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GUIDELINES AND BEST
PRACTISES FOR BATTERY
DATA MANAGEMENT AND
SHARING
BATTERY 2030+ CSA3

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At the heart of a connected green society

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TABLE OF CONTENTS

1	Introduction.....	4
2	Core Principles of Data Management and Sharing	5
2.1	The FAIR Principles of Data Management.....	5
2.1.1	Findable	5
2.1.2	Accessible	5
2.1.3	Interoperable.....	5
2.1.4	Reusable	6
2.2	Linked Data in Battery Research.....	6
2.2.1	Unique Identifiers for Entities	6
2.2.2	Structuring Data with RDF	6
2.2.3	Embedding Metadata with JSON-LD	6
2.2.4	Benefits for Battery Research.....	7
3	Guidelines and Best Practices.....	8
3.1	Best Practice: Use reliable and FAIR-aligned repositories for publishing data	8
3.2	Best Practice: Prioritize Non-Proprietary, Widely Supported Data Formats	8
3.3	Best Practice: Provide machine-readable and human-readable metadata	9
3.4	Best Practice: Validate datasets using controlled vocabularies and ontologies	9
3.5	Best Practice: Link datasets to external resources using RDF and URIs	10
4	Data sharing in Practice.....	11
4.1	The BIG-MAP data infrastructure	11
4.1.1	Towards the creation on a EUnified battery data space	11
4.2	Practical Checklist for Data Sharing.....	13
5	Conclusion	14
6	REFERENCES	15

1 INTRODUCTION

Data is the backbone of research, providing the critical foundation for discovery, analysis, and validation of results. High-quality, well-organized data ensures that research findings are accurate, reproducible, and reliable. However, research data encompasses far more than raw or processed numbers derived from experiments, simulations, or artificial intelligence. It also includes a wide range of associated materials such as physical samples, standard operating procedures, laboratory notebooks, images, and videos, as well as scripts and codes used in analysis. These resources are vital components of the research ecosystem and must be made accessible and usable far beyond the timeline of the projects in which they were generated.

Over the past decade, significant strides have been made in defining principles for data management and sharing, culminating in the development of the FAIR principles—Findable, Accessible, Interoperable, and Reusable. These principles are now widely accepted across research disciplines and provide a conceptual framework for organizing and sharing data. However, FAIR principles alone do not provide a detailed roadmap or practical tools for their implementation. Translating FAIR principles into actionable strategies remains a challenge for many research communities, especially those dealing with complex and interdisciplinary datasets.

Building on the foundation of the FAIR principles, the Battery 2030+ initiative has recognized the need for a unified approach to data management in battery research. As part of this vision, our work aims to standardize battery research data across the 15+ projects under the Battery 2030+ umbrella. This deliverable focuses on practical solutions for creating and sharing data within a dedicated and ontologized battery data space. A central element of this effort is the BIG-MAP data infrastructure developed under the H2020 BIG-MAP project, which provides the tools and platform needed to support a unified data ecosystem.

The BIG-MAP data infrastructure serves as the cornerstone of this effort, integrating tools to store, annotate, and share data while ensuring compliance with FAIR principles. It includes platforms for secure data storage, electronic laboratory notebooks for standardizing workflows, an app store for processing tools, and a comprehensive battery ontology to enable semantic interoperability. These components collectively contribute to the creation of a cohesive battery data space, where researchers can efficiently share and access high-quality, standardized data.

In this deliverable, we outline our progress toward establishing these unified data standards, with an emphasis on practical implementation and interoperability. We also describe how the BIG-MAP infrastructure facilitates data sharing across projects, ensuring that all participants in Battery 2030+ have access to a robust, secure, and FAIR-compliant data ecosystem. This report highlights the workshops, tools, and practices developed to enable researchers to adopt these standards and contribute to a more collaborative and data-driven future in battery research. Through these efforts, Battery 2030+ is setting a new benchmark for effective data management and sharing in the field of energy storage.

