are also shown in the top and second panels.

The large number of CPU cores available on Viking allows effective use of the parallel processing capabilities of the Montreal Forced Aligner (MFA) software. This significantly reduces the time taken to process thousands of recordings compared with researchers' laptop and desktop computers. The time savings have allowed exploration of the impact on the alignment accuracy of varying a range of MFA's parameters including different language models and dictionaries. This is particularly important as the recordings are of telephone calls with reduced quality and the language models are not optimised to the speakers' accents.

The development of a straightforward and simple to use pipeline for using Montreal Forced Aligner on Viking paves the way for other researchers in the Department of Language and Linguistic Science to use this tool in the future for larger-scale analyses. As researchers in the department are beginning to use increasingly larger speech corpora the need for such tools and the large processing capability of Viking will no doubt grow.

UNIVERSITY of York

Support and Training

Research Software Engineering Team

The Research and High Performance Computing Support Team continues to grow in the past year with two new research software engineers which broadens the existing available support and now adds robotics, environment, geography and The Plasma Institute knowledge into the mix. A new role of Research Software Engineer Team Lead has been created to manage and support the RSE team. These new positions increase the RSE team to 6 people.

Research Infrastructure Team

The Research Infrastructure Team continues to provide support for users across the university. We have 1 FTE devoted to Viking, with 1 FTE in physics and 1 FTE in CS.

York has continued its contribution to EasyBuild. EasyBuild is a software build and installation framework that simplifies software management on HPC systems. The Team has not only contributed significantly to the Easybuild community with code, but one of the Research Infrastructure Team members (Jasper Grimm) is now an EasyBuild maintainer. York has made 900 contributions in the last 12 months. Easybuild is a framework used in a number of HPC facilities both nationally and internationally, with York now being a major contributor.

These new team member additions have resulted in lower case creation to solution time for the Research IT team and a marked increase in positive user feedback. Service Level Agreements (SLAs) are being met for cases to receive responses in less than three days (accounting for weekends) and often cases are solved in one response with a friendly and informative approach. Additionally, some in-person sessions have been delivered when requested by users, this allowed us to deliver focused support tailored to the user's specific needs.

Research Coding Club continues its outreach for anyone who works with research software. Offering both informal drop-in style clinics, which not only invite participants to problem solve each other's work but also just a friendly chat, and also structured seminars where short talks of one hour or so on interesting topics are delivered by anyone within the University. Some more recent topics include version control through Git and parallel problem solving which often finish off with some lively discussion within the group.

MATLAB is a popular application in use on a range of University systems, but it can have a steep learning curve for some users when running it remotely on Viking as they are unfamiliar with the additional layers. Listening to user feedback, a new solution to streamlining this use case has recently been introduced, gaining recognition of its unique approach from the wider MATLAB community.

Finally, various user surveys have been conducted throughout the year focussing on their use of Viking to help the team better structure the upcoming Viking 2 project. Focusing on the users feedback here allows the upcoming Viking 2 to deliver on their use cases and overall needs, drawing from their day to day experiences with the current Viking HPC.

Regional and National Links

The N8 Centre of Excellence in Computationally Intensive Research (N8CIR) was awarded £3.1M in 2019 from EPSRC, supplemented by £5.3M from N8 member institutions, to establish a new research computing facility in the North of England. **Bede** offers access to a large GPGPU cluster using novel technology. You can find more information about this facility on the N8 CIR website. The University of York is one of the biggest users of the Bede facility. We have also contributed to a number of case studies with places for more in the future. The Director of N8 CIR is also a member of the University of York.

The ARCHER2 Service is a world class advanced computing resource for UK researchers. ARCHER2 is provided by UKRI, EPCC, HPE Cray and the University of Edinburgh. The new national facility, having received £79M of government funding in early 2019, went live in July 2021. There were delays due to the impact of Covid but ARCHER2 passed the benchmarking and user testing period and is now available for general use. ARCHER2 has the potential to benefit more computationally experienced University researchers, with Viking acting as a stepping stone on which to develop necessary skills. More information about the new ARCHER2 system can be found on the ARCHER2 website.

Plans for the Future

Viking entered its final year of operation in 2023. Viking has proven to be an important resource for research and teaching. Going forward we intend to build on this success with Viking2. Viking2 will follow in a similar vein to Viking except with improvements to the hardware technologies used, more cores, GPUs and some backup storage. The Research IT team also intends to improve the sustainability of the Viking service - the University aims to achieve net zero by 2030, therefore Viking2 has been designed with this in mind.

Viking2 will be housed in a carbon negative facility, in the nordic regions where greener and more cost effective power is available. The EcoDataCenter in Falun, Sweden, achieves this by using sustainable building materials and the heat produced by computer hardware to dry wood pellets that are used to provide heating to businesses and homes.

The Viking2 procurement has now been completed with an aim to go live September 2023.

In addition to Viking2 we have other initiatives in progress for Research IT which include:

- Trusted Research Environment for sensitive data (Azure cloud)
- Azure Virtual Desktop for research. To assist non Linux users who do not need a large HPC facility for their research.
- Two Research Software Engineer sustainability posts to improve code efficiency and sustainability.

Appendix

Publications & Outputs

Abdul-Wahab, Dina, Ezio Iacocca, Richard F. L. Evans, Amilcar Bedoya-Pinto, Stuart Parkin, Kostya S. Novoselov, and Elton J. G. Santos. 2021. "Domain Wall Dynamics in Two-Dimensional van Der Waals Ferromagnets." *Applied Physics Reviews* 8 (4): 041411. https://doi.org/10.1063/5.0062541.

Agatz, Annika, Roman Ashauer, Paul Sweeney, and Colin D. Brown. 2020. "A Knowledge-Based Approach to Designing Control Strategies for Agricultural Pests." *Agricultural Systems* 183 (August): 102865. https://doi.org/10.1016/j.agsy.2020.102865.

Alexander, Becky, Tomás Sherwen, Christopher D. Holmes, Jenny A. Fisher, Qianjie Chen, Mat J. Evans, and Prasad Kasibhatla. 2020. "Global Inorganic Nitrate Production Mechanisms: Comparison of a Global Model with Nitrate Isotope Observations." *Atmospheric Chemistry and Physics* 20 (6): 3859–77. https://doi.org/10.5194/acp-20-3859-2020.

Alharbi, Emad, Paul S. Bond, Radu Calinescu, and Kevin Cowtan. 2019. "Comparison of Automated Crystallographic Model-Building Pipelines." *Acta Crystallographica Section D Structural Biology* 75 (12): 1119–28. https://doi.org/10.1107/s2059798319014918.

Alharbi, Emad, Radu Calinescu, and Kevin Cowtan. 2020. "Pairwise Running of Automated Crystallographic Model-Building Pipelines." *Acta Crystallographica Section D Structural Biology* 76 (9): 814–23. https://doi.org/10.1107/s2059798320010542.

———. 2023. "*Buccaneer* Model Building with Neural Network Fragment Selection." *Acta Crystallographica Section D Structural Biology* 79 (4): 326–38. https://doi.org/10.1107/s205979832300181x.

Alrashdi, Reem, and Simon O'Keefe. 2019. "Robust Domain Adaptation Approach for Tweet Classification for Crisis Response." In *Learning and Analytics in Intelligent Systems*, 124–34. Springer International Publishing. https://doi.org/10.1007/978-3-030-36778-7_14.

Alrashdi, Reem, and Simon OKeefe. 2020. "Automatic Labeling of Tweets for Crisis Response Using Distant Supervision." In *Companion Proceedings of the Web Conference 2020*. ACM. https://doi.org/10.1145/3366424.3383757.

Augustin, Mathias, Sarah Jenkins, Richard F. L. Evans, Kostya S. Novoselov, and Elton J. G. Santos. 2021. "Properties and Dynamics of Meron Topological Spin Textures in the Two-Dimensional Magnet CrCl3." *Nature Communications* 12 (1). https://doi.org/10.1038/s41467-020-20497-2.

Backer, Adam S., Graeme A. King, Andreas S. Biebricher, Jack W. Shepherd, Agnes Noy, Mark C. Leake, Iddo Heller, Gijs J. L. Wuite, and Erwin J. G. Peterman. 2021. "Elucidating the Role of Topological Constraint on the Structure of Overstretched DNA Using Fluorescence Polarization Microscopy." *The Journal of Physical Chemistry B* 125 (30): 8351–61. https://doi.org/10.1021/acs.jpcb.1c02708.

Badia, Alba, Claire E. Reeves, Alex R. Baker, Alfonso Saiz-Lopez, Rainer Volkamer, Theodore K. Koenig, Eric C. Apel, et al. 2019. "Importance of Reactive Halogens in the Tropical Marine Atmosphere: A Regional Modelling Study Using WRF-Chem." *Atmospheric Chemistry and Physics* 19 (5): 3161–89. https://doi.org/10.5194/acp-19-3161-2019.

Baker, Amy, Robert Craighead, Emma Jarvis, Harriett Stenton, Athanasios Angeloudis, Lucas Mackie, Alexandros Avdis, Matthew Piggott, and Jon Hill. 2020. "Modelling the Ecological Impacts of Tidal Energy Barrages." *Earth ArXiv*. https://doi.org/10.31223/osf.io/vapmu.

