

Jon G. C. Kragoskow

PhD Student

Chilton Group, Department of Chemistry, School of Natural Sciences, University of Manchester, 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

- September 2018-present** **Ph.D.** (Expected submission March 2022)
Department of Chemistry, The University of Manchester, UK
Supervisor: Professor Nicholas F. Chilton
Thesis title: "Chemical Control of Spin-Phonon Coupling "
- September 2014-June 2018** **MChem in Chemistry** – 1st Class honours (2nd place in cohort)
Department of Chemistry, The University of Manchester, UK
Dissertation title: "Understanding the Crystal Field of Metal Complexes"

Research Experience

- September 2018-present** **Doctoral Research Project**
Chilton Group, Department of Chemistry, The University of Manchester, UK
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.
- September 2017-June 2018** **Master's Research Project**
Chilton Group, Department of Chemistry, The University of Manchester, UK
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**
Chilton Group, Department of Chemistry, The University of Manchester, UK
Explored the magnetic and electronic properties of transition metal single molecule magnets using *ab initio* calculations in tandem with 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

Mills Group, Department of Chemistry, The University of Manchester, UK

Synthesised and characterised novel f-block silylamide compounds and their derivatives using air-sensitive techniques. Funded by departmental research bursary.

Teaching

September 2019-
January 2021

Graduate Teaching Assistant

Department of Chemistry, The University of Manchester, UK

Taught MATLAB programming to 2nd year undergraduate students.

Marked student manuscripts and performed assessment interviews with students.

Co-developed an overhaul of the course material for virtual/distanced learning during COVID-19 and beyond.

September 2018-
Present

Developer/Maintainer

www.waveplot.com

Created Waveplot, an open-source python/flask based teaching tool for plotting 2D and 3D representations of different wavefunctions.

Other responsibilities

September 2018-
Present

Code oversight and maintenance

Chilton Group, Department of Chemistry, The University of Manchester, UK

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). 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).

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

Publications

1. C. A. P. Goodwin, B. L. L. Réant, J. G. C. Kragoskow, I. M. DiMucci, K. M. Lancaster, D. P. Mills and S. Sproules, *Dalt. Trans.*, 2018, **47**, 10613–10625
2. H. M. Nicholas, C. A. P. Goodwin, J. G. C. Kragoskow, S. J. Lockyer, D. P. Mills, *Molecules*, 2018, **23**, 1138
3. C. A. P. Goodwin, B. L. L. Réant, G. F. Vettese, J. G. C. Kragoskow, M. J. Giansiracusa, I. M. Dimucci, K. M. Lancaster, D. P. Mills, S. Sproules, *Inorg. Chem.*, 2020, **59**, 7571–7583
4. K.-X. Yu, J. G. C. Kragoskow, Y.-S. Ding, Y.-Q. Zhai, D. Reta, N. F. Chilton, Y.-Z. Zheng, *Chem*, 2020, **6**, 1–17
5. D. Reta, J. G. C. Kragoskow, N. F. Chilton, *J. Am. Chem. Soc.* 2021, 143, **15**, 5943–5950
6. C. A. Gould, K. R. McClain, D. Reta, J. G. C. Kragoskow, 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
7. J. G. C. Kragoskow, J. Marbey, C. D. Buch, J. Nehr Korn, M. Ozerov, S. Piligkos, S. Hill, N. F. Chilton, *Nat. Commun.*, 2022, 825, **18**

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

Talks

- 2018:** Midlands Computational Chemistry Conference, Nottingham Trent University
- 2021:** Department of Chemistry Staff Symposium, The University of Manchester
- 2021:** 17th International Conference on Molecule Based Magnets Rising Star Symposium, The University of Manchester
- 2022:** American Physical Society March Meeting, Chicago

Posters

- 2018:** National Training School in Theoretical Chemistry Summer School, University of Oxford
- 2019:** Royal Society of Chemistry Theoretical Chemistry Group Graduate Meeting, University of Nottingham

2019: CASTEP Users Meeting, University of Oxford

2019: European Conference on Molecular Magnetism, University of Florence