2 CORE PRINCIPLES OF DATA MANAGEMENT AND SHARING

Managing and sharing data effectively is critical for fostering collaboration, enhancing reproducibility, and driving innovation in battery research. This section outlines the foundational principles for battery data management and sharing, emphasizing the FAIR data principles and the adoption of linked data approaches. Together, these principles provide a robust framework for ensuring that battery data is discoverable, accessible, interoperable, and reusable.

2.1 The FAIR Principles of Data Management

The FAIR principles provide a guiding framework for optimizing the utility of research data. FAIR stands for Findable, Accessible, Interoperable, and Reusable, emphasizing the importance of structured, well-documented, and openly shared datasets. Adhering to these principles ensures that data can be utilized across disciplines and applications, maximizing its value in both research and industry settings.

2.1.1 Findable

Data must be easily discoverable for both humans and machines. Key to achieving findability is the inclusion of metadata—structured information that describes the content and context of a dataset. To ensure discovery:

- Assign persistent identifiers (e.g., DOIs) to datasets, ensuring a unique and permanent reference.
- Use searchable repositories and catalogues to host data.
- Include detailed metadata that describes the dataset's purpose, format, and origin.

Example: A dataset describing battery cycling data could include metadata fields such as the test conditions, electrode composition, and data collection dates, ensuring clarity for potential users.

2.1.2 Accessible

Research data must be available to those who need it, under clear terms and conditions. Accessibility involves:

- Hosting data on open-access platforms or repositories to eliminate barriers.
- Ensuring that data is stored in widely supported, non-proprietary formats, allowing easy access without specialized tools.
- Providing usage terms through clear licensing, such as Creative Commons licenses.

Example: A battery test dataset shared via Zenodo or a university repository with a CC BY 4.0 license ensures accessibility while maintaining proper attribution.

2.1.3 Interoperable

To maximize its potential, data should integrate seamlessly with other datasets and tools. Interoperability requires adherence to common standards and the use of controlled vocabularies to describe data:

- Employ widely adopted formats like JSON-LD, CSV, or RDF for structured data.
- Use ontologies, such as the Domain Battery Ontology, to ensure consistent terminology and definitions across datasets.

Example: A dataset on electrolyte properties described using RDF and linked to external material databases enables integration with other research platforms.

2.1.4 Reusable

Rich metadata and clear licensing ensure data can be reused effectively across projects and disciplines. Reusability involves:

- Providing comprehensive metadata, including details on the methodology, variables, and units of measurement.
- Documenting datasets with human-readable descriptions and machine-readable metadata to support diverse user needs.
- Using standardized, open data formats to maintain compatibility over time.

Example: A dataset with metadata detailing the experimental conditions of a battery degradation study—temperature, current density, and material properties—ensures that others can reproduce or build upon the study.

2.2 Linked Data in Battery Research

In the context of battery research, the adoption of linked data principles provides a transformative approach to organizing, sharing, and integrating data. Linked data enables disparate datasets to be connected in a meaningful, machine-readable way, enhancing their usability across research disciplines. This section explores key aspects of linked data relevant to battery research, including the use of unique identifiers, structured data frameworks, and embedded metadata.

2.2.1 Unique Identifiers for Entities

A foundational principle of linked data is the assignment of unique identifiers to entities. Uniform Resource Identifiers (URIs) serve as these unique identifiers, ensuring that each entity—whether it be a material, process, or dataset—is referenced unambiguously across datasets and systems.

For instance, a specific battery cell could be assigned a URI such as <http://example.org/batteryCell/123>. This identifier allows researchers to refer to the same entity consistently, regardless of the dataset or application in which it appears. URIs also facilitate linking related entities, such as connecting a battery cell to its manufacturer, performance data, or test results.

By ensuring that all entities have unique and persistent URIs, linked data practices eliminate ambiguities, making datasets interoperable and more reliable for both humans and machines.

