Plan Overview

A Data Management Plan created using DMPonline

Title: Chemical Control of Vibronic Coupling for Magnetic Materials

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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.

ID: 32267

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Chemical Control of Vibronic Coupling for Magnetic Materials

Manchester Data Management Outline

1. Is this project already funded?

- Yes

2. If you will be applying for funding from multiple sources who else will you be applying to?

- Not applicable

3. Is The University of Manchester the lead institution for this project?

- Yes – only institution involved

4. What data will you use in this project (please select all that apply)?

- 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

5. Where will the data be stored and backed-up during the project lifetime?

- University of Manchester Research Data Storage Service (Isilon)

6. If you will be using Research Data Storage, how much storage will you require?

- 1 - 8 TB

7. If you have a contractual agreement with a 3rd party data provider will any of the data associated with this project be sourced from, processed or stored outside of the institutions and groups stated on your agreement?

- Not applicable

8. How long do you intend to keep your data for after the end of your project (in years)?

- 5 - 10 years

Questions about personal information

Personal information or personal data, the two terms are often used interchangeably, relates to identifiable living individuals. Special category personal data is more sensitive information such as medical records, ethnic background, religious beliefs, political opinions, sexual orientation and criminal convictions or offences information. If you are not using personal data then you can skip the rest of this section.

Please note that in line with data protection law (the General Data Protection Regulation and Data Protection Act 2018), personal information should only be stored in an identifiable form for as long as is necessary for the project; it should be pseudonymised (partially de-identified) and/or anonymised (completely de—identified) as soon as practically possible. You must obtain the appropriate ethical approval in order to use identifiable personal data.

- No sensitive or personal data

10. Please provide details of how you plan to store, protect and ensure confidentiality of the participants' information as stated in the question above.

No personal information will be stored.

11. If you are storing personal information will you need to keep it beyond the end of the project?

- Not applicable

12. Sharing person identifiable information can present risks to participants' privacy, researchers and the institution. Will the participants' information (personal and/or sensitive) be shared with or accessed by anyone outside of the University of Manchester? This includes using 3rd party service providers such as cloud storage providers or survey platforms.

- No

13. If you will be sharing personal information outside of the University of Manchester, will the individual or organisation you are sharing with be outside the EEA?

- Not applicable

14. Are you planning to use the personal information for future purposes such as research?

- No

15. Who will act as the data custodian or information asset owner for this study?

Dr Nicholas F. Chilton

16. Please provide the date on which this plan was last reviewed (dd/mm/yyyy).

04/09/2019

Summary

Project Acronym

ContraVib

Project Number

ERC-STG-851504

Provide a dataset summary

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

FAIR data and resources

1. Making data findable

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

2. Making data openly accessible

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

3. Making data interoperable

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.

4. Increase data reuse

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

5. Allocation of resources and data security

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.