Graphene, MXene and ionic liquid-based sustainable supercapacitor

GREENCAP - Deliverable report

D7.2 – Data Management Plan

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Summary

This document is a deliverable of the GREENCAP project, funded under the European Union's Horizon Europe research and innovation programme under grant agreement No. 101091572.

The ultimate objective of GREENCAP is the realization of a Critical Raw Material-free technology exhibiting a battery-like energy density (>20 Wh/kg, >16 Wh/L), together with the distinctive superior power densities and high cycle life of traditional electrochemical double layer capacitors. By rationally exploiting layered 2D materials, including graphene and MXenes as electrode materials, and ionic liquids (ILs) as high-voltage electrolytes, GREENCAP aims to bring technological advancements in the SC fields, producing novel types of cylindrical cells, controlled via customized SC management system, at a TRL 6, while ensuring the creation/existence of the complete value chain from material to cell producers.

To implement its workplan, GREENCAP will collect and generate data obtained from different sources and experimental methodologies, and it is expected to provide datasets useful for research beyond the project itself. Most of the research data will be managed and processed, within the project life, through the internal project platform (METT), even though permanent and certified public repositories will be used for long-term storage to promote the re-usability of consolidated datasets. In this context, the Data Management Plan (DMP) identifies the type of project's research data, describing how to make them findable, accessible, interoperable, and reusable according to the Findable, Accessible, Interoperable ad Reusable (FAIR) principles. The present deliverable is the initial version of the DMP, aiming at proposing a general approach to handle the research data during and after the end of the GREENCAP project. It provides guidelines to specify which data will be generated in the project, the standards/methodology that will be used, how the data will be exploited and/or shared/made accessible for verification and re-use, and how this data will be curated and preserved (including after the end of the project). In accordance with the guidelines provided by the European Commission (EC), this initial DMP is intended to be a living document that will be continuously updated as the implementation of the project progresses and considering the discussions between the partner of the consortium.

This deliverable is structured following the Horizon Europe DMP template. After introducing the GREENCAP project summary and the importance to follow the approach "as open as possible, as closed as necessary" towards FAIR data (Section 1), the Data Summary (Section 2) provides general information about the data types and formats, as well as their utility in the project. Section 3 describes how GREENCAP adopts the principles of FAIR data. The next sections explain other aspects, such as the Allocation of resources (Section 4), Data security (Section 5), Ethical aspects and other issues (Section 6), and Risk Register (Section 7). This deliverable does not include any deviation from the objectives and timings planned in the Grant Agreement of the project.

Contents

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Abbreviations & Definitions

Abbreviation	Explanation
2D	Two-dimensional
CRM	Critical Raw Material
DMP	Data Management Plan
DOI	Digital Object Identifier
EC	European Commission
EM	Electrode material
EU	European Union
FAIR	Findable, Accessible, Interoperable ad Reusable
FLG	Few-layer graphene
HPH	High-pressure homogenization
IG	Ionogel
IL	Ionic liquid
IP	Intellectual Property
IPR	Intellectual Property Rights
LPE	Liquid-phase exfoliation
SC	Supercapacitor
SLG	Single-layer graphene
WJM	Wet-jet milling

1 Introduction

This deliverable, D7.2 – Data Management Plan, aims at proposing a general approach to handle the research data during and after the end of the GREENCAP project, providing practices and guidelines to indicate which data will be generated, processed, and collected, to what extent this data will be publicly available, and how data will be curated and preserved (including after the end of the project). The document also addresses several aspects on how to make the data produced in the GREENCAP project as FAIR as possible, following the guidelines provided by the EC. This deliverable does not include any deviation from the objectives and timings planned in the Grant Agreement of the project. Based on the guidelines provided by the EC, the Data Management Plan (DPM) of GREENCAP will be considered as a living document. If needed, it will be updated as the implementation of the project progresses and considering the discussions between the GREENCAP consortium.