Baker, N., C. M. C. Catta-Preta, R. Neish, J. Sadlova, B. Powell, E. V. C. Alves-Ferreira, V. Geoghegan, et al. 2021. "Systematic Functional Analysis of Leishmania Protein Kinases Identifies Regulators of Differentiation or Survival." *Nature Communications* 12 (1). https://doi.org/10.1038/s41467-021-21360-8.

Bateman, Mark D., Tim C. Kinnaird, Jon Hill, Robert A. Ashurst, Jenna Mohan, Rebecca B. I. Bateman, and Ruth Robinson. 2021. "Detailing the Impact of the Storegga Tsunami at Montrose, Scotland." *Boreas* 50 (4): 1059–78. https://doi.org/10.1111/bor.12532.

Bayfield, Oliver W., Andrey N. Shkoporov, Natalya Yutin, Ekaterina V. Khokhlova, Jake L. R. Smith, Dorothy E. D. P. Hawkins, Eugene V. Koonin, Colin Hill, and Alfred A. Antson. 2023. "Structural Atlas of a Human Gut Crassvirus." *Nature* 617 (7960): 409–16. https://doi.org/10.1038/s41586-023-06019-2.

Berenbeim, Jacob A., Natalie G. K. Wong, Martin C. R. Cockett, Giel Berden, Jos Oomens, Anouk M. Rijs, and Caroline E. H. Dessent. 2020. "Sodium Cationization Can Disrupt the Intramolecular Hydrogen Bond That Mediates the Sunscreen Activity of Oxybenzone." *Physical Chemistry Chemical Physics* 22 (35): 19522–31. https://doi.org/10.1039/d0cp03152f.

Binh, Nguyen Thanh, Sarah Jenkins, Sergiu Ruta, Richard F. L. Evans, and Roy W. Chantrell. 2023. "Higher-Order Magnetic Anisotropy in Soft-Hard Magnetic Materials." *Physical Review B* 107 (4). https://doi.org/10.1103/physrevb.107.l041410.

Binh, Nguyen Thanh, Sergiu Ruta, Ondrej Hovorka, Richard F. L. Evans, and Roy W. Chantrell. 2022. "Influence of Finite-Size Effects on the Curie Temperature of ***L*1-FePt**." *Physical Review B* 106 (5). https://doi.org/10.1103/physrevb.106.054421.

Blanchette, Robert A., Deborah Tear Haynes, Benjamin W. Held, Jonas Niemann, and Nathan Wales. 2021. "Fungal Mycelial Mats Used as Textile by Indigenous People of North America." *Mycologia* 113 (2): 261–67. https://doi.org/10.1080/00275514.2020.1858686.

Bond, Paul S., Keith S. Wilson, and Kevin D. Cowtan. 2020. "Predicting Protein Model Correctness in *Coot* Using Machine Learning." *Acta Crystallographica Section D Structural Biology* 76 (8): 713–23. https://doi.org/10.1107/s2059798320009080.

Brito, Francisco M. O., Linhu Li, João M. V. P. Lopes, and Eduardo V. Castro. 2022. "Edge Magnetism in Transition Metal Dichalcogenide Nanoribbons: Mean Field Theory and Determinant Quantum Monte Carlo." *Physical Review B* 105 (19). https://doi.org/10.1103/physrevb.105.195130.

Buchanan, Edgar, Léni K. Le Goff, Wei Li, Emma Hart, Agoston E. Eiben, Matteo De Carlo, Alan F. Winfield, et al. 2020. "Bootstrapping Artificial Evolution to Design Robots for Autonomous Fabrication." *Robotics* 9 (4): 106. https://doi.org/10.3390/robotics9040106.

Buenabad-Chavez, Jorge, Emma Rand, and James Chong. 2022a. "Cloud-SPAN Create Your Own AWS Instance: Overview." Zenodo. https://doi.org/10.5281/ZENODO.6782969.

———. 2022b. "Cloud-SPAN/Create-Aws-Instance-1-Open-Account: Cloud-SPAN Create Your Own AWS Instance Session 1: Open Your Account." Zenodo. https://doi.org/10.5281/ZENODO.6783169.

———. 2022c. "Cloud-SPAN/Create-Aws-Instance-2-Manage-Instance: Cloud-SPAN Create Your Own AWS Instance Session 2: Manage Your Instance." Zenodo. https://doi.org/10.5281/ZENODO.6783171.

———. 2022d. "Cloud-SPAN/Create-Aws-Instance-3-Costs-Explained: Cloud-SPAN Create Your Own AWS Instance Session 3: Costs Explained." Zenodo. https://doi.org/10.5281/ZENODO.6783175.

Burden, Thomas J., Kathryn P. R. Fernandez, Mary Kagoro, Jonathan B. Eastwood, Theo F. N. Tanner, Adrian C. Whitwood, Ian P. Clark, et al. 2023. "Coumarin c-h Functionalization by Mn(i) Carbonyls: Mechanistic Insight by Ultra-Fast IR Spectroscopic Analysis." *Chemistry A European Journal* 29 (25). https://doi.org/10.1002/chem.202203038.

Cansdale, Annabel, and Sarah Forrester. 2022a. "Cloud-SPAN Metagenomics Course Session 1: QC & Assembly." Zenodo. https://doi.org/10.5281/ZENODO.7504047.

———. 2022b. "Cloud-SPAN Metagenomics Course Session 2: Polishing." Zenodo. https://doi.org/10.5281/ZENODO.7506737.

———. 2022c. "Cloud-SPAN Metagenomics Course Session 3: Taxonomic Annotation." Zenodo. https://doi.org/10.5281/ZENODO.7506983.

———. 2022d. "Cloud-SPAN Metagenomics Course Session 4: Binning + Functional Annotation." Zenodo. https://doi.org/10.5281/ZENODO.7506988.

Carey, John J., and Keith P. McKenna. 2018. "Does Polaronic Self-Trapping Occur at Anatase TiO Surfaces?" *The Journal of Physical Chemistry C* 122 (48): 27540–53. https://doi.org/10.1021/acs.jpcc.8b09437.

———. 2019. "Screening Doping Strategies to Mitigate Electron Trapping at Anatase TiO Surfaces." *The Journal of Physical Chemistry C* 123 (36): 22358–67. https://doi.org/10.1021/acs.jpcc.9b05840.

Carey, John J., James A. Quirk, and Keith P. McKenna. 2021. "Hole Polaron Migration in Bulk Phases of TiO Using Hybrid Density Functional Theory." *The Journal of Physical Chemistry C* 125 (22): 12441–50. https://doi.org/10.1021/acs.jpcc.1c03136.

Carpenter, Lucy J., Rosie J. Chance, Tomás Sherwen, Thomas J. Adams, Stephen M. Ball, Mat J. Evans, Helmke Hepach, et al. 2021. "Marine Iodine Emissions in a Changing World." *Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences* 477 (2247): 20200824. https://doi.org/10.1098/rspa.2020.0824.

Catania, Theresa, Yi Li, Thilo Winzer, David Harvey, Fergus Meade, Anna Caridi, Andrew Leech, et al. 2022. "A Functionally Conserved STORR Gene Fusion in Papaver Species That Diverged 16.8 Million Years Ago." *Nature Communications* 13 (1). https://doi.org/10.1038/s41467-022-30856-w.

Ceballos, Alejandro, Akshay Pattabi, Amal El-Ghazaly, Sergiu Ruta, Christian P. Simon, Richard F. L. Evans, Thomas Ostler, et al. 2021. "Role of Element-Specific Damping in Ultrafast, Helicity-Independent, All-Optical Switching Dynamics in Amorphous (Gd,tb)co Thin Films." *Physical Review B* 103 (2). https://doi.org/10.1103/physrevb.103.024438.

Chance, Rosie J., Liselotte Tinel, Tomás Sherwen, Alex R. Baker, Thomas Bell, John Brindle, Maria Lucia A. M. Campos, et al. 2019. "Global Sea-Surface Iodide Observations, 19672018." *Scientific Data* 6 (1). https://doi.org/10.1038/s41597-019-0288-y.

Coakley, James, Andrew Higginbotham, David McGonegle, Jan Ilavsky, Thomas D. Swinburne, Justin S. Wark, Khandaker M. Rahman, et al. 2020. "Femtosecond Quantification of Void Evolution During Rapid Material Failure." *Science Advances* 6 (51). https://doi.org/10.1126/sciadv.abb4434.

Colville, Jonathan F., Colin M. Beale, Félix Forest, Res Altwegg, Brian Huntley, and Richard M. Cowling. 2020. "Plant Richness, Turnover, and Evolutionary Diversity Track Gradients of Stability and Ecological Opportunity in a Megadiversity Center." *Proceedings of the National Academy of Sciences* 117 (33): 20027–37. https://doi.org/10.1073/pnas.1915646117.

Community, The International GEOS-Chem User. 2019. "Geoschem/Geos-Chem: GEOS-Chem 12.6.0." Zenodo. https://doi.org/10.5281/ZENODO.3507501.

———. 2020. "Geoschem/Geos-Chem: GEOS-Chem 12.7.0." Zenodo. https://doi.org/10.5281/ZENODO.3634864.

