

# Molecular Magnetism investigations assisted by 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 molecular spintronics, magnetic cooling and information storage among other topics. The magnetic properties of such materials can be investigated by SQUID (Superconducting Quantum Interference Device) magnetometry and Electron Paramagnetic Resonance (EPR) spectroscopy. We have a current collaboration with Dr Grace Morgan (School of Chemistry, University College Dublin) whose group synthesise different molecular magnetic materials, which will be investigated in this project.

Machine-learning (ML) methods are becoming an extremely popular method to sift through extremely large data sets. In the field of molecular magnetism this can be applied to predicting which of the multitude of possible chemical compounds are more likely to have interesting magnetic properties. Dr Solveig Felton and Dr David Wilkins have been investigating how to utilise this predictive power for single molecule magnets, and the results of this will help guide sample choice in this project. Interested students may get involved in the machine learning process as well as the magnetic characterisation. This project will potentially involve visits to Dr. Grace Morgan (University College Dublin) to learn how to synthesise molecular magnetic materials.

For informal inquiries, please feel free to contact Dr. Solveig Felton ([s.felton@qub.ac.uk](mailto:s.felton@qub.ac.uk)) or Dr. David Wilkins ([d.wilkins@qub.ac.uk](mailto:d.wilkins@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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