Dr Jon G. C. Kragskow

Department of Chemistry, University of Bath, UK
www.kragskow.dev jgck20@bath.ac.uk

A fast and enthusiastic learner with a strong background in computational and theoretical chemistry, particularly as applied to magnetic and spectroscopic properties of transition metal and lanthanide systems. Passionate about building well-documented and open-source tools which make research easier, clearer, and more approachable. Committed to education, particularly through the creation of modern and interactive digital resources.

EMPLOYMENT

UNIVERSITY OF BATH Bath, UK

Post-Doctoral Research Associate January 2023-Ongoing

- EPSRC funded position in computational chemistry supervised by Dr Elizaveta Suturina.
- Implemented new computational tools for routine simulation and analysis of paramagnetic NMR spectra in both biological and chemical systems.
- Calculated and simulated of magnetic properties of exchange-coupled transition metal complexes using *ab initio* methods and spin-Hamiltonian modelling.
- Participation in academic exchange visits to Florence, Italy (protein NMR experiments) and Bordeaux, France (proton NMR and magnetochemistry experiments).
- Tutor in first year physical chemistry, and demonstrator/contributor for second year computational chemistry lab experiments.

THE UNIVERSITY OF MANCHESTER Manchester, UK

Post-Doctoral Research Associate April 2022-October 2022

- ERC funded position in computational chemistry supervised by Prof. Nicholas Chilton.
- Modelled magnetic behaviour of molecular nanomagnets using *ab initio* quantum chemistry, particularly in the solid-state.
- Led development of magnetochemistry software such as *ccfit2*, a python package for fitting experimental magnetic data.
- Trained of group members in python and Fortran software development and best practices for code deployment and version control through code-review sessions, documentation, and workshops.
- Maintained and architected group subversion and git code repositories and created automated pipelines for code documentation and release.

EDUCATION

THE UNIVERSITY OF MANCHESTER Manchester, UK

PhD in Chemistry Associate - "Chemical Control of Spin-Phonon Coupling" September 2018-April 2022

- PhD position in group of Prof. Nicholas Chilton funded by EPSRC studentship and University of Manchester President's Doctoral Scholarship.
- Calculated spin-phonon coupling (SPC) in lanthanide coordination complexes using *ab initio* quantum chemistry and spin-Hamiltonian approaches.
- Developed novel methodologies and software for the simulation of SPC-derived properties such as magnetic relaxation rates and magnetic field dependent infrared spectroscopy data.
- Collaborations with experimental groups in Xi'an Jiaotong University (China), the National High Magnetic Field lab (Florida, United States), and University of Copenhagen (Denmark).
- Instructed 2nd year undergraduates in MATLAB programming, marked lab scripts and carried out individual student assessment interviews. Overhauled course material and adapted course for distance learning during COVID-19.

THE UNIVERSITY OF MANCHESTER Manchester, UK

MChem in Chemistry September 2014-June 2018

- Degree Classification: **First Class**
- Outstanding Academic Achievement Award for top 0.5% of graduating students in Faculty of Science and Engineering.

COMPUTATIONAL SKILLS

Programming Languages

Beginner	JavaScript, Docker, flask, Apache, C++
Intermediate	HTML, CSS, Qt, Bash
Experienced	Python, Fortran90, Git, Subversion, make, MATLAB, GitLab CI/CD

Open-Source Software Development

ccfit2	A python package for working with experimental magnetometry data. Users can input a magnetometer output file and obtain a fitted plot of their data using a single command and an interactive interface. Thanks to its modular design and rich documentation, ccfit2 can be included in users own python code with ease.
Waveplot	An online wavefunction viewer which demonstrates simple concepts in quantum chemistry. Waveplot is built with students in mind and features the model quantum systems they encounter in introductory quantum chemistry. Students can manipulate input variables, plots, and download raw data to use in their own work.
AtomAccess	A python package which quantifies steric hindrance at chemical centres using raytracing. I wrote AtomAccess to be fast and user-friendly through either its simple web-interface, or through command-line and scripting.
Tau	A C++/Fortan90 program for the simulation of magnetic relaxation rates. Tau uses *ab initio* spin-phonon coupling data to accurately simulate magnetic relaxation under a range of conditions using a semi-classical master equation.
FIRMS_SIM	A Fortran90 program for the simulation of magnetic field dependent infrared spectroscopy. FIRMS_SIM uses *ab initio* spin-phonon coupling data to simulate the infrared spectra of molecules in varying magnetic fields.

