Plan Overview

A Data Management Plan created using DMPonline

Title: Searching Improved Magnetocaloric Materials for Hydrogen Liquefaction Exploiting Magnetic Anisotropy (MAGCALORICH)

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Project abstract:

Refrigeration based on the magnetocaloric effect relies on the variation of a material’s temperature or entropy when exposed to a changing magnetic field, through adiabatic or isothermal processes, respectively. This effect is inherently anisotropic, reaching its maximum when the applied magnetic field aligns with the easy magnetization axis of a single crystal. However, the fabrication of single crystals imposes significant limitations in terms of versatility, with restricted sizes and shapes unsuitable for practical applications.

Polycrystalline materials, on the other hand, can be produced in a wide range of shapes and sizes, an advantage that has been further enhanced by the rapid progress of additive manufacturing. However, polycrystals are generally isotropic, which diminishes the magnetocaloric effect due to the averaging of properties across all crystallographic directions.

This project aims to address these challenges through a two-phase approach:

1. **Phase 1:** Manufacturing of magnetic polycrystals based on rare-earth-transition-metal (R-MT) intermetallic alloys and magnetic shape memory alloys with phase transitions in the 20–80 K range. These materials will be produced with preferential crystallographic

orientation along the easy magnetization direction.

2. **Phase 2:** Utilizing the knowledge gained to develop hybrid anisotropic materials, extending the working range of precursor materials, and exploring the fabrication of optimized components for magnetic liquefaction via 3D printing.

The **University of Oviedo** and **BCMaterials** have extensive experience in the development of advanced magnetic materials with high productivity, both individually and in collaboration. Their expertise in researcher training and dissemination of scientific results, both within academic and public spheres, provides a strong foundation for tackling the challenges outlined in this project.

The **coordinator** is a tenured professor at the University of Oviedo, coauthor of 50 Q1 journal articles and a book chapter (h-index = 21). He has participated in **six national and four regional research projects** and has led an industry-funded project in the additive manufacturing sector. His scientific contributions also include a book chapter and two translated popular science books.

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Searching Improved Magnetocaloric Materials for Hydrogen Liquefaction Exploiting Magnetic Anisotropy (MAGCALORICH)

Data Collection

What data will you collect or create?

This project involves the development of low-temperature magnetocaloric materials for liquefaction applications. A wide range of data will be collected and generated, including experimental measurements, structural and magnetic characterization, and data related to the synthesis process of the materials.

1. Data Types

- **Experimental measurements**: These will include magnetization curves as a function of temperature and magnetic field, adiabatic temperature changes (ΔTad), and specific heat measurements.
- **Structural characterization**: Data obtained from **X-ray diffraction (XRD)** and **neutron diffraction** for phase identification and lattice parameters, as well as images from **Scanning Electron Microscopy (SEM)** and **Transmission Electron Microscopy (TEM)** for microstructure and morphology analysis.
- **Synthesis data**: Parameters related to the fabrication of the materials using techniques like **arc melting**, **melt spinning**, and **ball milling**, including temperature, time, and pressure conditions.

2. Format and Volume

- **Data formats**: The primary formats will include **CSV** for tabular data (e.g., magnetization curves, specific heat measurements), **TIFF/PNG/JPEG** for SEM and TEM images, and **TXT** for raw data such as experimental conditions or synthesis parameters.
- **Software compatibility**: All chosen formats ensure compatibility with widely-used data analysis tools such as **Scilab, FullProf,** or **Origin**. This ensures that data can be easily shared, analyzed, and visualized by other researchers.
- **Data volume**: The volume of data is expected to be moderate, mainly consisting of tabular data (e.g., a few megabytes per measurement set) and image files (which may range from several megabytes to gigabytes depending on resolution and number of samples).

