Plan Overview

A Data Management Plan created using DMPonline

Title: High throughput mechanochemical synthesis for sustainable advanced materials

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Project abstract:

Future technologies will rely on the ability to create designed materials with novel properties on-demand. Promising examples of such material families that have emerged over the past two decades include two-dimensional materials (2D materials), metal-organic frameworks (MOFs) and covalent-organic frameworks (COFs). These have shown enormous performance benefits in key technologies including energy storage (novel electrodes, supercapacitors), wearables (flexible electronics), pollution remediation (adsorption, advanced oxidation, membranes), and green hydrogen (photo- and electro-catalysis). Nearly all these materials have yet to reach significant commercial scales, limiting their impact and slowing deployment into new technologies that can benefit society. Furthermore, many of these are produced using chemical processes that use large volumes of toxic solvents which are harmful to the environment.

Mechanochemical approaches are emerging as an exciting, sustainable, and green alternative that can produce new materials using mechanical force – reducing or completely removing toxic solvent waste. This approach works with liquid dispersions, slurries, or dry powders and is a stark contrast to traditional manufacturing which relies on large volumes of toxic and dangerous solvents and oxidising agents. For example, it can produce 2D nanomaterials via mechanical exfoliation of layered precursor crystals. While this approach has shown promise, the synthesis pathway from the instigation of mechanical force to the formation of products requires a better understanding to ensure promising laboratory processes can be translated to industrial scale operations. The aim of this research project is to utilise and develop new mechanochemical processes that vastly improve the throughput over existing technologies such as ball milling. High-throughput experimental and computational approaches will be used to obtain a critical understanding of mechanochemical synthesis routines and products.

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High throughput mechanochemical synthesis for sustainable advanced materials

Data Collection

What data will you collect or create?

The main set of data collected will be chemical analysis data, including numerical spreadsheets for UV-Vis, SEM and TEM images, Raman and XPS spectra, and XRD patterns.

How will the data be collected or created?

Primarily, the data will be collected from labratory experiments, being grouped by analysis method, date and experimental conditions.

Documentation and Metadata

What documentation and metadata will accompany the data?

Datasets will be accompanied by:

- A description of experimental conditions
- Date of data creation
- Instrumentation and software used
- Documentation of methodology and protocols

Ethics and Legal Compliance

How will you manage any ethical issues?

Currently, there are no known ethical concerns regarding the project. If any are found they are to be discussed with the relavent ethics boards.

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

Copyright and Intellectual Property Rights will be recognised and any confidentiality agreements will be respected.

Storage and Backup

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

Primary storage of the data will be on a laptop's hard drive, with a copy of any data being stored on a seperate drive located in the university as well as backups being located on a cloud storage system.

How will you manage access and security?

The data is encrypted and access requires the use of a password as well as 2-factor authentication.

Selection and Preservation

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

Currently, it is unknown what data is of long-term value but experimental research data is to be to stored and maintained.

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

At the publication of a paper, a subset of the data that underpins the paper will be transferred to the UoB Research Data Archive (RDA). Once transferred the data will be set to read-only to prevent any inadvertent additions or deletions of the dataset, Any changes will result in a new dataset, which will be archived separately. The RDA solution has been created to be highly resilient and is located at two data centers in two different sites, with a backup placed in a third site. Data will be stored for 10 years, should access to the data be requested within a 10 year period, the 10 year clock is then reset from the point of last access. After the 10 year period the data will be deleted.

Data Sharing

How will you share the data?

Data will be shared through the University of Birmingham's eData repository (https://edata.bham.ac.uk/Opens in a new window) which makes the datasets discoverable through search engines like Google. Publications will include a data access statement, linking to the dataset deposited in the University of Birmingham’s data repository where the data can be accessed by anyone or reasons and access conditions will be provided if the data cannot be shared openly.

Are any restrictions on data sharing required?

Any commercially confidential data may be made available to others subject to a suitable legally enforceable non-disclosure agreement.

Responsibilities and Resources

Who will be responsible for data management?

Aadam Rabani and University of Birmingham

What resources will you require to deliver your plan?

Appropriate access and training to required instrumentation as well as any corresponding analytical software:

- UV-Vis
- SEM
- TEM
- XRD
- XPS
- Ramas Spectroscopy

Data management will require the use of the University of Birmingham's Research Data Store for the storage of any digital data required.