# Molecular Magnetism and Machine Learning

Molecular magnetic materials are a family of compounds that contain one or more magnetic metal ions, within a molecular framework. Examples of molecular magnetic materials are Single-molecule magnets (SMMs), complexes of metal ions which couple ferromagnetically or antiferromagnetically, exhibiting a large anisotropy in their magnetic response, and spin-crossover materials, where the magnetic ion changes between high and low spin states in response to external stimuli, such as temperature or pressure. Molecular magnetic materials are of current interest in information storage, molecular spintronics, and magnetic cooling. However, finding an compound with the desired properties (e.g. magnetic response and its anisotropy) currently requires experimental screening, which takes a large amount of time. Screening candidate SMMs with quantum-mechanical calculations is also possible, but decreases the screening time from weeks to days, meaning that a substantial outlay is still required.

Machine-learning (ML) methods are becoming an extremely popular method to circumvent time-intensive quantum-mechanical calculations, with modern ML approaches able to predict the results of solving the Schrödinger equation with high accuracy. The student will develop the methodology to predict the magnetic properties of molecular magnetic materials using ML, choosing the best ML method and descriptors to give a model that requires no specialist knowledge or computationally intensive calculations but nonetheless gives highly accurate results. In addition, the interested student may carry out experiments to characterise molecular magnetic materials, allowing a feedback between theory and experiment, with each strand of the project guiding the other. This project will potentially involve collaborations with the Quantum Technology group within the school who are interested in applications of these materials to quantum computing.

For informal inquiries, please feel free to contact Dr. David Wilkins (d.wilkins@qub.ac.uk) or Dr. Solveig Felton (s.felton@qub.ac.uk) at the Centre for Quantum Materials & Technologies, School of Mathematics & Physics, Queen's University Belfast.

**Entry requirements**

Applicants are expected to possess a first or upper-second class degree in physics, chemistry, materials science, or a relevant discipline (or an equivalent overseas qualification).

**How to apply**

Applications should be submitted via the Direct Applications Portal.

**References**

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