3. Long-term Access and Reusability

- **Reusability and open formats**: All data will be stored in **open formats** (e.g., **CSV**, **TIFF**, **PNG**) to maximize long-term usability and compatibility with existing repositories like **Zenodo** or **OpenAIRE**, ensuring that the data is readily accessible and reusable in the future.
- **Data storage and backup**: Data will be stored on institutional servers, with regular backups to ensure data integrity. Additionally, key datasets will be uploaded to public repositories for long-term preservation and sharing.
- **Complementary and reusable data**: Existing data from previous studies on magnetocaloric materials, available in public repositories (e.g., from **OpenAIRE** or **Zenodo**), will be reused where relevant. We will ensure compliance with any **copyright** and **IPR** issues, obtaining proper permissions for reuse and ensuring the data is made available with the least restrictions possible.

4. Long-term Value and Preservation

- Data on the **magnetocaloric properties** (e.g., ΔTad, magnetization) and **structural**

characteristics (e.g., XRD, SEM, TEM) are of long-term value and will be preserved and shared through open-access repositories to promote future research and development in this field.

- **Physical samples**: While physical samples may not be directly shared, the conditions and synthesis parameters used will be fully documented, enabling replication and further study.

How will the data be collected or created?

The data collection process will follow established methodologies for experimental research in the field of magnetocaloric materials. The key data types—magnetization, X-ray diffraction (XRD), neutron diffraction, SEM/TEM imaging, and adiabatic temperature change (ΔTad)—will be gathered using standard, well-established techniques in the field. Specifically:

- **Magnetization measurements** will be carried out using commercial systems such as **Quantum Design's PPMS** and **Physical Property Measurement System (PPMS)**, which are calibrated to meet community standards for magnetic property measurements.
- **XRD and neutron diffraction** experiments will be performed following established protocols, using high-resolution instruments like those available at the **ALBA synchrotron** and **Institut Laue-Langevin** facilities.
- **SEM/TEM imaging** will be done using electron microscopes equipped with energy-dispersive X-ray spectroscopy (EDX) to analyze the microstructure, morphology, and composition of the samples.
- **ΔTad data** will be collected using home-made systems.

While specific community standards for magnetocaloric materials may not be fully established, the data collection will align with best practices in material characterization and data reporting.

File and Folder Structure, Naming Conventions, and Versioning

The organization of data will follow a clear and consistent structure throughout the project to ensure traceability and easy access. The folder structure will be organized by data type and experimental phase, such as:

```
/ProjectName
  /Synthesis
    /Arc_Melting
    /Melt_Spinning
  /Characterization
    /XRD
    /Neutron_Diffraction
    /Magnetization
    /SEM_TEM
  /Data_Analysis
    /Raw_Data
    /Processed_Data
  /Reports
```

- **Naming conventions** will include a combination of sample identifiers, measurement type, and date to ensure clarity and consistency.
- **Versioning** will be managed using a combination of date-based naming for tracking major revisions in data processing scripts and analysis tools. Raw experimental data will be considered final once collected, while processed data will follow a versioning protocol that includes a date and version number for every new iteration.

Quality Assurance Processes

Quality assurance (QA) is critical to ensuring the consistency and reliability of the collected data. The following processes will be implemented to ensure the highest standards:

- **Calibration and Repeated Measurements**: All instruments will be calibrated regularly according to manufacturer instructions and standards. Repeated measurements will be taken at key points to ensure consistency, especially for **magnetization** measurements, which may be sensitive to experimental conditions.
- **Standardized Data Capture**: Data will be recorded using standardized templates for each type of measurement. For instance, magnetization curves will be recorded in a **CSV** format with specific columns for temperature, magnetic field, and magnetization.
- **Data Entry Validation**: Manual data entry, when required, will be validated by using cross-checks and independent review to minimize transcription errors.

Documentation and Metadata

What documentation and metadata will accompany the data?

To ensure that the data collected during this project can be correctly interpreted and reused, comprehensive documentation and metadata will accompany all datasets. This documentation will include basic details about the data as well as specific information on the methodology used, measurement units, and analytical processes.

1. Metadata to Enable Data Discovery and Interpretation

Each dataset will be accompanied by metadata that provides essential information to help other researchers understand and reuse the data effectively. The metadata will include:

- **Creator/Contributor Information**: Names of all researchers involved in data collection and processing, along with their affiliations and contact details.
- **Title and Description**: A clear and concise title and a description of the dataset, including its content and objectives.
- **Date of Creation and Versioning**: The date when the data was collected or processed, along with versioning information to track updates or changes in the dataset.
- **Conditions of Access**: Information on who can access the data, any restrictions (e.g., related to IPR or licensing), and the terms under which the data can be shared or reused.

