# Dr Jon G. C. Kragskow

Post-Doctoral Research Associate

Suturina Group, Department of Chemistry, University of Bath, UK

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I am a fast and enthusiastic learner, and thrive when solving complex, high-level problems. I have a broad interest in computational and theoretical chemistry and am passionate about communicating my research clearly and effectively.

## Education

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| September 2018- April 2022 | Ph.D.<br>Department of Chemistry, The University of Manchester, UK<br>Supervisor: Professor Nicholas F. Chilton<br>Thesis title: “Chemical Control of Spin-Phonon Coupling” |
| September 2014- June 2018 | MChem in Chemistry – 1st Class honours (2nd place in cohort)<br>Department of Chemistry, The University of Manchester, UK<br>Dissertation title: “Understanding the Crystal Field of Metal Complexes” |

## Research Experience

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| January 2023- Present | Post-Doctoral Research Associate<br>Suturina Group, Department of Chemistry, University of Bath, UK<br>Development of new computational tools for the routine simulation and analysis of paramagnetic nuclear magnetic resonance spectra.<br>Funded by EPSRC. |
| April 2022- October 2023 | Post-Doctoral Research Associate<br>Chilton Group, Department of Chemistry, The University of Manchester, UK<br>Continuation of doctoral research, with an emphasis on extending previously developed approaches to the understanding of relaxation dynamics of solid-state materials and surface-bound single molecule magnets. Funded by ERC. |
| September 2018-April 2022 | Doctoral Research Project<br>Chilton Group, Department of Chemistry, The University of Manchester, UK<br>Investigation and simulation of the electronic structure and spin dynamics of lanthanide based single molecule magnets, with particular focus on developing custom computer code and novel theoretical approaches. Funded by EPSRC studentship and University of Manchester President’s Doctoral Scholarship scheme. |

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| September 2017-June 2018 | Master's Research Project<br>Chilton Group, Department of Chemistry, The University of Manchester, UK<br>Developed a new technique for the parameterisation of high-level *ab initio* calculations in terms of simple crystal field models. |
| June 2017-September 2017 | 3rd Year Summer Research Project<br>Chilton Group, Department of Chemistry, The University of Manchester, UK<br>Explored the magnetic and electronic properties of transition metal single molecule magnets using *ab initio* calculations and spin-hamiltonian modelling methods and experimental data. Funded by a competitive Royal Society of Chemistry research bursary. |
| June 2016-September 2016 | 2nd Year Summer Research Project<br>Mills Group, Department of Chemistry, The University of Manchester, UK<br>Synthesised and characterised novel f-block silylamide compounds and their derivatives using air-sensitive techniques. Funded by departmental research bursary. |

Teaching

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| September 2019-January 2021 | Graduate Teaching Assistant<br>Department of Chemistry, The University of Manchester, UK<br>Taught MATLAB programming to 2nd year undergraduate students.<br>Marked student manuscripts and performed assessment interviews with students.<br>Co-developed an overhaul of the course material for virtual/distanced learning during COVID-19 and beyond. |
| September 2018-Present | Developer/Maintainer<br>www.waveplot.com<br>Created Waveplot, an open-source python/flask-based teaching tool for plotting 2D and 3D representations of different wavefunctions. |
| February 2022-Present | Developer/Maintainer<br>www.magnetism-tools.manchester.ac.uk<br>Created, with Prof. Nicholas Chilton, a web-based tool for calculating and plotting Tanabe-Sugano diagrams. |

Other responsibilities

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| September 2018-October 2022 | Code oversight and maintenance<br>Chilton Group, Department of Chemistry, The University of Manchester, UK<br>Responsible for maintenance of group subversion and git code repositories and for automated code documentation and release. Championed the use of good programming practice through style guides and documentation. Lead education of others in the group on best practices for code development through tutorials and manuals. |

Technical Skills

Quantum Chemistry: High-level knowledge of computational and quantum chemistry methods (HF, DFT, CASSCF, CASPT2), theoretical molecular magnetism and spin-phonon coupling, and experience in using established programs (Gaussian, OpenMOLCAS, ORCA). Implementation of original theory in both compiled and interpreted programming languages, and deployment of said code on large scale high-performance computing hardware.

