Plan Overview

A Data Management Plan created using DMPonline

Title: Collaboration data plan

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Affiliation: University of Manchester

Template: The Royal Society Template

Project abstract:

Density functional theory (DFT) is the principal workhorse in atomistic modelling of molecules and materials. DFT is appealing because it is scalable to systems with thousands of atoms, and because it is straightforward to obtain predictions for electronic, optical, and magnetic properties of these systems. Two main challenges of DFT are that (1) its accuracy strongly depends on the employed density functional approximation (DFA), and that (2) it is not well suited for describing systems with strong (static) correlation, e.g. with near-degenerate energy levels.

Nanoscale organic systems with extensive π-electron delocalisation, such as π-magnetic graphene nanoribbons and d-magnetic porphyrin nanostructures, are promising candidates for optoelectronics, spintronics, and quantum information processing. Optical, electronic, and magnetic properties of these conjugated systems can be manipulated by chemical design, but the space of possible structures is practically infinite. Modelling can offer predictions about properties and new functionalities (e.g. efficient light emission or length-independent conductance), but the credibility of such predictions has been limited by the limitations of presently available DFAs. As a result, DFT for magnetic organic systems is usually used only reactively, i.e., a DFA is chosen according to agreement with already known experimental results.

The main objective of this project is to develop a highly accurate DFA tailored for organic conjugated systems with π- and/or d-magnetism, which would enable us to make reliable predictions. This is ambitious, but it builds upon prior successful work on tuning DFAs done in both Peking (Chen Li) and Manchester (Igor Roncevic). This project will enable us to connect the complementary approaches that have been employed by these two groups. Our first goal is to enhance and integrate range-separated hybrid DFAs (developed in Manchester) with the localised orbital scaling correction (LOSC) functional (developed in Peking). Our second goal is to explore solutions for strongly correlated systems using DFT by imposing rigorous constraints derived from semiclassical limits. Finally, our third goal is to use our tailored DFA to identify systems in which the spin state can be read-out by light emission or electrical conductance, which is important for applications in optoelectronics and quantum information technologies.

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Copyright information:

Collaboration data plan

Manchester Data Management Outline

1. Will this project be reviewed by any of the following bodies (please select all that apply)?

- Funder

2. Is The University of Manchester collaborating with other institutions on this project?

- Yes - Part of a collaboration and owning or handling data

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

- Acquire new data

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

- Other storage system (please list below)
- University of Manchester Research Data Storage Service (Isilon)

Data generated in the Roncevic group will be shared within the group on the Manchesters's Research Data Storage system.
A subset of this data will be shared with our collaborators through a GitHub repository.

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

- 1 - 8 TB

6. Are you going to be receiving data from, or sharing data with an external third party?

- Yes

We will share data with Peking University through a GitHub repository.

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

- 5 - 10 years

Guidance for questions 8 to 13

Highly restricted information defined in the Information security classification, ownership and secure information handling SOP is information that requires enhanced security as unauthorised disclosure could cause significant harm to individuals or to the University and its ambitions in respect of its purpose, vision and values. This could be: information that is subject to export controls; valuable intellectual property; security sensitive material or research in key industrial fields at particular risk of being targeted by foreign states. See more examples of highly restricted information .

Personal information, also known as personal data, relates to identifiable living individuals. Personal data is classed as special category personal data if it includes any of the following types of information about an identifiable living individual: racial or ethnic origin; political opinions; religious or similar philosophical beliefs; trade union membership; genetic data; biometric data; health data; sexual life; sexual orientation.

Please note that in line with data protection law (the UK 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.

8. What type of information will you be processing (please select all that apply)?

- No confidential or personal data

Data will be composed of electronic structure code, and input and output files for electronic software programs.

9. How do you plan to store, protect and ensure confidentiality of any highly restricted data or personal data (please select all that apply)?

- Not applicable

10. If you are storing personal information (including contact details) will you need to keep it beyond the end of the project?

- Not applicable

11. Will the participants' information (personal and/or sensitive) be shared with or accessed by anyone outside of the University of Manchester?

- No

12. 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?

- Yes

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

- No

Not applicable.

14. Will this project use innovative technologies to collect or process data?

- No

15. Who will act as the data custodian for this study, and so be responsible for the information involved?

Igor Roncevic

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

2026-03-17

Data outputs

What data outputs will be generated by the research that are of value to the public?

Data generated by this project will consist of code for running density functional theory calculations, and outputs of such calculations.

Data access

How will others be able to access the data?

Through a private GitHub repository.

If the data is of high public interest, how will it be made accessible not only for those in the same or linked field, but also to a wider public audience?

Data accompanying publications will be hosted on Zenodo.

Specify whether any limits will be placed on the data to be shared, for example, for the purposes of safeguarding commercial interests, personal information, safety or security of the data.

Not applicable.

Where and when will you make the data available?

All relevant data accompanying publications will be hosted on repositories such as Zenodo.

Preservation

How will datasets be preserved to ensure they are of long-term benefit?

Manchester data service guarantees >5 years of storage after project conclusion (in practice much longer). Zenodo guarantees 20 years.