Connor, Jack P., Steven D. Quinn, and Charley Schaefer. 2022. "Sticker-and-Spacer Model for Amyloid Beta Condensation and Fibrillation." *Frontiers in Molecular Neuroscience* 15 (October). https://doi.org/10.3389/fnmol.2022.962526.

Dale, Matthew, Julian F. Miller, Susan Stepney, and Martin A. Trefzer. 2019. "A Substrate-Independent Framework to Characterize Reservoir Computers." *Proceedings of the Royal Society A: Mathematical, Physical and Engineering Sciences* 475 (2226): 20180723. https://doi.org/10.1098/rspa.2018.0723.

Dale, Matthew, Simon O'Keefe, Angelika Sebald, Susan Stepney, and Martin A. Trefzer. 2020. "Reservoir Computing Quality: Connectivity and Topology." *Natural Computing* 20 (2): 205–16. https://doi.org/10.1007/s11047-020-09823-1.

———. 2021. "Computing with Magnetic Thin Films: Using Film Geometry to Improve Dynamics." In *Unconventional Computation and Natural Computation*, 19–34. Springer International Publishing. https://doi.org/10.1007/978-3-030-87993-8_2.

Darby, John F., Amelia K. Gilio, Beatriz Piniello, Christian Roth, Elena Blagova, Roderick E. Hubbard, Carme Rovira, Gideon J. Davies, and Liang Wu. 2020. "Substrate Engagement and Catalytic Mechanisms of n-Acetylglucosaminyltransferase v." *ACS Catalysis* 10 (15): 8590–96. https://doi.org/10.1021/acscatal.0c02222.

Davesne, D., A. Pastore, and J. Navarro. 2021. “Linear Response Theory with Finite-Range Interactions.” *Progress in Particle and Nuclear Physics* 120 (September): 103870. https://doi.org/10.1016/j.ppnp.2021.103870.

Davey, John W, Carolina M C Catta-Preta, Sally James, Sarah Forrester, Maria Cristina M Motta, Peter D Ashton, and Jeremy C Mottram. 2020. “Chromosomal Assembly of the Nuclear Genome of the Endosymbiont-Bearing Trypanosomatid *Angomonas Deanei*.” Edited by B Andrews. *G3 GenesGenomesGenetics* 11 (1): 1–7. https://doi.org/10.1093/g3journal/jkaa018.

Davies, R, D Dickinson, and H Wilson. 2022. “Kinetic Ballooning Modes as a Constraint on Plasma Triangularity in Commercial Spherical Tokamaks.” *Plasma Physics and Controlled Fusion* 64 (10): 105001. https://doi.org/10.1088/1361-6587/ac8615.

Daza-Cajigal, Vanessa, Adriana S. Albuquerque, Joanna Pearson, Jennifer Hinley, Andrew S. Mason, Jens Stahlschmidt, Adrian J. Thrasher, Vibhash Mishra, Jennifer Southgate, and Siobhan O. Burns. 2019. “Loss of Janus Associated Kinase 1 Alters Urothelial Cell Function and Facilitates the Development of Bladder Cancer.” *Frontiers in Immunology* 10 (September). https://doi.org/10.3389/fimmu.2019.02065.

Debgupta, Joyashish, Leonardo Lari, Mark Isaacs, John Carey, Keith P. McKenna, Vlado K. Lazarov, Victor Chechik, and Richard E. Douthwaite. 2022. “Predictive Removal of Interfacial Defect-Induced Trap States Between Titanium Dioxide Nanoparticles via Sub-Monolayer Zirconium Coating.” *The Journal of Physical Chemistry C* 127 (1): 660–71. https://doi.org/10.1021/acs.jpcc.2c06927.

Delius, G. W., B. J. Powell, M. A. Bees, G. W. A. Constable, N. J. MacKay, and J. W. Pitchford. 2020. “More Prevalent, Less Deadly? Bayesian Inference of the COVID19 Infection Fatality Ratio from Mortality Data.” *medRxiv*. https://doi.org/10.1101/2020.04.19.20071811.

Dobaczewski, J, P Bączyk, P Becker, M Bender, K Bennaceur, J Bonnard, Y Gao, et al. 2021. “Solution of Universal Nonrelativistic Nuclear DFT Equations in the Cartesian Deformed Harmonic-Oscillator Basis. (IX) HFODD (V3.06h): A New Version of the Program.” *Journal of Physics G: Nuclear and Particle Physics* 48 (10): 102001. https://doi.org/10.1088/1361-6471/ac0a82.

Doeveren, Thomas, Jose A. Nakauma-Gonzalez, Andrew S. Mason, Geert J. L. H. Leenders, Tahlita C. M. Zuiverloon, Ellen C. Zwarthoff, Isabelle C. Meijssen, et al. 2020. “The Clonal Relation of Primary Upper Urinary Tract Urothelial Carcinoma and Paired Urothelial Carcinoma of the Bladder.” *International Journal of Cancer* 148 (4): 981–87. https://doi.org/10.1002/ijc.33327.

Dubanevics, Igors, and Tom C. B. McLeish. 2021. “Computational Analysis of Dynamic Allostery and Control in the SARS-CoV-2 Main Protease.” *Journal of The Royal Society Interface* 18 (174): 20200591. https://doi.org/10.1098/rsif.2020.0591.

———. 2022. “Optimising Elastic Network Models for Protein Dynamics and Allostery: Spatial and Modal Cut-Offs and Backbone Stiffness.” *Journal of Molecular Biology* 434 (17): 167696. https://doi.org/10.1016/j.jmb.2022.167696.

Dudson, B D, W A Gracias, R Jorge, A H Nielsen, J M B Olsen, P Ricci, C Silva, et al. 2021. “Edge Turbulence in ISTTOK: A Multi-Code Fluid Validation.” *Plasma Physics and Controlled Fusion* 63 (5): 055013. https://doi.org/10.1088/1361-6587/abe21d.

Dulias, Katharina, M. George B. Foody, Pierre Justeau, Marina Silva, Rui Martiniano, Gonzalo Oteo-García, Alessandro Fichera, et al. 2022. “Ancient DNA at the Edge of the World: Continental Immigration and the Persistence of Neolithic Male Lineages in Bronze Age Orkney.” *Proceedings of the National Academy of Sciences* 119 (8). https://doi.org/10.1073/pnas.2108001119.

Eastwood, Jonathan B., L. Anders Hammarback, Thomas J. Burden, Ian P. Clark, Michael Towrie, Alan Robinson, Ian J. S. Fairlamb, and Jason M. Lynam. 2023. “Understanding Precatalyst Activation and Speciation in Manganese-Catalyzed ch Bond Functionalization Reactions.” *Organometallics*, April. https://doi.org/10.1021/acs.organomet.3c00004.

Eftaxias, Giorgos, Mirjam Weilenmann, and Roger Colbeck. 2023. “Advantages of Multicopy Nonlocality Distillation and Its Application to Minimizing Communication Complexity.” *Physical Review Letters* 130 (10). https://doi.org/10.1103/physrevlett.130.100201.

Elser, Michael J., Ellie Neige, Thomas Berger, Mario Chiesa, Elio Giamello, Keith McKenna, Thomas Risse, and Oliver Diwald. 2023. “On the Importance of Nanoparticle Necks and Carbon Impurities for Charge Trapping in TiO.” *The Journal of Physical Chemistry C* 127 (18): 8778–87. https://doi.org/10.1021/acs.jpcc.3c00430.

Evans, Richard F. L., Levente Rózsa, Sarah Jenkins, and Unai Atxitia. 2020. “Temperature Scaling of Two-Ion Anisotropy in Pure and Mixed Anisotropy Systems.” *Physical Review B* 102 (2). https://doi.org/10.1103/physrevb.102.020412.

Fagan, Brennen T., Marina I. Knight, Niall J. MacKay, and A. Jamie Wood. 2020. “Change Point Analysis of Historical Battle Deaths.” *Journal of the Royal Statistical Society Series A: Statistics in Society* 183 (3): 909–33. https://doi.org/10.1111/rssa.12578.

Fagan, Brennen T., Niall J. MacKay, Dmitri O. Pushkin, and A. Jamie Wood. 2021. “Stochastic Gel-Shatter Cycles in Coalescence-Fragmentation Models.” *Europhysics Letters* 133 (5): 53001. https://doi.org/10.1209/0295-5075/133/53001.

Fewster, Christopher J., Eli Hawkins, Christoph Minz, and Kasia Rejzner. 2021. “Local Structure of Sprinkled Causal Sets.” *Physical Review D* 103 (8). https://doi.org/10.1103/physrevd.103.086020.

Forrester, Sarah, and Annabel Cansdale. 2022. “Cloud-SPAN Metagenomics Course: Overview.” Zenodo. https://doi.org/10.5281/ZENODO.7505859.

Forster, Piers M., Harriet I. Forster, Mat J. Evans, Matthew J. Gidden, Chris D. Jones, Christoph A. Keller, Robin D. Lamboll, et al. 2020. “Current and Future Global Climate Impacts Resulting from COVID-19.” *Nature Climate Change* 10 (10): 913–19. https://doi.org/10.1038/s41558-020-0883-0.

