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## Plan Overview

*A Data Management Plan created using DMPonline*

**Title:** Molecular and mesoscopic simulations incorporating chemical reactivity: applications to reverse aggregation

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**Affiliation:** University of Manchester

**Funder:** Engineering and Physical Sciences Research Council (EPSRC)

**Template:** EPSRC Data Management Plan Customised By: University of Manchester

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### Project abstract:

This proposal aims at the development of new simulation tools to model complex systems in which chemical reactions play crucial roles and where the length and time scales of interest are beyond the reach of standard, atomistic modelling techniques. The plan is two-pronged. The first prong involves small scale ab initio simulations, using machine learning techniques to train a many-body, reactive forcefield. This forcefield will then be used to obtain a molecular-scale description of the system. The second prong is to conduct meso-scale simulations incorporating chemical reactivity. While our chosen application is in the field of liquid-liquid extraction, this approach will be applicable to a wide variety of systems, such as surfactants, coatings, cell wall interactions and, with some extensions, explosions.

**ID:** 172139

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### Copyright information:

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# Molecular and mesoscopic simulations incorporating chemical reactivity: applications to reverse aggregation

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## Manchester Data Management Outline

### 1. Is this project already funded?

- No

### 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

The project involves the creation of new simulations for which pre-existing data are not required.

### 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

We will need to store history files from our simulations in order to conduct our analysis.

### 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 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**

We will have no such information.

### **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?**

Andrew John Masters

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

03/03/2025

## Data Collection

### What data will you collect or create?

Numerical data, such as molecular co-ordinates generated by a simulation.

### How will the data be collected or created?

It will be created by a molecular dynamics or Monte Carlo simulation code. The data will be lists of numbers, stored typically in a binary format. The volume of data to be stored per simulation will be typically 10 - 100 MByte.

## Documentation and Metadata

### What documentation and metadata will accompany the data?

All necessary documentation as to the use of our simulations will be published online, along with useful metadata to help other potential users. Access will be free. All publications will contain required meta-data and documentation in supplementary documentation.

## Ethics and Legal Compliance

### How will you manage any ethical issues?

No ethical issues are anticipated, but if they arise, we will seek advice from the University of Manchester.

### How will you manage copyright and Intellectual Property Rights (IPR) issues?

This will be managed via University of Manchester institutions (e.g. UMIP).

## Storage and Backup

### How will the data be stored and backed up during the research?

On repositories provided by the University of Manchester's Computer Shared Facility. We will work with Research IT on this.

### How will you manage access and security?

There is no restricted access to our data. Storage of data and access to it will be managed by the investigator, taking advice from the University of Manchester's Research IT team.

## Selection and Preservation

### Which data are of long-term value and should be retained, shared, and/or preserved?

We anticipate that we will generate no data of long-term value. The project is about general physical behaviour, such as the symmetry of a phase. In case we do need to retain any data long-term, we will seek advice from Manchester's Research IT.

**What is the long-term preservation plan for the dataset?**

Again we foresee no need for long-term preservation of data. In the unlikely event this is needed, we will again make use of the University of Manchester's long-term storage facilities.

## **Data Sharing**

**How will you share the data?**

Data will be made freely available on request. Supplementary information provided in our papers will also give free access to data. All our publications will be free access.

**Are any restrictions on data sharing required?**

No

## **Responsibilities and Resources**

**Who will be responsible for data management?**

Andrew John Masters

**What resources will you require to deliver your plan?**

Only the data management resources already provided by the University of Manchester.