

Jon G. C. Kragoskow

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Personal Profile

I am a self-motivated 1st year Chemistry PhD student at the University of Manchester, and am particularly interested in the development of novel methods in theoretical and computational chemistry. I have experience working both in a group and as an individual with a wide range of people in different research environments including synthetic, measurement and computational laboratories.

Skills

- Experience in using MATLAB, FORTRAN, and Python for data-processing, generation of publication quality figures, and GUI development.
- Specialised knowledge in Quantum Mechanics, Quantum Chemistry and Molecular Magnetism.
- Production of high quality research reports using the LaTeX document preparation system.
- Previous experience performing *ab initio* calculations (CASSCF, HF, DFT) in Gaussian and Molcas packages.

Education

Postgraduate Studies - University of Manchester - September 2018 – Present

President's Doctoral Scholar - PhD Chemistry - Chilton Group

- Investigating the effects of dynamic vibrational motion on the magnetic properties of single molecule magnets.
- Created the OrbiPlot software for displaying radial wave functions in a graphical user interface.

Undergraduate Studies - University of Manchester - September 2014 – June 2018

MChem Chemistry - 1st Class Degree graduating within top 0.5% of faculty (>1000 total graduates)

- Undertook a Masters research project in the field of 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. This 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.
- The above projects required self-driven enquiry into branches of chemistry which are not taught in the main undergraduate course, such as mathematical treatments of *ab initio* theory, quantum mechanics and molecular spectroscopy, followed by presenting or explaining this knowledge to my peers.

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 all three sciences.
- Awarded Duncan Tweed prize for outstanding contribution to the scientific life of the school.

Practical experience

Chilton group, School of Chemistry, University of Manchester. June 2017 – September 2017

- Summer internship centred around the theory and modelling of the magnetic properties of a family of near-linear transition metal complexes.
- Gained first-hand experience in multi-configurational *ab initio* calculations (CASSCF), wrote Fortran programs to produce publication quality figures, and employed spin-Hamiltonian modelling methods in order to analyse experimental SQUID magnetometry data.

Mills group, School of Chemistry, University of Manchester. June 2016 – August 2016

- Summer internship involving the synthesis of air-sensitive novel f-block silylamide compounds and their derivatives via glove box and Schlenk line techniques.
- Characterisation of compounds by use of single-crystal x-ray diffraction and NMR.
- Placed 57 reactions in a 7-week period, generating 6 novel compounds in the process.

Awards and Achievement

- Outstanding academic achievement award 2018 - presented to the top 0.5% of graduates from the Faculty of Science and Engineering at the University of Manchester - (>1000 total graduates).
- Several awards pertaining to academic achievement -
 - 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.
 - President's Doctoral Scholar Award for being among the top incoming PhD students at the University of Manchester (~100 are selected across the entire University each year.).

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