

THE UNIVERSITY OF MANCHESTER
PARTICULARS OF APPOINTMENT
FACULTY OF SCIENCE & ENGINEERING
SCHOOL OF NATURAL SCIENCES
DEPARTMENT OF CHEMISTRY
RESEARCH ASSOCIATE IN COMPUTATIONAL CHEMISTRY
VACANCY REF: S&E-14950

Salary:	£32,816 to £40,322 per annum, depending on relevant experience
Hours:	Full Time
Duration:	Fixed Term, from 1 February 2020 until 31 January 2023
Location:	Oxford Road, Manchester

Enquiries about the vacancy, shortlisting and interviews:

Contact: Dr Nicholas Chilton

Email: nicholas.chilton@manchester.ac.uk

BACKGROUND

Applications are invited for an ERC-funded Research Associate position to undertake research in the field of molecular magnetism and vibronic coupling. This position is part of the “ContraVib: Chemical Control of Vibronic Coupling for Magnetic Materials” project, funded by an ERC Starting Grant, which seeks to use high quality physical measurements and state-of-the-art computational techniques to develop guidelines for the chemical control of vibronic coupling. The successful candidate will join the multidisciplinary Chilton group at The University of Manchester in the UK, and tackle the elementary questions of: how can molecular vibronic coupling be controlled and how can it be exploited?

Relevant publications:

- Goodwin *et al.*, [Molecular magnetic hysteresis at 60 kelvin in dysprosocenium](#), *Nature*, 2017, **548**, 439.
- Ding *et al.*, [Field- and temperature-dependent quantum tunnelling of the magnetisation in a large barrier single-molecule magnet](#), *Nature Commun.*, 2018, **9**, 3134.
- F. Ortu *et al.*, [Studies of Hysteresis and Quantum Tunnelling of the Magnetisation in Dysprosium\(III\) Single Molecule Magnets](#), *Dalton Trans.*, 2019, **48**, 8541.
- Evans *et al.*, [A Bis-Monophospholyl Dysprosium Cation Showing Magnetic Hysteresis at 48 Kelvin](#), *ChemRxiv*, 2019, preprint.

Overall Purpose of the Job

You will lead the computational studies for the project, performing density-functional theory (DFT) and complete active space self-consistent field spin-orbit (CASSCF-SO) calculations to determine the anharmonic phonon spectra, phonon-phonon coupling, and vibronic coupling of molecular magnets in the solid state. This is part of a combined physical, computational and theoretical study, aimed at realising chemical control of vibronic coupling.

You will be a highly capable, motivated and independent researcher who is able to manage multiple facets of a large project. You will be expected to take a leading role in the research group including supervising PhD and MChem students, and presenting findings at international conferences.

Key Responsibilities, Accountabilities or Duties

The range of duties will include:

- Conduct individual and collaborative research projects.
- Write up research work for publication.
- Continually update knowledge and understanding in field or specialism.
- Translate knowledge of advances in the subject area into research activity.
- Use new research techniques and methods.
- Use initiative and creativity to identify areas for research, develop new research methods and extend the research portfolio.
- Use creativity to analyse and interpret research data and draw conclusions on the outcomes.
- Contribute to collaborative decision making with colleagues in areas of research.
- Plan and manage own research activity in collaboration with others.
- Work with colleagues on joint projects, as required.
- Collaborate with academic colleagues on areas of shared research interest.
- Attend and contribute to relevant meetings.
- Liaise with colleagues and students.
- Be involved in the supervision of student projects.
- Assist in the development of student research skills.
- Deal with routine communication using a range of media.
- Communicate complex information, orally, in writing and electronically.
- Communicate material of a specialist or highly technical nature.

- Prepare proposals and applications to external bodies, e.g. for funding and contractual purposes.
- Build internal contacts and participate in internal networks for the exchange of information and to form relationships for future collaboration.
- Use research resources, laboratories and workshops as appropriate.
- Balance, with help, the competing pressures of research and administrative demands and deadlines.
- Be aware of the risks in the work environment and their potential impact on their own work and that of others.

PERSON SPECIFICATION

Essential Knowledge, Skills and Experience

- Have, or be about to obtain, a relevant PhD (or equivalent).
- Expertise in one of: periodic DFT, lattice dynamics or CASSCF-SO calculations.
- Excellent communication and interpersonal skills.
- Excellent time management and organisational skills.
- Ability to work independently and as part of a team.
- Ability to liaise confidently and effectively with a range of individuals.
- Flexible approach to dealing with research problems as they arise.
- Willingness to learn and develop.
- Ability to present in both written and oral publications.
- Ability to meet deadlines.
- The ability to evaluate complex data.
- Understand equal opportunity issues as they may impact on areas of research content.

Desirable Knowledge, Skills, Experience and Qualifications

- Experience in molecular magnetism.
- Experience in lattice dynamics.
- Experience in periodic DFT calculations.

- Experience in CASSCF-SO calculations.
- Experience with a range of HPC resources.
- Knowledge of scripting and/or coding.
- Experience in supervision of undergraduate and postgraduate researchers.
- Strong journal publication record.