Chemical Control of Vibronic Coupling for Magnetic Materials

A Data Management Plan created using DMPonline

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Template: ERC DMP Customised By: University of Manchester

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Project abstract:

Coupling of molecular vibrations to electronic states (vibronic coupling) is a fundamental process that profoundly affects the outcome of chemical reactions and physical processes, but our knowledge of this coupling is remarkably poor. Gaining fuller understanding will allow deliberate tailoring of the vibronic coupling, providing design criteria for high-performance magnetic memories and qubits, and in future, improved catalysts and optical materials. This research programme will develop a comprehensive computational framework for calculating the molecular origins of vibronic coupling and employ a range of physical measurements to support development of a modern theory of the effect. Thus, the programme will yield rules for how vibrational motions of functional groups and structural motifs couple to electronic states, leading to the rapid development of a new research field of vibronic control.

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Manchester Data Management Outline

- Yes
- Not applicable
- Yes – only institution involved
- Acquire new data

Optimised molecular/crystal/amorphous geometries
Anharmonic and harmonic vibrational modes
Electronic structures at equilibrium and for distortions along normal mode coordinates
Vibronic coupling coefficients
Magnetic relaxation times for molecular magnets in different phases
Quantum tunnelling rates for molecular magnetis in different phases

- University of Manchester Research Data Storage Service (Isilon)
- 1 - 8 TB
- Not applicable
- 5 - 10 years
- No sensitive or personal data

No personal information will be stored.

- Not applicable
- No
- Not applicable
- No

Dr Nicholas F. Chilton

04/09/2019

Summary

ContraVib

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FAIR data and resources

All data relevant to individual publications will be made publicly available, indefinitely, through Mendeley Data, with a persistent and unique Digital Object Identifier.

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Data will be in compressed plain text format as much as possible, but if it must be stored in a unique manner access instructions will be provided with the dataset.

By publishing the digtal data for the experimental measurements in the publications/project, which is not currently common practise in the community, others will be able to directly comapre models or re-interpret data in the future.

All data sets generated from this research will be curated in a database in line with UoM's data management policy. I have been allocated 8 TB of resilient storage for this project, which is managed through the University of Manchester Library. This data will be archived and backed-up for a minimum of 10 years, and storage will be expanded as necessary.