2. Methodology and Analytical Information

The metadata will include detailed information on the methodology used for data collection, processing, and analysis. This will help secondary users understand the experimental setup and ensure that the data is reproducible. Key elements include:

- **Data Collection Methods**: A description of the experimental techniques used, such as **magnetization measurement**, **X-ray diffraction (XRD)**, **neutron diffraction**, **SEM/TEM imaging**, and **melt spinning** or **ball milling** methods.
- **Measurement Units and Variables**: Clear definitions of the variables measured (e.g., magnetization, temperature, magnetic field, adiabatic temperature change) along with the units used (e.g., A/m, K, Tesla).
- **Calibration and Standardization**: Information on how instruments were calibrated and any standard procedures followed to ensure data consistency and accuracy.
- **Assumptions and Limitations**: Any assumptions made during the data collection or analysis

process (e.g., assumptions about sample homogeneity) and known limitations of the methods used (e.g., resolution limits for TEM).

3. Metadata Standards

To ensure consistency, interoperability, and long-term usability, metadata standards widely recognized in the scientific community, ensuring compatibility with data repositories like **Zenodo**, **Figshare**, and **OpenAIRE**, and improving the discoverability and reuse of the data, will be used. In particular,

- **Dublin Core Metadata Initiative (DCMI)**: This widely adopted standard will be used for basic metadata elements such as title, creator, and date of creation.
- **Material Data Interchange Format (MDIF)**: A specialized standard for materials science data that includes details such as crystal structures, compositions, and processing conditions.
- **Machine-Readable Metadata**: Metadata will be stored in machine-readable formats (e.g., XML, JSON) to facilitate automated processing and integration with data repositories.

4. Documentation Formats and Location

The metadata and documentation will be stored in **separate README files** or embedded in the headers of the data files themselves (for example, in **CSV** files or **TIFF** images). This will include:

- **README Files**: For each data folder or experiment, a **readme** file will be created that summarizes the dataset content, measurement conditions, and relevant metadata.
- **File Headers**: For tabular data and image files, key metadata (e.g., experiment date and sample ID) will be embedded in the file header for easy retrieval and context.
- **Repositories**: The metadata and documentation will also be stored in **repositories** linked to each dataset, ensuring centralized access and easy retrieval.

Ethics and Legal Compliance

How will you manage any ethical issues?

The data to be collected during this project involves well-established techniques such as **X-ray diffraction**, **neutron diffraction**, **SEM/TEM imaging**, and **magnetization**. These are standard materials science methods that do not involve human subjects, animals, or sensitive personal data.

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

1. Ownership of Data

In this project, the **University of Oviedo** will be the primary owner of the data generated, as the institution is the leading partner. Any data produced through collaborations with other partners or external entities (e.g., companies, research institutes) will be governed by specific **collaborative agreements** that detail the ownership rights. In the case of multi-partner collaboration, ownership and IPR will be clearly outlined in a **consortium agreement** to avoid any ambiguity and to ensure fair distribution of rights.

As the lead researcher, I, Pablo Álvarez-Alonso, will retain the rights to manage and share the data in line with the institution's policies. Any intellectual property arising from the project, such as innovations in the magnetocaloric materials developed, will be subject to the **University’s IPR policy**

and **national IP laws**.

2. Licensing for Data Reuse

The data generated during this project will be made available for reuse under an **open access license** to promote transparency, accessibility, and collaboration. The exact license will depend on the nature of the data, but it is expected to be one of the following:

- **CC BY** license will be applied, allowing others to freely use, share, and adapt the data, as long as proper attribution is given to the original creators.