1.1 GREENCAP project summary

A paradigm shift in energy storage technology is needed to support the transition towards the climate neutrality set by the EU's international commitments under the Paris Agreement while ensuring the targets of EU's Action Plan on Critical Raw Materials (CRMs). In this context, GREENCAP joins a multi-disciplinary consortium with 5 Universities, 1 R&D Institute, 5 companies, located in 7 European countries including Italy, Germany, France, Ireland, United Kingdom, Estonia, and the Netherlands, to unlock the full potential of supercapacitors (SCs) as electrochemical energy storage systems. The ultimate objective of GREENCAP is the realization of a CRM-free technology exhibiting a battery-like energy density (>20 Wh/kg, >16 Wh/L), together with the distinctive superior power densities and high cycle life of traditional electrochemical double layer capacitors. GREENCAP will exploit layered two-dimensional (2D) materials, including graphene and MXenes as electrode materials, and ionic liquids (ILs) as high-voltage electrolytes. The main objectives of GREENCAP are: i) to synthesize/functionalize graphene and MXenes via facile, scalable, and sustainable (CRM-free) methodologies, assuring both high surface area and ion accessibility, introducing Faradaic charge storage mechanisms, and improving their quantum capacitance; ii) to produce novel non-/low-toxic and non-/low-flammable IL-based electrolyte with high conductivities, and a high electrochemical/thermal stability, ensuring SC operation at voltage > 3.5 V within -50°C to +100 °C temperature range, thus eliminating the need for sophisticated cooling systems; iii) to validate the novel SC technology at industrial scale by fabricating cylindrical cells at a TRL 6 while ensuring the creation/existence of the complete value chain from material to cell producers; iv) to produce a novel supercapacitor management system, enabling the full potential of the GREENCAP's SCs in high-end applications, and ensuring their integration into the circular economy. Accordingly, different types of data are expected to be produced during the project, coming from the development of electrode materials and ILs, the characterization of SCs, and the development of a supercapacitor management system. This DMP aims at defining the procedures and practices to handle the research data during and after the end of the project, specifying which data will be generated, processed, and collected, to what extent this data will be publicly available, and how data will be curated and preserved (including after the end of the project).

1.2   Structure of this document

This DMP first provides a summary of the data that will be collected (and monitored) during the project (Chapter 2). Chapter 3 discusses how the project will implement the Findable, Accessible, Interoperable and Reusable (FAIR) principles for data. Chapter 4 deals with the allocation of resources to implement the FAIR principles and data management as well as data security. Ethical aspects are reported in Chapter 5. In Chapter 6 Conclusions and Recommendations are given.

1.3   Background on FAIR Data

According to EC's guidelines, publishing research data must follow the approach "as open as possible, as closed as necessary" [2]. The objective behind this EC's incentive is to maximise the impact of EU-funded research projects and accelerate the technological implementation of findings through the interaction of the data produced in several research projects. Nevertheless, ensuring usefulness of the produced research data beyond the objectives of the single project is a challenging task [3]. The concepts of Findable, Accessible, Interoperable and Reusable (FAIR) data raised to ensure [4]: 1) proper collection, annotation, and archival of project data; 2) long-term care of valuable digital assets, with the goal that they should be discovered and re-used for downstream investigations, either alone or in combination with newly generated data. Thus, the DPM must ensure high-quality digital publications that facilitate and simplify the process of discovery, evaluation, and reuse in downstream studies.