Technical Skills

Quantum Chemistry	High-level knowledge of computational and quantum chemistry methods (HF, DFT, CASSCF, CASPT2), and experience in using established programs (Gaussian, OpenMOLCAS, ORCA).
Magnetism	Experienced in analysis and workup of experimental magnetometry data (AC susceptibility, DC Decay, magnetisation and susceptibility). Expert knowledge of phenomenological and spin-Hamiltonian modelling techniques.
HPC	Proficient HPC user, familiar with a variety of schedulers and systems of differing scale (AWS, Azure, local clusters, Tier-2 HPC). Experience in creating and maintaining group-level clusters/systems.

FUNDING SECURED

2023 **British Council** – Exchange program between Universities of Bath and Bordeaux (**£7k**)
2022 **Royal Society of Chemistry** –Researcher Mobility Grant (**£500**)
2017 **Royal Society of Chemistry** - Undergraduate Summer Research Bursary (**£1.5k**)
2016 **The University of Manchester** - Undergraduate Departmental Research Bursary (**£1k**)

AWARDS

2021 **The University of Manchester** – Outstanding Postgraduate Academic Achievement Award
2018 **The University of Manchester** – President's Doctoral Scholarship
2018 **The University of Manchester** – Outstanding Undergraduate Academic Achievement Award

PUBLICATIONS

13. G. K. Gransbury, S. C. Corner, **J. G. C. Kragskow**, P. Evans, H. Yeung, W. J. A. Blackmore, G. F. S. Whitehead, I. J. Vitorica-Yrezabal, Meagan S. Oakley, N. F. Chilton and D. P. Mills, *J. Am. Chem. Soc.*, 2023, **145**, 41, 22814–22825
12. R. Nabi, J. K. Staab, A. Mattioni, **J. G. C. Kragskow**, D. Reta, J. M. Skelton and N. F. Chilton, *J. Am. Chem. Soc.*, 2023, **145**, 45, 24558–24567

11. B. Alnami, **J. G. C. Kragskow**, J. K. Staab, J. M. Skelton and N. F. Chilton, *J. Am. Chem. Soc.*, 2023, **145**, 25, 13632-13639
10. **J. G. C. Kragskow**, A. Mattioni, J. K. Staab, D. Reta, J. M. Skelton and N. F. Chilton, *Chem. Soc. Rev.*, 2023, **52**, 4567
9. W J. A. Blackmore, G. K. Gransbury, P. Evans, **J. G. C. Kragskow**, D. P. Mills, N. F. Chilton, *Phys. Chem. Chem. Phys.*, 2023, **25**, 16735-16744
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 and N. F. Chilton, *Nat. Commun.*, 2022, **13**, 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, **375**, 198-202
5. D. Reta, **J. G. C. Kragskow**, N. F. Chilton, J. Am. Chem. Soc., 2021, **143**, 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, *Dalton Trans.*, 2018, **47**, 10613–1062

PRESENTATIONS

Contributed Talks

2022 **Ultrahard magnetism from mixed-valence dilanthanide complexes with metal-metal bonding**
7th European Conference on Molecular Magnetism, Rennes

2022 **Vibronic coupling in a 4f qubit**
American Physical Society March Meeting, Chicago

2021 ***Ab initio* relaxation dynamics in Lanthanide Single Molecule Magnets**
Department of Chemistry Postgraduate Symposium, The University of Manchester

2021 **Vibronic coupling in a 4f qubit**
17th International Conference on Molecule Based Magnets Rising Star Symposium, The University of Manchester

2021 **Enhancing Magnetic Hysteresis in Single-Molecule Magnets by Ligand Functionalization**
Department of Chemistry Staff Symposium, The University of Manchester

2018 **Understanding the Crystal Field of Metal Complexes**
Midlands Computational Chemistry Conference, Nottingham Trent University

Posters

2024 **Understanding the Electronic Structures of Transition Metal Complexes using Paramagnetic NMR Spectroscopy**
Spin Meeting 2024, The University of Manchester

2023 **Understanding the Electronic Structures of Transition Metal Complexes using Paramagnetic NMR Spectroscopy**
19th European Magnetic Resonance Congress, Glasgow

2019 **Ab initio Relaxation Dynamics of Dysprosium(III) Single Molecule Magnets**
7th European Conference on Molecular Magnetism, University of Florence

2019 **Ab initio Relaxation Dynamics of Dysprosium(III) Single Molecule Magnets**
CASTEP Users Meeting, University of Oxford

2019 **Ab initio Relaxation Dynamics of Dysprosium(III) Single Molecule Magnets**
Royal Society of Chemistry Theoretical Chemistry Group Graduate Meeting, University of Nottingham

2018 **Understanding the Crystal Field of Metal Complexes**
National Training School in Theoretical Chemistry Summer School, University of Oxford