3. Restrictions on Reuse of Third-Party Data

If any **third-party data** are used in the project (e.g., commercial data or data from other research groups), we will ensure that:

- The data is used **under the terms and conditions** specified by the third party.
- Proper **attribution** is given to the original creators of the data.
- Any **IPR restrictions** are respected, and we will obtain the necessary **permissions or licenses** to reuse the data, if required.
- The data will only be used for the purposes outlined in the project and will not be shared beyond the scope of the agreement without prior approval from the third-party data owner.

For any third-party data that are **subject to commercial restrictions or non-disclosure agreements (NDAs)**, we will ensure that these limitations are clearly stated and adhered to in the project documentation.

4. Data Sharing and Postponement

Data sharing will primarily be **open and accessible**, but there are some cases where sharing may be postponed or restricted:

- **Patents or Proprietary Information**: If the data generated in the project results in new, patentable discoveries (such as novel materials or processes), the sharing of certain data may be delayed to allow time for **patent filing**. This delay would not exceed **6 months** from the discovery date to allow for the patent process to be initiated, after which the data will be made publicly available.
- **Sensitive Data**: In cases where data is considered **commercially sensitive** or includes unpublished results that could jeopardize a future patent or proprietary application, access to the data may be temporarily restricted. The length of the restriction will depend on the specifics of the data and will be determined on a case-by-case basis.

Once any intellectual property protection (such as a patent) or sensitive data concerns are addressed, the data will be **deposited in an open-access repository** and made available under the selected license for reuse.

Storage and Backup

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

1. **Storage and Backup Plan**

- **Data Storage Location**:
  - **OneDrive Cloud storage service** will be used. This system allow the data to be backed up automatically and access to different versions of the document.

- The final version of each file will be kept in the researcher's computer, connected to OneDrive.

2. **Backup Responsibility**

- **Data Backup Responsibility**:
  - The **Principal Investigators** will oversee the backup process, with **research staff** ensuring that data is consistently uploaded and properly backed up.

3. **Backup and Recovery Procedures**

- **Incident Recovery**:
  - In the event of an incident, such as data loss, the following process will be followed:
    - **Step 1**: The **research staff** will notify the **PIs** immediately, as they are responsible for restoring data from the backups.
    - **Step 2**: The **PIs** and **research staff** will initiate the **recovery process** from the most recent backup and ensure the data is restored to its original location.
    - **Step 3**: The **research staff** will confirm the recovery of the data.

How will you manage access and security?

1. **Data Security and Compliance**

- **Sensitive Data Protection**:
  - If sensitive data is involved, such as proprietary experimental methods or unpublished results, extra measures will be taken, including **encryption** of data before storage and using **encrypted backups**.
- **Data Security Risks**:
  - The main risks involve **data theft**, **data corruption**, or **accidental deletion**. These will be mitigated through:
    - **Encryption** of sensitive files.
    - **Access controls** to limit who can modify or access the data.

2. **Access Control**

- **Who Can Access the Data?**:
  - **Research Team**: the research team will have access to data related to experiments.
  - **Collaborators**: Collaborators from other institutions will be granted access via secure cloud repositories or cloud storage services.
- **Access Control Mechanisms**:
  - **Password Protection & MFA**: All accounts and systems containing research data will require strong passwords and multi-factor authentication (MFA) to prevent unauthorized access.

3. **Data Security Monitoring**

- **Security Monitoring**: Continuous monitoring of data storage systems will be undertaken to detect any unauthorized access, unusual patterns, or possible breaches.
- **Incident Response**: A detailed incident response plan will be in place to ensure quick action in case of a security breach. The plan includes notifying relevant stakeholders, investigating the incident, and taking corrective action.

Selection and Preservation

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

1. Data to be Kept

- **Core Experimental Data**: Key datasets that directly contribute to the published results and validation of findings should be retained for long-term use. These include:
  - **Experimental Data**: X-ray, neutron diffraction data, magnetization measurements, adiabatic temperature change, and SEM/TEM images.
  - **Synthesis Data**: Parameters from techniques like arc furnace, melt spinning, and ball milling, including the conditions under which samples were produced.
  - **Characterization Data**: The results of structural and magnetic characterization of the materials, such as lattice parameters, magnetic moment, entropy variation, and thermal measurements.
- **Models and Simulation Data**: Simulations used to predict material properties or performance, model input files and results should also be kept.
- **Documentation**: Data related to the methodologies and procedures used, including calibration data, equipment logs, and experimental protocols.
- **Data from Public or Third-Party Sources** : If external data are used in your research, these should be retained as long as the original terms of use allow, and any relevant documentation (licenses, citations) should be stored.