To univocally reference and cite data in research communications, it is essential to assign a unique and persistent identifier that enables persistent linkages to be established between the data, metadata, and other related materials to assist their discovery and reuse. Related materials may include the code or models necessary to use the data, research literature that provides further insights into the creation and interpretation of the data, and other related information. Thus, data that are "Findable" means that data can be easily found through appropriate search tools, including search engines on the Internet. Data must then be "Accessible" by humans and machines upon appropriate authorisation and through a well-defined and universally implementable protocol. Noteworthy, accessibility does not mean that data are provided in open and reusable formats without any constraint. Accessibility means that the human or machine is provided - through metadata - with the precise conditions by which the data are accessible and that the mechanisms and technical protocols for data access are implemented such that the data and/or metadata can be accessed and used. To be "Interoperable", data and metadata must also use a formal, accessible, shared, and broadly applicable language for knowledge representation. Thus, according to FAIR principles, the (meta)data are described using normative- and community-recognised specifications, vocabularies, and standards that determine the precise meaning of concepts and qualities that the data represent. Interoperability is a key feature in the value and usability of data. In FAIR principles, technical interoperability means that the (meta)data and related information are encoded using a standard that can be read on all applicable systems. Instead, legal interoperability means that (meta)data should be "Reusable". To be "Reusable", (meta)data must meet community standards and provide information about their sources. Thus, data must be accompanied by their creation methods (e.g., survey protocols and experimental processes) and information about data processing. Open community-endorsed formats also play a key role in

reusability. The conditions under which the data can be used should be transparent to both humans and machines. This means that data must be released with a clear and accessible data usage license. Based on these considerations, the main goal of this DMP is to provide indications on how to make the data generated within the GREENCAP project as FAIR as possible. The development of vocabulary/ontologies used in the SC-related disciplines, and the development of other tools for metadata generation are some topics that will be further discussed among GREENCAP. For example, in Part B of Grant Agreement No. 101091572 – GREENCAP, the identification of proper performance metrics and their accurate calculation have been already identified as essential methodological aspects to guarantee a reliable benchmarking of GREENCAP's SC technologies with commercially available ones.

In accordance with the guidelines provided by the EC, this DMP will be considered a living document in which information will be made available on a finer level of granularity through updates as the implementation of the project progresses and when significant changes occur [1]. More in particular, the DMP will be updated over the course of the project whenever significant changes arise, such as (but not limited to): new data; changes in consortium policies (e.g., new innovation potential, decision to file for a patent); changes in consortium composition and external factors (e.g., new consortium members joining or old members leaving).

2 Data Summary

Within the GREENCAP project, a vast amount of data will be generated and collected across all work packages and activities. The purpose of the data collection within GREENCAP is to propose an innovative energy storage system, which is a CRM-free SC technology exhibiting a battery-like energy density (>20 Wh/kg, >16 Wh/L), together with the distinctive superior power densities and high cycle life of traditional electrochemical double layer capacitors. This chapter will specify the types and formats of data that will be collected and re-used in the project (Section 2.1), and to whom it will be useful outside of the GREENCAP project (Section 2.2).

2.1 Data Types and Formats

In order to monitor and collect the data generated during the project, the coordination team (UNR and BED) defined a dedicated template that will be discussed and updated during project General Assemblies (GAs). The template will be stored and accessible at the data-sharing platform *Mett*.

The file collects all necessary information as requested by the official template (selection in the list below):
- Data Summary
    - Type and format
    - Origin of the data
    - Quantity and storage of data set
- Fair data
    - Naming used
    - Identifiability/mechanism used
    - Which data will be available and how
    - Possible restrictions
    - Timing for re-use
- Allocation of resources
    - Costs
    - Responsibilities

Table 1 enlists the main data types that are being generated or collected within GREENCAP. It also contains the purpose of the data, the production methods, the format, and the users or stakeholders for whom the data might be useful.

2.2 Data Utility

The aggregated data from this project may be useful to a wide variety of stakeholders: nanomaterial and SC manufacturers, the scientific community of hybrid stationary energy storage systems, decision makers (for the new designs), policymakers, experts in standardization and legislation sector, system operators, academia, potential end users, etc.

In addition, the raw data sets may also be useful for other complementary or future research projects.

Naturally, project data is useful for the different GREENCAP partners. Data from data owners may be shared upon reasonable request by other partners. A reasonable request excludes company secrets or company-sensitive information.