Furlan, Chris, Nipa Chongdar, Pooja Gupta, Wolfgang Lubitz, Hideaki Ogata, James N Blaza, and James A Birrell. 2022. “Structural Insight on the Mechanism of an Electron-Bifurcating [FeFe] Hydrogenase.” *eLife* 11 (August). https://doi.org/10.7554/elife.79361.

Grace, Cooper Alastair, Kátia Silene Sousa Carvalho, Mayara Ingrid Sousa Lima, Vladimir Costa Silva, João Luís Reis-Cunha, Matthew J. Brune, Sarah Forrester, et al. 2022. “Parasite Genotype Is a Major Predictor of Mortality from Visceral Leishmaniasis.” Edited by Louis M. Weiss. *mBio* 13 (6). https://doi.org/10.1128/mbio.02068-22.

Grace, Cooper Alastair, Sarah Forrester, Vladimir Costa Silva, Kátia Silene Sousa Carvalho, Hannah Kilford, Yen Peng Chew, Sally James, et al. 2021. “Candidates for Balancing Selection in *Leishmania Donovani* Complex Parasites.” Edited by Bonnie Fraser. *Genome Biology and Evolution* 13 (12). https://doi.org/10.1093/gbe/evab265.

Greaves, Richard B., Sabine Dietmann, Austin Smith, Susan Stepney, and Julianne D. Halley. 2017. “A Conceptual and Computational Framework for Modelling and Understanding the Non-Equilibrium Gene Regulatory Networks of Mouse Embryonic Stem Cells.” Edited by Scott Markel. *PLOS Computational Biology* 13 (9): e1005713. https://doi.org/10.1371/journal.pcbi.1005713.

Groote, R. P. de, J. Moreno, J. Dobaczewski, Á. Koszorús, I. Moore, M. Reponen, B. K. Sahoo, and C. Yuan. 2022. “Precision Measurement of the Magnetic Octupole Moment in 45Sc as a Test for State-of-the-Art Atomic- and Nuclear-Structure Theory.” *Physics Letters B* 827 (April): 136930. https://doi.org/10.1016/j.physletb.2022.136930.

Hall, Rebecca J., Stephen Thorpe, Gavin H. Thomas, and A. Jamie Wood. 2019. “Simulating the Evolutionary Trajectories of Metabolic Pathways for Insect Symbionts in the *Sodalis* Genus,” October. https://doi.org/10.1101/819946.

Hammarback, L. Anders, Jonathan B. Eastwood, Thomas J. Burden, Callum J. Pearce, Ian P. Clark, Michael Towrie, Alan Robinson, Ian J. S. Fairlamb, and Jason M. Lynam. 2022. “A

Comprehensive Understanding of Carboncarbon Bond Formation by Alkyne Migratory Insertion into Manganacycles.” *Chemical Science* 13 (34): 9902–13. https://doi.org/10.1039/d2sc02562k.

Hao, Ning-Jing, Rui-Xue Ding, Chuan-Jia Tong, and Keith P. McKenna. 2023. “Heterogeneity of Grain Boundary Properties in CuZnSnS: A First-Principles Study.” *Journal of Applied Physics* 133 (14): 145002. https://doi.org/10.1063/5.0147435.

Harper, Andrea L., Zhesi He, Swen Langer, Lenka Havlickova, Lihong Wang, Alison Fellgett, Vibha Gupta, Akshay Kumar Pradhan, and Ian Bancroft. 2020. “Validation of an Associative Transcriptomics Platform in the Polyploid Crop Species*brassica Juncea*by Dissection of the Genetic Architecture of Agronomic and Quality Traits.” *The Plant Journal* 103 (5): 1885–93. https://doi.org/10.1111/tpj.14876.

He, Zhesi, Ruiqin Ji, Lenka Havlickova, Lihong Wang, Yi Li, Huey Tyng Lee, Jiaming Song, et al. 2021. “Genome Structural Evolution in Brassica Crops.” *Nature Plants* 7 (6): 757–65. https://doi.org/10.1038/s41477-021-00928-8.

Hennius, Andreas, John Ljungkvist, Steven P. Ashby, Richard Hagan, Samantha Presslee, Tom Christensen, Rudolf Gustavsson, Jüri Peets, and Liina Maldre. 2022. “Late Iron Age Whaling in Scandinavia.” *Journal of Maritime Archaeology* 18 (1): 1–22. https://doi.org/10.1007/s11457-022-09349-w.

Hill, Jon. 2019. “Resolving the Tsunami Wave: Interpreting Palaeotsunami Deposits by Integrating Numerical Modelling and Sedimentology.” figshare. https://doi.org/10.6084/M9.FIGSHARE.9771917.V3.

Hill, Jon, Alexandros Avdis, Geoff Bailey, and Kurt Lambeck. 2022. “Sea-Level Change, Palaeotidal Modelling and Hominin Dispersals: The Case of the Southern Red Sea.” *Quaternary Science Reviews* 293 (October): 107719. https://doi.org/10.1016/j.quascirev.2022.107719.

Ho, Hon Eong, Angela Pagano, James A. Rossi-Ashton, James R. Donald, Ryan G. Epton, Jonathan C. Churchill, Michael J. James, Peter OBrien, Richard J. K. Taylor, and William P. Unsworth. 2020. “Visible-Light-Induced Intramolecular Charge Transfer in the Radical Spirocyclisation of Indole-Tethered Ynones.” *Chemical Science* 11 (5): 1353–60. https://doi.org/10.1039/c9sc05311e.

Holland, L. A., A. Köhn-Seemann, and R. G. L. Vann. 2023. “Parametric Dependence of Microwave Beam Broadening by Plasma Density Turbulence.” *Nuclear Fusion* 63 (5): 056013. https://doi.org/10.1088/1741-4326/acc25e.

Hung, Shih-Hsuan. 2019. “First Principles Investigation of the Structure and Properties of Au Nanoparticles Supported on ZnO.” [Data set] University of York. https://doi.org/10.15124/E4ABC92F-2363-4B8E-B5CA-F77C0E9E5967.

Hung, Shih-Hsuan, and Keith McKenna. 2019. “First-Principles Investigation of the Structure and Properties of Au Nanoparticles Supported on ZnO.” *The Journal of Physical Chemistry C* 123 (34): 21185–94. https://doi.org/10.1021/acs.jpcc.9b02639.

Iacocca, E., T.-M. Liu, A. H. Reid, Z. Fu, S. Ruta, P. W. Granitzka, E. Jal, et al. 2019. “Spin-Current-Mediated Rapid Magnon Localisation and Coalescence After Ultrafast Optical Pumping of Ferrimagnetic Alloys.” *Nature Communications* 10 (1). https://doi.org/10.1038/s41467-019-09577-0.

Inamdar, S., L. Tinel, R. Chance, L. J. Carpenter, P. Sabu, R. Chacko, S. C. Tripathy, et al. 2020. “Estimation of Reactive Inorganic Iodine Fluxes in the Indian and Southern Ocean Marine Boundary Layer.” *Atmospheric Chemistry and Physics* 20 (20): 12093–114. https://doi.org/10.5194/acp-20-12093-2020.

Inamdar, Swaleha, Liselotte Tinel, Rosie Chance, Lucy J. Carpenter, Prabhakaran Sabu, Racheal Chacko, Sarat C. Tripathy, et al. 2020. “Estimation of Reactive Inorganic Iodine Fluxes in the Indian and Southern Ocean Marine Boundary Layer.” *Atmospheric Chemistry and Physics* 20 (20): 12093–114. https://doi.org/10.5194/acp-20-12093-2020.

Ingram, Claire, Jenn Chubb, Claire Boardman, and Marian Ursu. 2020. “Generating Real-World Impact from Academic Research.” In *Proceedings of the IEEE/ACM 42nd International*

Conference on Software Engineering Workshops. ACM. https://doi.org/10.1145/3387940.3391479.

Ivatt, Peter D., and Mathew J. Evans. 2020. “Improving the Prediction of an Atmospheric Chemistry Transport Model Using Gradient-Boosted Regression Trees.” *Atmospheric Chemistry and Physics* 20 (13): 8063–82. https://doi.org/10.5194/acp-20-8063-2020.

Ivatt, Peter D., Mathew J. Evans, and Alastair C. Lewis. 2022. “Suppression of Surface Ozone by an Aerosol-Inhibited Photochemical Ozone Regime.” *Nature Geoscience* 15 (7): 536–40. https://doi.org/10.1038/s41561-022-00972-9.

Jalal, Adam S. B., Ngat T. Tran, Clare E. Stevenson, Elliot W. Chan, Rebecca Lo, Xiao Tan, Agnes Noy, David M. Lawson, and Tung B. K. Le. 2020. “Diversification of DNA-Binding Specificity by Permissive and Specificity-Switching Mutations in the ParB/Noc Protein Family.” *Cell Reports* 32 (3): 107928. https://doi.org/10.1016/j.celrep.2020.107928.

Jenkins, Sarah, Roy W. Chantrell, Timothy J. Klemmer, and Richard F. L. Evans. 2019. “Magnetic Anisotropy of the Noncollinear Antiferromagnet **IrMn**.” *Physical Review B* 100 (22). https://doi.org/10.1103/physrevb.100.220405.