2. **Data Retention Period**

- **Research Data**: In accordance with the funding body and university policies, **research data should be retained for a minimum of 5-10 years** after the publication of the final project results. This ensures that the data is available for replication, review, and further analysis by the research community.
- **Sensitive Data**: Any sensitive or proprietary data, particularly related to intellectual property, should be retained until the patent process is complete or until there are no further commercialization interests.
- **Long-Term Preservation**: Even after the mandatory retention period, key datasets, especially those with potential for reuse in future research, should be preserved in a **long-term archive**.

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

1. **Repository for Data Storage**

- **Repository**: The dataset will be deposited in a **well-established, trusted repository**. It will provide:
  - **Long-term, secure access** to scientific datasets
  - **DOI (Digital Object Identifier)** for easy citation and permanent linking.
  - **Open-access** policies ensuring broad availability of the data.
  - **Version control** for tracking updates to the dataset.
- **Institutional Repository**: In addition to or instead of an open-access repository, the dataset

related to experiments carried out in large facilities or external laboratorios may be archived in the **corresponding institutional repository** (if available). This ensures long-term curation and institutional support for the preservation of the data.

3. **Costs for Repository or Archive**

- A **free access** repository for academic datasets will be selected.

4. **Timeline for Data Preparation**

- **During Project Phase**: Data preparation for sharing will begin during the data collection phase, particularly ensuring that files are organized and properly formatted as the research progresses.
- **Post-Project Phase**: Once the main experimental work is completed and publications are prepared, the final dataset, along with its metadata and documentation, will be uploaded to the chosen repository. A timeline will be set to ensure that data sharing happens promptly after publication to ensure its long-term accessibility.
- **Post-Project Updates**: Any updates to the dataset (e.g., new data resulting from follow-up experiments) will be tracked using version control in the repository.

5. **Long-Term Data Management After Grant Completion**

- **Repository Curation**: After the project ends, the selected repository will ensure the curation of the dataset. Both **Zenodo** and **Figshare** have been proven to be sustainable platforms for long-term data archiving and will maintain the datasets with minimal risk of data loss or inaccessibility.
- **Periodic Updates**: The dataset will be updated, if necessary, to ensure it remains accessible and accurate. Any updates or improvements to the dataset will be logged as part of version control.

6. **Effort**

- The preparation of data for sharing and long-term preservation will be integrated into the regular workflow of the research team. A portion of the research team's time will be dedicated to cleaning and formatting the data, creating comprehensive metadata, and preparing the documentation.

Data Sharing

How will you share the data?

1. **Potential users and conditions**

- **Open Access**: The data will be shared **openly** with the academic and scientific community, as well as with any interested stakeholders, without restrictions. The use of **open-access repositories** ensures that the data can be accessed by anyone, without paywalls or subscription barriers.
- **Conditions for Use**: The dataset will be released under **CC BY**.

2. M**echanism followed for data sharing**

- **Primary Method - Repository**: The **primary method for data sharing** will be via the chosen open-access repository.
    - **DOI and Citation**: The dataset will be assigned a **persistent identifier**, making it easy for researchers to find and cite the data. The DOI will be included in relevant publications,

research articles, and project reports, allowing users to track the data.

- **Secondary Method - Direct Requests**: If specific data or a subset of data is needed and is not readily available via the repository, data will be shared **directly upon request**.
    - A dedicated contact email will be provided for such requests on the repository and publications.
- **Data will be available:**
-
    - **Post-Publication**: The dataset will be made available **immediately after the publication** of related research findings. This aligns with the expectation that data should be accessible at the time of publication to allow for full transparency, validation, and reproducibility of the results.
    - **During Ongoing Research**: In some cases, preliminary datasets (with proper documentation and clear labeling) may be shared during the research process if they can add value to the research community, particularly in open-access platforms or conferences.

