

---

## Plan Overview

*A Data Management Plan created using DMPonline*

**Title:** Insights into confinement effects on structural properties of liquids by total neutron scattering

**Creator:** Marta Falkowska

**Principal Investigator:** Marta Falkowska

**Affiliation:** University of Manchester

**Template:** University of Manchester Generic Template

**ORCID ID:** 0000-0003-0888-005X

### Project abstract:

Investigating structuring and dynamics of molecules constituting liquids by neutron scattering techniques have been revealing the causes of different macroscopic properties e.g. as a function of temperature or composition. These properties for liquids upon confinement in porous materials, narrow slits or channels are frequently very different than for their corresponding unrestricted phases.

This project is aiming to unravel the influence of surface chemistry of confining material (hydrophilic and hydrophobic materials) and pores topology (incl. pore size) on the structural properties of the geometrically restricted liquids. Understanding these effects will advance the design of systems in various fields utilising nanotechnology, such as porous materials used as drug carriers, catalysts used for preventing greenhouse gases emission, complex membranes for water purification.

The project will focus on designing a new Liquid Delivery System used at NIMROD instrument at ISIS Neutron and Muon Source. This new setup will enable preparation of a broad spectrum of confined liquid samples including less volatile compounds which is not possible at the moment and hence will extend the pool of samples that can be probed by the instrument with high confidence. Additionally, new workflows for data analysis collected for confined fluids will be implemented into existing software to increase the accessibility of these systems studies to the wider user community.

**ID:** 108702

**Start date:** 01-03-2023

**End date:** 29-02-2024

**Last modified:** 25-10-2022

**Grant number / URL:** <https://royalsociety.org/grants-schemes-awards/grants/research-grants/>

### Copyright information:

The above plan creator(s) have agreed that others may use as much of the text of this plan

as they would like in their own plans, and customise it as necessary. You do not need to credit the creator(s) as the source of the language used, but using any of the plan's text does not imply that the creator(s) endorse, or have any relationship to, your project or proposal

# Insights into confinement effects on structural properties of liquids by total neutron scattering

---

## 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?**

- No - only institution involved

**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?**

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

Raw total neutron scattering data will be accessible via STFC ISIS Neutron and Muon Source repository: <https://data.isis.stfc.ac.uk/> - data collected during each experiment receives specific doi numbers

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

- < 1 TB

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

- Yes

Raw total neutron scattering data will be shared by STFC ISIS Neutron and Muon Source (Harwell Campus, UK) with the PI via data repository: <https://data.isis.stfc.ac.uk/>

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

- 11 - 20 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

**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?**

- Not applicable

**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?**

- Not applicable

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

- No

**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?**

Marta Falkowska

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

2022-10-13

## **Project details**

### **What is the purpose of your research project?**

The aim of the project is to build an understanding of confinement effects on structural properties of liquids. This will be achieved by total neutron scattering experiments realised at STFC facility - ISIS Neutron and Muon Source.

Raw data will be collected during the experiments and will be accessible through ISIS repository (with assigned doi numbers). The processed data will be stored at Research Data Storage Service at UoM.

### **What policies and guidelines on data management, data sharing, and data security are relevant to your research project?**

The University of Manchester Research Data Management Policy

ISIS Data Policy

The University of Manchester Records Management Policy

<http://documents.manchester.ac.uk/display.aspx?DocID=14916>

The University of Manchester Publications Policy

<http://documents.manchester.ac.uk/display.aspx?DocID=28526>

The University of Manchester IT policies and guidelines

<http://www.itservices.manchester.ac.uk/aboutus/policy/>

The University of Manchester Intellectual Property Policy

<http://documents.manchester.ac.uk/display.aspx?DocID=24420>

## **Responsibilities and Resources**

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

Marta Falkowska and her future PhD students - data capture, metadata production, data quality, data quality, storage and backup. PI is responsible for data archiving and data sharing

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

Research Data Storage Service <1 TB

## **Data Collection**

### **What data will you collect or create?**

Data file format RAW/Nexus

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

Raw neutron scattering data will be stored in folders with specific 'RB number' that is assigned by ISIS Neutron and Muon Source in online catalogue at <https://data.isis.stfc.ac.uk/>

## Documentation and Metadata

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

Raw data from each experiment is automatically described in the online catalogue (<https://data.isis.stfc.ac.uk/>), additionally each data file within the folder is clearly described (automatically generated title, time of experiment, amount of neutron beam received, configuration of the instrument, etc.) which allows secondary users to re-process the data, if needed.

## Ethics and Legal Compliance

### How will you manage any ethical issues?

not applicable

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

The University of Manchester

## Storage and backup

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

Raw data will be stored on <https://data.isis.stfc.ac.uk/> and processed data will be stored at UoM Research Data Storage Service (uploaded quarterly).

### How will you manage access and security?

not applicable

## Selection and Preservation

### Which data should be retained, shared, and/or preserved?

The raw data is shared publicly after 5 years after the experiment. The processed data will be shared with interested researchers upon request.

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

5 years

## **Data Sharing**

### **How will you share the data?**

Data will be shared upon request with interested researchers

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

UoM IP Policy