Jenkins, Sarah, and Richard F L Evans. 2020. “Scalable Space and Time Hierarchical Dipole- Dipole Interactions in the VAMPIRE Code.” https://doi.org/10.5281/ZENODO.3669966.

João, S M, J M Viana Parente Lopes, and Aires Ferreira. 2022. “High-Resolution Real-Space Evaluation of the Self-Energy Operator of Disordered Lattices: Gade Singularity, Spinorbit Effects and p-Wave Superconductivity.” *Journal of Physics: Materials* 5 (4): 045002. https://doi.org/10.1088/2515-7639/ac91f9.

João, Simão M., Miša Anelković, Lucian Covaci, Tatiana G. Rappoport, João M. V. P. Lopes, and Aires Ferreira. 2020. “KITE: High-Performance Accurate Modelling of Electronic Structure and Response Functions of Large Molecules, Disordered Crystals and Heterostructures.” *Royal Society Open Science* 7 (2): 191809. https://doi.org/10.1098/rsos.191809.

João, Simão Meneses, Miša Anđelković, Lucian Covaci, Tatiana Rappoport, João M. V. P. Lopes, and Aires Ferreira. 2019. “KITE: High-Performance Quantum Transport Software.” Zenodo. https://doi.org/10.5281/ZENODO.3245011.

Kampanos, Georgios, and Siamak F. Shahandashti. 2021. “Accept All: The Landscape of Cookie Banners in Greece and the UK.” In *ICT Systems Security and Privacy Protection*, 213–27. Springer International Publishing. https://doi.org/10.1007/978-3-030-78120-0_14.

Karaca, E., P. J. P. Byrne, P. J. Hasnip, and M. I. J. Probert. 2022. “Prediction of Phonon-Mediated Superconductivity in New Ti-Based MAX Phases.” *Scientific Reports* 12 (1). https://doi.org/10.1038/s41598-022-17539-8.

———. 2023. “CrAlN and the Search for the Highest Temperature Superconductor in the MAX Family.” *Scientific Reports* 13 (1). https://doi.org/10.1038/s41598-023-33517-0.

Karaca, E, P J P Byrne, P J Hasnip, H M Tütüncü, and M I J Probert. 2021. “Electronphonon Interaction and Superconductivity in Hexagonal Ternary Carbides Nb AC (A: Al, S, Ge, As and Sn).” *Electronic Structure* 3 (4): 045001. https://doi.org/10.1088/2516-1075/ac2c94.

Keller, Christoph A., Mathew J. Evans, K. Emma Knowland, Christa A. Hasenkopf, Sruti Modekurty, Robert A. Lucchesi, Tomohiro Oda, et al. 2021. “Global Impact of COVID-19 Restrictions on the Surface Concentrations of Nitrogen Dioxide and Ozone.” *Atmospheric Chemistry and Physics* 21 (5): 3555–92. https://doi.org/10.5194/acp-21-3555-2021.

Kelly, Jamie M., Peter D. Ivatt, Mathew J. Evans, Jesse H. Kroll, Amy I. H. Hrdina, Ishwar N. Kohale, Forest M. White, Bevin P. Engelward, and Noelle E. Selin. 2021. “Global Cancer Risk from Unregulated Polycyclic Aromatic Hydrocarbons.” *GeoHealth* 5 (9). https://doi.org/10.1029/2021gh000401.

Ker, De-Sheng, Huw T. Jenkins, Sandra J. Greive, and Alfred A. Antson. 2021. “CryoEM Structure of the Nipah Virus Nucleocapsid Assembly.” *PLOS Pathogens* 17 (7). https://doi.org/10.1371/journal.ppat.1009740.

Kerrigan, A., K. Pande, D. Pingstone, S. A. Cavill, M. Gajdardziska-Josifovska, K. P. McKenna, M. Weinert, and V. K. Lazarov. 2022. “Nano-Faceted Stabilization of Polar-Oxide Thin Films: The Case of MgO(111) and NiO(111) Surfaces.” *Applied Surface Science* 596 (September): 153490. https://doi.org/10.1016/j.apsusc.2022.153490.

Kristoffersen, Emil Laust, Matthew Burman, Agnes Noy, and Philipp Holliger. 2022. “Rolling Circle RNA Synthesis Catalyzed by RNA.” *eLife* 11 (February). https://doi.org/10.7554/elife.75186.

Kyle-Davidson, Cameron, Adrian Bors, and Karla Evans. 2019. “Predicting Visual Memory Schemas with Variational Autoencoders.” arXiv. https://doi.org/10.48550/ARXIV.1907.08514.

Lacy, Stuart E., Sharon L. Barrans, Philip A. Beer, Daniel Painter, Alexandra G. Smith, Eve Roman, Susanna L. Cooke, et al. 2020. “Targeted Sequencing in DLBCL, Molecular Subtypes, and Outcomes: A Haematological Malignancy Research Network Report.” *Blood* 135 (20): 1759–71. https://doi.org/10.1182/blood.2019003535.

Lall, Gurdeep Matharu, Maarten H. D. Larmuseau, Jon H. Wetton, Chiara Batini, Pille Hallast, Tunde I. Huszar, Daniel Zadik, et al. 2020. “Subdividing y-Chromosome Haplogroup R1a1 Reveals Norse Viking Dispersal Lineages in Britain.” *European Journal of Human Genetics* 29 (3): 512–23. https://doi.org/10.1038/s41431-020-00747-z.

Lawrence, Robert A., Scott J. Donaldson, and Matt I. J. Probert. 2023. “Magnetic Transition State Searching: Beyond the Static Ion Approximation.” *Magnetochemistry* 9 (2): 42. https://doi.org/10.3390/magnetochemistry9020042.

Leadbeater, Daniel R., Neil C. Bruce, and Thierry Tonon. 2022. “In Silico Identification of Bacterial Seaweed-Degrading Bioplastic Producers.” *Microbial Genomics* 8 (9). https://doi.org/10.1099/mgen.0.000866.

Lee, Katherine C., Jody M. Webster, Tristan Salles, Eleanor E. Mawson, and Jon Hill. 2022. “Tidal Dynamics Drive Ooid Formation in the Capricorn Channel Since the Last Glacial Maximum.” *Marine Geology* 454 (December): 106944. https://doi.org/10.1016/j.margeo.2022.106944.

Li, Xiaoguang, Laichuan Shen, Yuhao Bai, Junlin Wang, Xichao Zhang, Jing Xia, Motohiko Ezawa, et al. 2020. “Bimeron Clusters in Chiral Antiferromagnets.” *Npj Computational Materials* 6 (1). https://doi.org/10.1038/s41524-020-00435-y.

Liu, Wen-Zhao, Ming-Han Li, Sammy Ragy, Si-Ran Zhao, Bing Bai, Yang Liu, Peter J. Brown, et al. 2021. “Device-Independent Randomness Expansion Against Quantum Side Information.” *Nature Physics* 17 (4): 448–51. https://doi.org/10.1038/s41567-020-01147-2.

Luik, H, J Peets, J Ljungkvist, L Maldre, R Maldre, R Allmäe, M Muñoz-Rodríguez, K McGrath, C Speller, and S Ashby. 2020. “ANTLER COMBS FROM THE SALME SHIP BURIALS: FIND CONTEXT, ORIGIN, DATING AND MANUFACTURE.” *Estonian Journal of Archaeology* 24 (1): 3. https://doi.org/10.3176/arch.2020.1.01.

Mandle, Richard J., Nerea Sebastián, Josu Martinez-Perdiguero, and Alenka Mertelj. 2021. “On the Molecular Origins of the Ferroelectric Splay Nematic Phase.” *Nature Communications* 12 (1). https://doi.org/10.1038/s41467-021-25231-0.

Mason, Andrew S., Ashlee R. Lund, Paul M. Hocking, Janet E. Fulton, and David W. Burt. 2020. “Identification and Characterisation of Endogenous Avian Leukosis Virus Subgroup e (ALVE) Insertions in Chicken Whole Genome Sequencing Data.” *Mobile DNA* 11 (1). https://doi.org/10.1186/s13100-020-00216-w.

Mason, Andrew S., Claire L. Varley, Olivia M. Foody, Xiang Li, Katie Skinner, Dawn Walker, Tony R. Larson, Daisuke Wakamatsu, Simon C. Baker, and Jennifer Southgate. 2022. “LPCAT4 Knockdown Alters Barrier Integrity and Cellular Bioenergetics in Human Urothelium.” *International Journal of Molecular Sciences* 23 (19): 11871. https://doi.org/10.3390/ijms231911871.

Mawson, Eleanor E., Katherine C. Lee, and Jon Hill. 2022. “Sea Level Rise and the Great Barrier Reef: The Future Implications on Reef Tidal Dynamics.” *Journal of Geophysical Research: Oceans* 127 (8). https://doi.org/10.1029/2021jc017823.

McGregor, Nicholas G. S., Marta Artola, Alba Nin-Hill, Daniël Linzel, Mireille Haon, Jos Reijngoud, Arthur Ram, et al. 2020. “Rational Design of Mechanism-Based Inhibitors and Activity-Based Probes for the Identification of Retaining -L-Arabinofuranosidases.” *Journal of the American Chemical Society* 142 (10): 4648–62. https://doi.org/10.1021/jacs.9b11351.