Table 1 - Type of data per WP with its purpose, the data production method, format, and users

WP	Data type	Purpose	Data production methods	Data format	Useful for which stakeholders/users
1-5	Literature review	Updating on recent progresses in the SC field	Researching, reading, analyzing, evaluating, and summarizing literature (typically journals and articles) about a specific topic	.docx, .pdf., .ppt, etc…	Nanomaterial manufacturers, SC manufacturers, energy industries, EU project coordinators, scientific community, etc…
1-4	Experimental data – linked to D1.3 (see WP1, task 1.3 in Annex I)	Evaluation of SC materials and device configurations	Compositional characterizations, structural/morphological and other physical characterizations, electrical and electrochemical characterizations	.csv, .xlsx, .opj, .txt., .rtf, etc…	Nanomaterial manufacturers, SC manufacturers, energy industries, EU project coordinators, scientific community, etc…
1-5	Methods	Ensuring data reproducibility and reusability	Description of methods used for the data creation (*e.g.*, survey protocols and experimental processes) and information about data processing	.docx, .rtf, .txt, etc…	Nanomaterial manufacturers, SC manufacturers, energy industries, EU project coordinators, scientific community, etc…
1-4	Component designs	Realization of innovative SC devices	Description of the component specifications as measured through experimental protocols (*e.g.*, standards)	.docx, .rtf, .txt, etc…	Nanomaterial manufacturers, SC manufacturers, scientific community
5	Environmental and socio-economic impact assessment	Evaluation of the benefits resulting from GREENCAP technologies	International Standard Organization 14040–14044 standards and other relevant methods identified during the project	.docx, .rtf, .txt, etc…	Nanomaterial manufacturers, SC manufacturers, energy industries, EU project coordinators,

	e.g., life cycle assessment				Scientific community, general audience
7	Project internal communications	Effective coordination of the GREENCAP activities	Elaboration of minutes and document reporting relevant project internal communication to partners	.docx, .rtf, .txt, etc…	All project partners
1-7	Official project reports	Evaluation of project's progresses and elaboration of mitigation measures in presence of delays	Drafting and approval of project's deliverables and project's reports	.docx, .rtf, .txt, etc…	Project officer, EC. For public deliverables: EU project coordinators, scientific community, general audience
7	Peer-reviewed research articles	Disclosing the technological progresses of GREENCAP activities, stimulating advancements in SC state of the art, and preparing the industrial uptake of innovative technologies	Data elaboration and analysis through suitable data analysis and graphing software (*e.g.*, Origin, MatLab Excel and PowerPoint), elaboration of the drafts to submit to the journals	.docx, .ppt., .opj, .xlsx, .mat, .rtf, .txt, etc…	Nanomaterial manufacturers, SC manufacturers, energy industries, EU project coordinators, scientific community, general audience
7	Stakeholder contacts	Data will be used to contact the stakeholders for communicating and dissemination results of the project	Stakeholder database generated based on contacts of all project partners	Data: text format table (.txt, .xls)	All project partners

3 FAIR Data

The following sections describe how GREENCAP adopts the principles of FAIR data.

3.1 Making data findable, including provisions for metadata

All data generated and collected within GREENCAP will be made easily findable by providing a rich set of metadata describing the dataset and a standard, unique and persistent identifier, in case of scientific publications preferably DOI (Digital Object Identifier). All deliverables that are intended for public use will also be made available for download *via* the GREENCAP website.

The basic metadata that will be defined for each dataset and or document are the following:
- Title
- Description
- Creator and contributors
- Specification of the data identifier(s)
- Publisher (if relevant)
- Date of data collection
- Dates of document creation and last revision
- Language
- Keywords (defined by GREENCAP partners)
- Acknowledgement of the EC funding of the GREENCAP project

3.1.1 Naming conventions for file identification

To enable findability of data/research outputs the naming convention will be GREENCAP-DATA_TYPE-DATE.EXTENSION.

In order to facilitate quick identification and indexing, the consistent naming of all the data will function as metadata. Deliverables will be named and numbered in the following way:
GREENCAP-DXX_TYPE-DATE.EXTENSION for an easy data identification within the project, andGREENCAP_<dnum>_<sdis>_<orgshortname>_v<ver>.pdf to connect the type of data to the deliverable and organization when necessary.