Computer Software: Proficient in Fortran, Python, Bash, make, and MATLAB languages, and in git and subversion version control systems and CI/CD. Experience deploying/maintaining web servers (apache/wsgi) and scientific websites (dash/flask/js).

Computer Hardware/Systems: Experienced in assembly and management of computer systems for research and personal use.

Publications


8. K. R. McClain, H. Kwon, K. Chakarawet, R. Nabi, J. G. C. Kragskow, N. F. Chilton, R. D. Britt, J. R. Long, and B. G. Harvey , *J. Am. Chem. Soc.*, 2023, **145**, 8996–9002.
7. J. G. C. Kragskow, J. Marbey, C. D. Buch, J. Nehrkorn, M. Ozerov, S. Piligkos, S. Hill, N. F. Chilton, *Nat. Commun.*, 2022, **18**, 825.
6. C. A. Gould, K. R. McClain, D. Reta, J. G. C. Kragskow, D. A. Marchiori, E. Lachman, E.-S. Choi, J. G. Analytis, R. D. Britt, N. F. Chilton, B. G. Harvey and J. R. Long, *Science*, 2022, 6577, 198, **375**, 198-202.
5. D. Reta, J. G. C. Kragskow, N. F. Chilton, *J. Am. Chem. Soc.*, 2021, **15**, 5943–5950
4. K.-X. Yu, J. G. C. Kragskow, Y.-S. Ding, Y.-Q. Zhai, D. Reta, N. F. Chilton, Y.-Z. Zheng, *Chem*, 2020, **6**, 1–17.
3. C. A. P. Goodwin, B. L. L. Réant, G. F. Vettese, J. G. C. Kragskow, M. J. Giansiracusa, I. M. Dimucci, K. M. Lancaster, D. P. Mills, S. Sproules, *Inorg. Chem.*, 2020, **59**, 7571–7583
2. H. M. Nicholas, C. A. P. Goodwin, J. G. C. Kragskow, S. J. Lockyer, D. P. Mills, *Molecules*, 2018, **23**, 1138.

1. C. A. P. Goodwin, B. L. L. Réant, J. G. C. Kragskow, I. M. DiMucci, K. M. Lancaster, D. P. Mills and S. Sproules, *Dalt. Trans.*, 2018, **47**, 10613–10625.

Awards

2021: Department of Chemistry, Outstanding Academic Achievement Award

2018: The University of Manchester, President's Doctoral Scholarship

2018: Department of Chemistry, Outstanding Academic Achievement award for undergraduate study

2017: Royal Society of Chemistry, summer research project bursary

2016: Department of Chemistry, summer research project bursary

Presented work

Contributed Talks

2022: 7th European Conference on Molecular Magnetism, Rennes

2022: American Physical Society March Meeting, Chicago

2021: 17th International Conference on Molecule Based Magnets Rising Star Symposium, The University of Manchester

2021: Department of Chemistry Staff Symposium, The University of Manchester

2018: Midlands Computational Chemistry Conference, Nottingham Trent University

Posters

2019: 7th European Conference on Molecular Magnetism, University of Florence

2019: CASTEP Users Meeting, University of Oxford

2019: Royal Society of Chemistry Theoretical Chemistry Group Graduate Meeting, University of Nottingham

2018: National Training School in Theoretical Chemistry Summer School, University of Oxford

## Funding

2022: Royal Society of Chemistry Researcher Mobility Grant (~£500)

2017: Royal Society of Chemistry Undergraduate Research Bursary (~1.5k)

2016: University of Manchester Chemistry Undergraduate Departmental Research Bursary (~£1k)