McGregor, Nicholas G. S., Joan Coines, Valentina Borlandelli, Satoko Amaki, Marta Artola, Alba Nin-Hill, Daniël Linzel, et al. 2021. “Cysteine Nucleophiles in Glycosidase Catalysis: Application of a Covalent -L-Arabinofuranosidase Inhibitor.” *Angewandte Chemie International Edition* 60 (11): 5754–58. https://doi.org/10.1002/anie.202013920.

McKenna, Keith Patrick. 2019. “Forming-Free Grain Boundary Engineered Hafnium Oxide Resistive Random Access Memory Devices.” [Data set] University of York. https://doi.org/10.15124/DDD777F1-0E57-41DC-B843-449D7268E617.

———. 2021. “Self-Healing of Broken Bonds and Deep Gap States in SbSe and SbS.” *Advanced Electronic Materials* 7 (3): 2000908. https://doi.org/10.1002/aelm.202000908.

McNeill, Rhiannon, Andrew Mason, Mark Hodson, James Catto, and Jennifer Southgate. 2019. “Specificity of the Metallothionein-1 Response by Cadmium-Exposed Normal Human Urothelial Cells.” *International Journal of Molecular Sciences* 20 (6): 1344. https://doi.org/10.3390/ijms20061344.

Meek, Richard W., James N. Blaza, Jil A. Busmann, Matthew G. Alteen, David J. Vocadlo, and Gideon J. Davies. 2021. “Cryo-EM Structure Provides Insights into the Dimer Arrangement of the o-Linked -n-Acetylglucosamine Transferase OGT.” *Nature Communications* 12 (1). https://doi.org/10.1038/s41467-021-26796-6.

Meo, A, P Chureemart, R W Chantrell, and J Chureemart. 2022. “The Role of Interfacial Intermixing on HAMR Dynamics in Bilayer Media.” *Journal of Physics: Condensed Matter* 34 (46): 465801. https://doi.org/10.1088/1361-648x/ac916d.

Meo, Andrea, K. Pituso, P. Kampun, K. Pornpitakpong, A. Suntives, S. E. Rannala, R. W. Chantrell, P. Chureemart, and J. Chureemart. 2023. “Signal-to-Noise Ratio in Heat-Assisted-Recording Media: A Comparison Between Simulations and Experiments.” *Physical Review Applied* 19 (5). https://doi.org/10.1103/physrevapplied.19.054010.

Meo, A., W. Pantasri, W. Daeng-am, S. E. Rannala, S. I. Ruta, R. W. Chantrell, P. Chureemart, and J. Chureemart. 2020. “Magnetization Dynamics of Granular Heat-Assisted Magnetic Recording Media by Means of a Multiscale Model.” *Physical Review B* 102 (17). https://doi.org/10.1103/physrevb.102.174419.

Moreno, Roberto, Samuel Poyser, Daniel Meilak, Andrea Meo, Sarah Jenkins, Vlado K. Lazarov, Gonzalo Vallejo-Fernandez, Sara Majetich, and Richard F. L. Evans. 2020. “The Role of Faceting and Elongation on the Magnetic Anisotropy of Magnetite Fe3O4 Nanocrystals.” *Scientific Reports* 10 (1). https://doi.org/10.1038/s41598-020-58976-7.

Morozs, Nils, Paul D. Mitchell, and Roee Diamant. 2020. “Scalable Adaptive Networking for the Internet of Underwater Things.” *IEEE Internet of Things Journal* 7 (10): 10023–37. https://doi.org/10.1109/jiot.2020.2988621.

Mortimer, Luke, Marta P. Estarellas, Timothy P. Spiller, and Irene DAmico. 2021. “Evolutionary Computation for Adaptive Quantum Device Design.” *Advanced Quantum Technologies* 4 (8): 2100013. https://doi.org/10.1002/qute.202100013.

Muller, Bruce, and William Smith. 2020. “A Hierarchical Loss for Semantic Segmentation.” In *Proceedings of the 15th International Joint Conference on Computer Vision, Imaging and Computer Graphics Theory and Applications*. SCITEPRESS - Science; Technology Publications. https://doi.org/10.5220/0008946002600267.

Nascimento, Júlio César A. do, Adam Kerrigan, Philip J. Hasnip, and Vlado K. Lazarov. 2022. “Significant Improvement of the Seebeck Coefficient of Fe2VAl with Antisite Defects.” *Materials Today Communications* 31 (June): 103510. https://doi.org/10.1016/j.mtcomm.2022.103510.

Naydenov, G A, P J Hasnip, V K Lazarov, and M I J Probert. 2019. “Huge Power Factor in p-Type Half-Heusler Alloys NbFeSb and TaFeSb.” *Journal of Physics: Materials* 2 (3): 035002. https://doi.org/10.1088/2515-7639/ab16fb.

Nelson, Beth S., Daniel J. Bryant, Mohammed S. Alam, Roberto Sommariva, William J. Bloss, Mike J. Newland, Will S. Drysdale, et al. 2023. “Extreme Concentrations of Nitric Oxide Control Daytime Oxidation and Quench Nocturnal Oxidation Chemistry in Delhi During Highly Polluted Episodes.” *Environmental Science & Technology Letters* 10 (6): 520–27. https://doi.org/10.1021/acs.estlett.3c00171.

Newland, Mike J., Daniel J. Bryant, Rachel E. Dunmore, Thomas J. Bannan, W. Joe F. Acton, Ben Langford, James R. Hopkins, et al. 2021. “Low-NO Atmospheric Oxidation Pathways in a Polluted Megacity.” *Atmospheric Chemistry and Physics* 21 (3): 1613–25. https://doi.org/10.5194/acp-21-1613-2021.

Oddy, Meghan J., Daniel A. Kusza, Ryan G. Epton, Jason M. Lynam, William P. Unsworth, and Wade F. Petersen. 2022. “Visible-Light-Mediated Energy Transfer Enables the Synthesis of -Lactams via Intramolecular Hydrogen Atom Transfer.” *Angewandte Chemie International Edition* 61 (48). https://doi.org/10.1002/anie.202213086.

Padilha, A. C. M., and K. P. McKenna. 2019. “First Principles Investigation of YO-doped HfO.” *Journal of Applied Physics* 126 (8): 084105. https://doi.org/10.1063/1.5110669.

Padilha, Antonio Claudio Claudio. 2019. “First Principles Investigation of YO-doped HfO.” [Data set] University of York. https://doi.org/10.15124/6AF02367-39F8-4577-BCD9-4BD7BD0F9E77.

Parks, Brad, Ahmed Abdelgawad, Thomas Wong, Richard F. L. Evans, and Sara A. Majetich. 2020. “Magnetoresistance Dynamics in Superparamagnetic **Co-Fe-B** Nanodots.” *Physical Review Applied* 13 (1). https://doi.org/10.1103/physrevapplied.13.014063.

Petzold, Stefan, Alexander Zintler, Robert Eilhardt, Eszter Piros, Nico Kaiser, Sankaramangalam Ulhas Sharath, Tobias Vogel, et al. 2019. “Forming-Free Grain Boundary Engineered Hafnium Oxide Resistive Random Access Memory Devices.” *Advanced Electronic Materials* 5 (10): 1900484. https://doi.org/10.1002/aelm.201900484.

Pires, J.P. Santos, S.M. João, Aires Ferreira, B. Amorim, and J.M. Viana Parente Lopes. 2022. “Anomalous Transport Signatures in Weyl Semimetals with Point Defects.” *Physical Review Letters* 129 (19). https://doi.org/10.1103/physrevlett.129.196601.

Pound, R. J., D. P. Durcan, M. J. Evans, and L. J. Carpenter. 2023. “Comparing the Importance of Iodine and Isoprene on Tropospheric Photochemistry.” *Geophysical Research Letters* 50 (8). https://doi.org/10.1029/2022gl100997.

Pound, Ryan J., Tomás Sherwen, Detlev Helmig, Lucy J. Carpenter, and Mat J. Evans. 2020. “Influences of Oceanic Ozone Deposition on Tropospheric Photochemistry.” *Atmospheric Chemistry and Physics* 20 (7): 4227–39. https://doi.org/10.5194/acp-20-4227-2020.

Quirk, James A., Vlado K. Lazarov, and Keith P. McKenna. 2019. “Electronic Properties of 112 and 110 Twin Boundaries in Anatase TiO.” *Advanced Theory and Simulations* 2 (12): 1900157. https://doi.org/10.1002/adts.201900157.

Quirk, James A., and Keith P. McKenna. 2023. “Small-Polaron Mediated Recombination in Titanium Dioxide from First Principles.” *Physical Review Research* 5 (2). https://doi.org/10.1103/physrevresearch.5.023072.

Quirk, James A., Bin Miao, Bin Feng, Gowoon Kim, Hiromichi Ohta, Yuichi Ikuhara, and Keith P. McKenna. 2021. “Unveiling the Electronic Structure of Grain Boundaries in Anatase with Electron Microscopy and First-Principles Modeling.” *Nano Letters* 21 (21): 9217–23. https://doi.org/10.1021/acs.nanolett.1c03099.

Quirk, James. A., Vlado K. Lazarov, and Keith P. McKenna. 2020. “First-Principles Modeling of Oxygen-Deficient Anatase TiO Nanoparticles.” *The Journal of Physical Chemistry C* 124 (43): 23637–47. https://doi.org/10.1021/acs.jpcc.0c06052.