- <dnum> represents the code of the deliverable
- <sdis> is filled with the acronyms related to dissemination level (e.g., SEN = sensitive, PU = public)
- <orgshortname> organization that is performing the changes on the version.
- <ver> the version of the document.

Versions 0.X will indicate that the document is still a draft. The first official document to be sent to the EC will be numbered v1.0. Further revisions or new issues of a deliverable will make use of the following format: v1.X when drafting and v2.0 when submitting and successively.

3.2   Making data openly accessible

GREENCAP follows the principle "as open as possible, as closed as necessary". Therefore, data generated and collected throughout the project will be stored in an open repository as far as possible to be accessible to a wider community.

The data which will be made openly available will correspond to the Public Deliverables (those deliverables classified as PU). Such deliverables will be in the Public Domain. Data that is made openly available will be on an Open Access website at the end of the project. Should any specific instructions be required to facilitate data access, such as information relating to the nature and origin of the data, then these will be provided when the data is deposited. The data selected for open access will be made available without restrictions. The data relating to deliverables that are classified at the consortium level will be stored within the internal project platform (METT) with access restricted to the partners in the consortium.

It is worth noticing that **23 out of a total of 29 GREENCAP deliverables are public**, highlighting the commitment from the consortium to ensure data and results from the project are openly available to and reusable by all interested parties.

3.3   Making data interoperable

To make our data interoperable, all GREENCAP (meta)data will use a formal, accessible, shared, and broadly applicable language for knowledge representation.

All data collected during the project will be exported to standard data formats (when possible) to facilitate interoperability. These may include .rtf, .txt, and .docx for reports, and .csv and .xlsx for numerical datasets. (Note, that .docx and .xlsx are Microsoft Office specific and hence, not necessarily standard format – but are included due to the wide distribution of Microsoft Office.)

3.4   Increase data re-use

At present, there is no standard regarding the licensing of data generated by GREENCAP and it is likely that data licensing will be decided on a case-by-case basis. Where possible, the most liberal approach will be used in accordance with Horizon Europe recommendations, except for data that is of commercially confidential nature, which will necessarily be subject to more restricted licensing. If licensing the use of data arises, this will be noted in a future DMP update. Typically, data will remain usable for 24 months after the project's completion.

4   Allocation of resources for FAIR data and data security

4.1   Allocation of resources

The responsibility for data management rests with the principal investigator at each of the project partners/host institutions. The storage of project data (in for example PubMed, ArXiv, ChemRxiv, TechRxiv, Preprints.org, Qucosa, Zenodo, OpenAIRE, univOAK, Partners' own servers, project sharepoint, public website, EOSC) is free, however, person-months will need to be allocated for the preparation of files. Personnel costs for efforts for data handling are included in the project's budget. The costs corresponding to the open-access provision of research publications and research data have been included as *other goods and services* in the budget. The potential value associated with the long-term preservation of data and the costs, including how data will be kept beyond the project, how long (at least 2 to 5 years), and how the costs will be met, will be discussed by the consortium in the coming months.

4.2   Data security

Project data will be stored in an open repository to make it accessible to a wider community based on the following classification level:
- **Public:** project data that can be published on GREENCAP website/registries of scientific repositories and disseminated to a wider community.
- **Confidential:** project data for which there is some obligation to third parties not to fully disclose; this data, therefore, will be disseminated to the public only upon the project partners' agreement and in a restrictive way; this classification level includes deliverables categorized as "sensitive" in terms of dissemination level and listed as such in the Grant Agreement.
- **Internal:** project raw data used by consortium partners during the project, which is not available for publishing.

Each consortium partner is responsible for the proper storage, processing, and sharing of the data created during their project activities. Each consortium partner is responsible for storage capacities of the data created during their project activities, for such data backup and recovery according to the partner's organisation internal rules.

