

Jon G. C. Kragoskow

Email: Jonkragoskow@gmail.com Jon.Kragoskow@manchester.ac.uk

Personal Profile

I am a self-motivated 2nd year Chemistry PhD student at the University of Manchester. I have programming experience in both individual and group environments, and am currently particularly interested in the development of software for all themes of chemistry.

Skills

Programming ability and experience in Python, Fortran, Matlab, Bash, and make.

Specialised knowledge in Quantum Mechanics, Quantum Chemistry and Molecular Magnetism.

Production of publication quality reports and papers.

Experience in performing *ab initio* calculations (CASSCF, HF, DFT) in Gaussian and Molcas packages.

Education

PhD Studies - Chilton Group - School of Chemistry - University of Manchester

September 2018 – Present

Project Title: Chemical Control of Spin-Phonon coupling

Funding: EPSRC and President's Doctoral Scholar Award

One of the top incoming PhD students at the University of Manchester (~100 selected across the University *per annum*.).

One paper published, and several under preparation.

Numerous codes written including *Tau - A program for calculating relaxation dynamics of Single Molecule Magnets*

Active maintenance of the group's code base using an SVN based repository system.

Created the OrbiPlot software for displaying radial wave functions in a graphical user interface.

Undergraduate Studies (MChem. Hons.) - School of Chemistry - University of Manchester

September 2014 – June 2018

First Class Degree (top 0.5% of Faculty >1000 total graduates)

Astra-Zeneca award for top organic chemist in first year (2015).

R.F. Warren memorial prize for the top physical chemist in second year (2016).

Kenneth Waugh memorial prize for the top physical chemist in fourth year (2018).

Masters research project in computational/theoretical chemistry, developing a novel method for the extraction of a crystal field Hamiltonian from a CASSCF calculation.

Lead a team of four in a 12-week investigation of gas phase polyatomic compounds using high-resolution infrared spectroscopy. Involved the design of a high vacuum gas line apparatus, followed by computational analysis of data using self-written code, and the production of a 30-page report.

Manshead Sixth Form and Upper School

September 2009 - June 2014

A-Level Mathematics (A), Chemistry (A), Physics (A).

AS-Level Ethics & Philosophy (B).

GCSEs (7A*, 3A) including English, Maths and Sciences.

Awarded Duncan Tweed prize for outstanding contribution to the scientific life of the school.

Practical Experience

Summer internship - Chilton group - School of Chemistry - University of Manchester

June 2017 – September 2017

Modelled the magnetic properties of a family of near-linear transition metal complexes.

Performed multi-configurational *ab initio* calculations (CASSCF), wrote code to produce publication quality figures, and employed spin-Hamiltonian modelling methods in order to analyse experimental data.

Summer internship - Mills group - School of Chemistry - University of Manchester

June 2016 – August 2016

Synthesised air-sensitive novel f-block silylamide compounds and their derivatives via glove box and Schlenk line techniques.

Placed 57 reactions in a 7-week period, generating 6 novel compounds in the process.

Three publications from this project.

Publications to date

1. H. Nicholas, C. Goodwin, **J. G. C. Kragoskow**, S. Lockyer and D. P. Mills, *Molecules*, 2018, **23**, 1138.
2. C. A. P. Goodwin, B. L. L. Réant, **J. G. C. Kragoskow**, I. M. DiMucci, K. M. Lancaster, D. P. Mills and S. Sproules, *Dalton Trans.*, 2018, **47**, 10613.
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 and 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 and Y.-Z. Zheng, *Chem*, 2020, **6**, 1–17.