Rand, Emma, James Chong, Jorge Buenabad-Chavez, Annabel Cansdale, Sarah Forrester, and Evelyn Greeves. 2022a. "Cloud-SPAN/00genomics: Cloud-SPAN Genomics Course Overview." Zenodo. https://doi.org/10.5281/ZENODO.6564314.

———. 2022b. "Cloud-SPAN/01genomics: Cloud-SPAN Genomics Session 1: Project Management for Cloud Genomics." Zenodo. https://doi.org/10.5281/ZENODO.6575972.

———. 2022c. "Cloud-SPAN/02genomics: Cloud-SPAN Genomics Session 2: Data Preparation and Organisation." Zenodo. https://doi.org/10.5281/ZENODO.6576002.

———. 2022d. "Cloud-SPAN/03genomics: Cloud-SPAN Genomics Session 3: Assessing Read Quality Then Trimming and Filtering Reads." Zenodo. https://doi.org/10.5281/ZENODO.6576024.

———. 2022e. "Cloud-SPAN/04genomics: Cloud-SPAN Genomics Session 4: Finding Sequence Variants." Zenodo. https://doi.org/10.5281/ZENODO.6576038.

Rannala, S. E., A. Meo, S. Ruta, W. Pantasri, R. W. Chantrell, P. Chureemart, and J. Chureemart. 2022. "Models of Advanced Recording Systems: A Multi-Timescale Micromagnetic Code for Granular Thin Film Magnetic Recording Systems." *Computer Physics Communications* 279 (October): 108462. https://doi.org/10.1016/j.cpc.2022.108462.

Rigby, O. M., T. Richards-Hlabangana, Q. M. Ramasse, I. MacLaren, R. A. Lomas-Zapata, M. S. Rumsey, K. P. McKenna, and B. G. Mendis. 2022. "Structure and Electronic Properties of Domain Walls and Stacking Fault Defects in Prospective Photoferroic Materials Bournonite and Enargite." *Journal of Applied Physics* 132 (18): 185001. https://doi.org/10.1063/5.0095091.

Rogerio, Luana Aparecida, Talita Yuri Takahashi, Luria Cardoso, Nayore Tamie Takamiya, Enaldo Vieira de Melo, Amelia Ribeiro de Jesus, Fabricia Alvisi de Oliveira, et al. 2023. "Co-Infection of Leishmania Infantum and a Crithidia-Related Species in a Case of Refractory Relapsed Visceral Leishmaniasis with Non-Ulcerated Cutaneous Manifestation in Brazil." *International Journal of Infectious Diseases* 133 (August): 85–88. https://doi.org/10.1016/j.ijid.2023.05.012.

Rose, Nicholas C., Anaïs V. Sanchez, Eve F. Tipple, Jason M. Lynam, and Christopher D. Spicer. 2022. "Insight into *Ortho*-Boronoaldehyde Conjugation *via* a FRET-Based Reporter Assay." *Chemical Science* 13 (43): 12791–98. https://doi.org/10.1039/d2sc04574e.

Sassarini, P L, J Dobaczewski, J Bonnard, and R F Garcia Ruiz. 2022. "Nuclear DFT Analysis of Electromagnetic Moments in Odd Near Doubly Magic Nuclei." *Journal of Physics G: Nuclear and Particle Physics* 49 (11): 11LT01. https://doi.org/10.1088/1361-6471/ac900a.

Savchenko, Tatiana M., Michele Buzzi, Ludovic Howald, Sergiu Ruta, Jaianth Vijayakumar, Martin Timm, David Bracher, et al. 2020. "Single Femtosecond Laser Pulse Excitation of Individual Cobalt Nanoparticles." *Physical Review B* 102 (20). https://doi.org/10.1103/physrevb.102.205418.

Schaefer, Charley, Peter R. Laity, Chris Holland, and Tom C. B. McLeish. 2021. "Stretching of Bombyx Mori Silk Protein in Flow." *Molecules* 26 (6): 1663. https://doi.org/10.3390/molecules26061663.

Schaefer, Charley, and Tom C. B. McLeish. 2022. "Theoretical Rheo-Physics of Silk: Intermolecular Associations Reduce the Critical Specific Work for Flow-Induced Crystallization." *Journal of Rheology* 66 (3): 515–34. https://doi.org/10.1122/8.0000411.

Scheck, Marcus, Robert Chapman, Jacek Dobaczewski, Claude Ederer, Peter Ivanov, Guiseppe Lorusso, David O'Donnell, and Christian Schröder. 2023. "A New Avenue in the Search for CP Violation: Mössbauer Spectroscopy of Ac." *The European Physical Journal A* 59 (5). https://doi.org/10.1140/epja/s10050-023-01000-z.

Schwab, Thomas, Daniel Thomele, Korbinian Aicher, John W. C. Dunlop, Keith McKenna, and Oliver Diwald. 2021. "Rubbing Powders: Direct Spectroscopic Observation of Triboinduced Oxygen Radical Formation in MgO Nanocube Ensembles." *The Journal of Physical Chemistry C* 125 (40): 22239–48. https://doi.org/10.1021/acs.jpcc.1c05898.

Shahi, Farah, Sarah Forrester, Kelly Redeker, James P. J. Chong, and Gavin Barlow. 2022. "Case Report: The Effect of Intravenous and Oral Antibiotics on the Gut Microbiome and Breath Volatile Organic Compounds over One Year." *Wellcome Open Research* 7 (February): 50. https://doi.org/10.12688/wellcomeopenres.17450.1.

Sheikh, J A, J Dobaczewski, P Ring, L M Robledo, and C Yannouleas. 2021. “Symmetry Restoration in Mean-Field Approaches.” *Journal of Physics G: Nuclear and Particle Physics* 48 (12): 123001. https://doi.org/10.1088/1361-6471/ac288a.

Shepherd, Jack W, Robert J Greenall, Matt I J Probert, Agnes Noy, and Mark C Leake. 2020. “The Emergence of Sequence-Dependent Structural Motifs in Stretched, Torsionally Constrained DNA.” *Nucleic Acids Research* 48 (4): 1748–63. https://doi.org/10.1093/nar/gkz1227.

Sherwen, T., R. J. Chance, L. Tinel, D. Ellis, M. J. Evans, and L. J. Carpenter. 2019. “A Machine-Learning-Based Global Sea-Surface Iodide Distribution.” *Earth System Science Data* 11 (3): 1239–62. https://doi.org/10.5194/essd-11-1239-2019.

Sherwen, Tomás. 2019. “Tsherwen/Sparse2spatial: Sparse2spatial v.0.1.1 - Predictions for Iodide, CH2Br2 and CHBr3.” Zenodo. https://doi.org/10.5281/ZENODO.3369212.

Sherwen, Tomás, Rosie J. Chance, Liselotte Tinel, Daniel Ellis, Mat J. Evans, and Lucy J. Carpenter. 2019. “A Machine-Learning-Based Global Sea-Surface Iodide Distribution.” *Earth System Science Data* 11 (3): 1239–62. https://doi.org/10.5194/essd-11-1239-2019.

Smith, Kate R., Peter M. Edwards, Peter D. Ivatt, James D. Lee, Freya Squires, Chengliang Dai, Richard E. Peltier, Mat J. Evans, Yele Sun, and Alastair C. Lewis. 2019. “An Improved Low-Power Measurement of Ambient NO and O Combining Electrochemical Sensor Clusters and Machine Learning.” *Atmospheric Measurement Techniques* 12 (2): 1325–36. https://doi.org/10.5194/amt-12-1325-2019.

Squire, Imogen A. Z., Christopher A. Goult, Benedict C. Thompson, Elias Alexopoulos, Adrian C. Whitwood, Theo F. N. Tanner, and Luke A. Wilkinson. 2022. “Enhancing the Air Stability of Dimolybdenum Paddlewheel Complexes: Redox Tuning Through Fluorine Substituents.” *Inorganic Chemistry* 61 (48): 19144–55. https://doi.org/10.1021/acs.inorgchem.2c02746.

Strungaru, Mara, Matthew O. A. Ellis, Sergiu Ruta, Oksana Chubykalo-Fesenko, Richard F. L. Evans, and Roy W. Chantrell. 2021. “Spin-Lattice Dynamics Model with Angular Momentum Transfer for Canonical and Microcanonical Ensembles.” *Physical Review B* 103 (2). https://doi.org/10.1103/physrevb.103.024429.

Strungaru, Mara, Sergiu Ruta, Richard F. L. Evans, and Roy W. Chantrell. 2020. “Model of Magnetic Damping and Anisotropy at Elevated Temperatures: Application to Granular FePt Films.” *Physical Review Applied* 14 (1). https://doi.org/10.1103/physrevapplied.14.014077.

Strungaru, M., B. T. Nguyen, K. Yuanmae, R. F. L. Evans, R. W. Chantrell, P. Chureemart, and J. Chureemart. 2022. “HAMR Switching Dynamics and the Magnetic Recording Quadrilemma.” *Journal of Magnetism and Magnetic Materials* 564 (December): 170041. https://doi.org/10.1016/j.jmmm.2022.170041.