As previously stated, the report deliverables to the EU are planned to be openly accessible on the public website of the GREENCAP project. These reports and other project-related documents will be stored by the coordination team (BED and UNR) using the internal project platform (METT). UNR has a contract with METT detailing provisions for data security, continuity, and availability.

5 Ethical aspects and other issues

Based on the ethics self-assessment, there are no ethical issues that may arise from the research activities of GREENCAP, and no ethical or legal issues have been identified that could have an impact on data sharing. An appropriate Consortium Agreement has been elaborated to manage the ownership of results and access to key knowledge (Intellectual Properties Rights -IPR- and research data). The IPR strategy considers diverse commercialization channels including patents, copyrights, and trade secrets. IPR is handled in line with general EC policies regarding ownership, exploitation rights, confidentiality, commercial utilization of results, availability of the information, and deliverables. The critical Intellectual Property (IP) required for the successful completion of the GREENCAP project are either owned by the consortium members or the consortium has preliminary checked the freedom to operate, and IPR protection measures have been defined in the Consortium Agreement. A list of the most relevant patents by GREENCAP partners can be found in Part B of Grant Agreement No. 101091572 – GREENCAP. The background IP brought by partners will be available for use, remaining the property of the original owner. IP developed during the project will be owned by the partner(s) who develop it. The decision to publish IP will be made by the GREENCAP consortium and the strategy for exploitation of the results will vary on a case-by-case basis, ranging from free access to licensing. Ownership agreements will be set up whenever necessary to proceed with commercialization.

6 Conclusion and Recommendation

This deliverable report presents a preliminary Data Management Plan outlining the production, handling, preservation, and re-use of the (research) data generated in the GREENCAP project. In addition, the methods that allow to make those data FAIR are demonstrated. The GREENCAP consortium commits to abide by the provisions described in this report. It is worth noting that this is a living document, which will be modified and updated throughout the lifetime of the project.

7 Risks and deviations from Annex I

No risks have arisen related to this deliverable. There are no deviations from the description of this deliverable as given in Annex I of the Grant Agreement.

7.1 Interconnections with other deliverables

This Data Management Plan also describes data that will lead to results that might have possible exploitable value. Therefore, this DMP can also be seen as making clear which partner(s) will produce specific data for possible future exploitation and intellectual property protection. The DMP serves as the initial guidance for these exploitations, and it will be updated throughput the project.

8 References

[1] European Commission, "Guidelines on Fair Data Management in Horizon 2020," no. July, 2016

[2] European Research Council (ERC), "Guidelines on Implementation of Open Access to Scientific Publications and Research Data in projects supported by the European Research Council under Horizon 2020," no. April, pp. 1–7, 2017.

[3] European Commission, "Turning FAIR into reality: final report and action plan from the European Commission Expert Group on FAIR Data," 2018.

[4] M. D. Wilkinson et al., "The FAIR Guiding Principles for scientific data management and stewardship," Sci. Data, vol. 3, no. 1, p. 160018, Dec. 2016, doi: 10.1038/sdata.2016.18.

9 Acknowledgement

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Project partners:

#	Partner short name	Partner Full Name
1	BED	BEDIMENSIONAL SPA
2	SOLV	SOLVIONIC
3	FSU	FRIEDRICH-SCHILLER-UNIVERSITAT JENA
4	SKL	SKELETON TECHNOLOGIES OU
5	TCD	THE PROVOST, FELLOWS, FOUNDATION SCHOLARS & THE OTHER MEMBERS OF BOARD, OF THE COLLEGE OF THE HOLY & UNDIVIDED TRINITY OF QUEEN ELIZABETH NEAR DUBLIN
6	TUD	TECHNISCHE UNIVERSITAET DRESDEN
7	UNISTRA	UNIVERSITE DE STRASBOURG
8	SM	SKELETON MATERIALS GMBH
9	UNR	UNIRESEARCH BV
10	CNR	CONSIGLIO NAZIONALE DELLE RICERCHE
11	UCAM	THE CHANCELLOR MASTERS AND SCHOLARS OF THE UNIVERSITY OF CAMBRIDGE