Are any restrictions on data sharing required?

1. **Expected Difficulties**

- **Intellectual Property Rights (IPR)**: Certain results or insights obtained from the magnetocaloric materials may be at risk of being used by third parties before patents are filed.
    - **Action to Overcome**: To address this, we will consider the option of postponing public release of specific sensitive data until patents or related intellectual property protection have been secured. This will be managed by collaborating with the institution's **Technology Transfer Office (TTO)** to ensure compliance with IP laws and regulations.
- **Exclusive Use Period**: We may need **exclusive use of the data for up to 12-18 months** after the collection period to complete the necessary patent applications and avoid jeopardizing the IP's commercial potential.
    - **Data Ownership and Control**: During this exclusive period, the data will remain under the control of the research team and institution, with the understanding that once the exclusive period expires, the data will be shared openly. The **institutional repository** will be notified of the data release to ensure it is properly archived and accessible.
- **Data Sharing Agreement (DSA)**: If the data includes collaborations with external partners, a formal DSA will be required to clarify the conditions under which the data can be shared, who can access it, and the terms of reuse. This agreement will include clauses about the duration of data confidentiality, the conditions under which data can be accessed, and how it will be handled if it is deemed sensitive.

Responsibilities and Resources

Who will be responsible for data management?

1. **Responsibility for Implementing and Reviewing the Data Management Plan (DMP)**

- **Primary Responsible**: The **Principal Investigator (PI)**, **Pablo Álvarez-Alonso**, will be responsible for implementing the Data Management Plan (DMP) and ensuring it is reviewed and revised as necessary throughout the project. The PI will ensure the DMP aligns with institutional

policies and funder requirements and will oversee periodic reviews to ensure it reflects any changes in the project or data management needs.

- **Review of DMP**: The DMP will be reviewed and updated at regular project milestones (e.g., at 6-month intervals or following major data collection events), and any required updates will be made to ensure the plan remains aligned with project goals and evolving data needs.

2. **Responsibility for Specific Data Management Activities**

- **Data Capture**: Individual researchers and technicians in the institutions will be responsible for capturing data in their respective experimental setups. Each researcher will follow the established data capture protocols and formats outlined in the DMP.
- **Metadata Production**: Individual researchers and technicians in the institutions will be primarily responsibles for ensuring that their data are properly documented with metadata according to the agreed-upon standards.
- **Data Storage and Backup**: Each research member will store their data in their dedicated, OneDrive folder.
- **Data Archiving and Sharing**: The **IP** will coordinate the archiving of data at the end of the project. They will ensure that data is deposited in an appropriate **public repository** after publication and patenting, ensuring compliance with the DMP.

What resources will you require to deliver your plan?

1. **Training**

- **Research Team**: The research team will need training on **best practices for data management**, such as standardized data capture methods, proper metadata documentation, and the use of the selected data repository. Training will be provided by the **IP**.

2. **Hardware and Software Requirements**

- - **Data Management Software**: A repository software will be required to manage, store, and share the data.
  - **Metadata and Documentation Tools**: Software for metadata creation and documentation will be essential for ensuring that each dataset is described comprehensively. The research team may also require software like **Origin, Kaleida Graph, or Scilab** for organizing and analyzing data before sharing.
  - **Cloud-based storage solutions** will be used to store on-going data.

3. **Data Repositories**

- **Repository Fees**: The selected **public data repositories** will not charge for data deposition.
- **Institutional Repository**: The institutional repositories that will be used are free of charge.

4. **Legal resources**

- **Legal and Compliance Resources**: Legal or compliance experts may be required to ensure that the project adheres to **data protection** and **IPR laws**, especially when dealing with proprietary data or sensitive information. In this case, we will consult with the university's legal department to draft data sharing agreements or non-disclosure agreements (NDAs) for collaborators.
- **Data Sharing Agreements (DSA)**: In the case of sharing data with external partners or institutions, dedicated legal resources will be required to draft and review **Data Sharing Agreements** to clarify rights, obligations, and restrictions.