Tong, Chuan-Jia, Holly J. Edwards, Theodore D. C. Hobson, Ken Durose, Vinod R. Dhanak, Jonathan D. Major, and Keith P. McKenna. 2020. “Density Functional Theory and Experimental Determination of Band Gaps and Lattice Parameters in Kesterite CuZnSn(SSe).” *The Journal of Physical Chemistry Letters* 11 (24): 10463–68. https://doi.org/10.1021/acs.jpclett.0c03205.

Tong, Chuan-Jia, and Keith P. McKenna. 2019. “Passivating Grain Boundaries in Polycrystalline CdTe.” *The Journal of Physical Chemistry C* 123 (39): 23882–89. https://doi.org/10.1021/acs.jpcc.9b08373.

Toseeb, Umar, John Vincent, Olakunle A. Oginni, Kathryn Asbury, and Dianne F. Newbury. 2023. “The Development of Mental Health Difficulties in Young People with and Without Developmental Language Disorder: A Geneenvironment Interplay Study Using Polygenic Scores.” *Journal of Speech, Language, and Hearing Research* 66 (5): 1639–57. https://doi.org/10.1044/2023_jslhr-22-00664.

Ulrich-Oltean, Felix, Peter Nightingale, and James Alfred Walker. 2022. “Selecting SAT Encodings for Pseudo-Boolean and Linear Integer Constraints.” In. Schloss Dagstuhl - Leibniz-Zentrum für Informatik. https://doi.org/10.4230/LIPICS.CP.2022.38.

Velasco-Berrelleza, Victor, Matthew Burman, Jack W. Shepherd, Mark C. Leake, Ramin Golestanian, and Agnes Noy. 2020. “SerraNA: A Program to Determine Nucleic Acids Elasticity from

Simulation Data." *Physical Chemistry Chemical Physics* 22 (34): 19254–66. https://doi.org/10.1039/d0cp02713h.

Vernon, A. R., R. F. Garcia Ruiz, T. Miyagi, C. L. Binnersley, J. Billowes, M. L. Bissell, J. Bonnard, et al. 2022. "Nuclear Moments of Indium Isotopes Reveal Abrupt Change at Magic Number 82." *Nature* 607 (7918): 260–65. https://doi.org/10.1038/s41586-022-04818-7.

Wahab, Dina Abdul, Mathias Augustin, Samuel Manas Valero, Wenjun Kuang, Sarah Jenkins, Eugenio Coronado, Irina V. Grigorieva, et al. 2020. "Quantum Rescaling, Domain Metastability, and Hybrid Domain-Walls in 2D CrI Magnets." *Advanced Materials* 33 (5): 2004138. https://doi.org/10.1002/adma.202004138.

Walker, Richard, Setareh Chong, and James Chong. 2021. "Facilitating Peer-Led Group Research Through Virtual Collaboration Spaces: An Exploratory Research Study." *Research in Learning Technology* 29 (March). https://doi.org/10.25304/rlt.v29.2520.

Wang, Junlin, Guanqi Li, Bosen Zhang, Kunpeng Zhang, Kaiyu Tong, Bo Liu, Hao Meng, Jing Wu, and Yongbing Xu. 2023. "Atomistic Investigation of Interface Edge Defect in CoFeB/MgO Ferromagnetic Nano-Dots." *IEEE Transactions on Magnetics* 59 (2): 1–4. https://doi.org/10.1109/tmag.2022.3218138.

Wang, Junlin, Mara Strungaru, Sergiu Ruta, Andrea Meo, Yifan Zhou, András Deák, László Szunyogh, et al. 2021. "Spontaneous Creation and Annihilation Dynamics of Magnetic Skyrmions at Elevated Temperature." *Physical Review B* 104 (5). https://doi.org/10.1103/physrevb.104.054420.

Wang, Qing Hua, Amilcar Bedoya-Pinto, Mark Blei, Avalon H. Dismukes, Assaf Hamo, Sarah Jenkins, Maciej Koperski, et al. 2022. "The Magnetic Genome of Two-Dimensional van Der Waals Materials." *ACS Nano* 16 (5): 6960–7079. https://doi.org/10.1021/acsnano.1c09150.

Wang, Xuan, Daniel J. Jacob, Sebastian D. Eastham, Melissa P. Sulprizio, Lei Zhu, Qianjie Chen, Becky Alexander, et al. 2019. "The Role of Chlorine in Global Tropospheric Chemistry." *Atmospheric Chemistry and Physics* 19 (6): 3981–4003. https://doi.org/10.5194/acp-19-3981-2019.

Ward, S. H., R. Akers, L. Li, Y. Q. Liu, A. Loarte, S. D. Pinches, A. R. Polevoi, R. G. L. Vann, and M. A. Van Zeeland. 2022. "LOCUST-GPU Predictions of Fast-Ion Transport and Power Loads Due to ELM-Control Coils in ITER." *Nuclear Fusion* 62 (12): 126014. https://doi.org/10.1088/1741-4326/ac904f.

Watson, George D., Elliot W. Chan, Mark C. Leake, and Agnes Noy. 2022. "Structural Interplay Between DNA-Shape Protein Recognition and Supercoiling: The Case of IHF." *Computational and Structural Biotechnology Journal* 20: 5264–74. https://doi.org/10.1016/j.csbj.2022.09.020.

Watts, D. P., J. Bordes, J. R. Brown, A. Cherlin, R. Newton, J. Allison, M. Bashkanov, N. Efthimiou, and N. A. Zachariou. 2021. "Photon Quantum Entanglement in the MeV Regime and Its Application in PET Imaging." *Nature Communications* 12 (1). https://doi.org/10.1038/s41467-021-22907-5.

Williams, Rhys E., Quentin M. Ramasse, Keith P. McKenna, Laurie J. Phillips, Peter J. Yates, Oliver S. Hutter, Ken Durose, Jonathan D. Major, and Budhika G. Mendis. 2020. "Evidence for Self-Healing Benign Grain Boundaries and a Highly Defective SbseCdS Interfacial Layer in Sbse Thin-Film Photovoltaics." *ACS Applied Materials & Interfaces* 12 (19): 21730–38. https://doi.org/10.1021/acsami.0c03690.

Winkler, Robert, Alexander Zintler, Stefan Petzold, Eszter Piros, Nico Kaiser, Tobias Vogel, Déspina Nasiou, Keith P. McKenna, Leopoldo Molina-Luna, and Lambert Alff. 2022. "Controlling the Formation of Conductive Pathways in Memristive Devices." *Advanced Science* 9 (33): 2201806. https://doi.org/10.1002/advs.202201806.

Wong, Natalie G. K., Jacob A. Berenbeim, and Caroline E. H. Dessent. 2019. "Direct Observation of Photochemical Free Radical Production from the Sunscreen 2-Phenylbenzimidazole-5-Sulfonic Acid via Laser-Interfaced Mass Spectrometry." *ChemPhotoChem* 3 (12): 1231–37. https://doi.org/10.1002/cptc.201900149.

Wong, Natalie G. K., and Caroline E. H. Dessent. 2022. “Illuminating the Effect of the Local Environment on the Performance of Organic Sunscreens: Insights from Laser Spectroscopy of Isolated Molecules and Complexes.” *Frontiers in Chemistry* 9 (January). https://doi.org/10.3389/fchem.2021.812098.

Wong, Natalie G. K., Conor D. Rankine, and Caroline E. H. Dessent. 2021. “Measurement of the Population of Electrosprayed Deprotomers of Coumaric Acids Using UVvis Laser Photodissociation Spectroscopy.” *The Journal of Physical Chemistry A* 125 (31): 6703–14. https://doi.org/10.1021/acs.jpca.1c04880.

Xia, Tian, Jeremy Cosgrove, Jane Alty, Stuart Jamieson, and Stephen Smith. 2019. “Application of Classification for Figure Copying Test in Parkinsons Disease Diagnosis by Using Cartesian Genetic Programming.” In *Proceedings of the Genetic and Evolutionary Computation Conference Companion*. ACM. https://doi.org/10.1145/3319619.3326822.

Xie, Haiyan, John F. Dawson, Jiexiong Yan, Andy C. Marvin, and Martin P. Robinson. 2020. “Numerical and Analytical Analysis of Stochastic Electromagnetic Fields Coupling to a Printed Circuit Board Trace.” *IEEE Transactions on Electromagnetic Compatibility* 62 (4): 1128–35. https://doi.org/10.1109/temc.2019.2954303.

Yang, Zhongzhen, Illya Zalessky, Ryan G. Epton, Adrian C. Whitwood, Jason M. Lynam, and William P. Unsworth. 2023. “Ring Expansion Strategies for the Synthesis of Medium Sized Ring and Macrocyclic Sulfonamides.” *Angewandte Chemie International Edition* 62 (13). https://doi.org/10.1002/anie.202217178.

Zhu, Lei, Daniel J. Jacob, Sebastian D. Eastham, Melissa P. Sulprizio, Xuan Wang, Tomás Sherwen, Mat J. Evans, et al. 2019. “Effect of Sea Salt Aerosol on Tropospheric Bromine Chemistry.” *Atmospheric Chemistry and Physics* 19 (9): 6497–507. https://doi.org/10.5194/acp-19-6497-2019.