2.2.2 Structuring Data with RDF

The Resource Description Framework (RDF) provides the backbone for representing linked data. RDF structures information as triples—subject, predicate, and object—creating a graph that defines relationships between entities. This graph-like representation enables complex, interconnected datasets to be expressed in a way that machines can understand and process.

This structured representation enables the aggregation of data from different sources into a cohesive graph. Researchers can query and analyse the relationships within the graph, extracting insights that would be difficult or impossible with traditional tabular data formats.

The flexibility of RDF also allows it to describe a wide variety of entities and relationships, from materials and their properties to test methods and experimental results. This makes it an ideal framework for battery research, where datasets often span multiple disciplines and levels of detail.

2.2.3 Embedding Metadata with JSON-LD

JSON-LD (JavaScript Object Notation for Linked Data) is a practical and widely used format for implementing linked data. By embedding linked data directly into JSON—a format familiar to developers and researchers alike—JSON-LD makes it easier to adopt linked data principles without requiring extensive technical expertise.

JSON-LD enriches datasets by including metadata that describes the context and relationships of the data. For instance, a JSON-LD representation of a battery cell might include its name, manufacturer, and capacity, along with links to related entities such as the materials used in its electrodes. An example JSON-LD snippet for a battery cell could look like this:

```
{
  "@context": "https://w3id.org/emmo/domain/battery/context",
  "@type": "CR2032",
  "schema:name": "My CR2032 Coin Cell",
  "schema:manufacturer": {
    "@id": "https://www.wikidata.org/wiki/Q3041255",
    "schema:name": "SINTEF"
  },
  "hasProperty": {
    "@type": ["NominalCapacity", "ConventionalProperty"],
    "hasNumericalPart": {
      "@type": "Real",
      "hasNumericalValue": 230
    },
    "hasMeasurementUnit": "emmo:MilliAmpereHour"
  }
}
```

In this example, the @context field specifies the vocabulary used to interpret the data (Schema.org), while @type defines the entity being described (a CR2032 battery cell). The inclusion of a capacity object provides structured information about the battery's capacity, including its value and unit of measurement.

JSON-LD's ability to integrate metadata seamlessly into datasets makes it an indispensable tool for battery research. It ensures that datasets are both human-readable and machine-readable, enabling better data sharing and collaboration.

2.2.4 Benefits for Battery Research

Adopting linked data practices allows researchers in the battery domain to address key challenges such as data silos, inconsistent formats, and the lack of interoperability that often hinder progress. These practices facilitate integration across domains, enabling connections between diverse datasets, such as linking materials science data with performance metrics or environmental impact assessments. By breaking down barriers between datasets, linked data creates opportunities for interdisciplinary collaboration and comprehensive analysis.

Additionally, linked data enhances discoverability. Researchers can query interconnected datasets to identify specific relationships, such as understanding how a material's properties influence a battery's lifespan. This interconnectedness ensures that critical insights can be uncovered more efficiently, without requiring manual assembly of disparate datasets.

Linked data also supports automated analysis by providing computational tools with access to structured, machine-readable graphs. These tools can navigate and analyse complex data structures with precision, unlocking patterns and relationships that might otherwise remain hidden. For instance, a researcher might query a linked data graph to identify all battery cells with capacities exceeding 3.0 Ah and using lithium-ion chemistry. By leveraging RDF and JSON-LD, this information can be extracted seamlessly from multiple datasets, demonstrating the power and utility of linked data in advancing battery research.

3 GUIDELINES AND BEST PRACTICES

Effective data management is essential for ensuring the utility, interoperability, and reusability of battery research data. By adhering to best practices for publishing, annotating, and sharing data, researchers can improve collaboration, support reproducibility, and enhance the impact of their work. This chapter outlines actionable guidelines and a practical checklist to help researchers manage their data effectively.

3.1 Best Practice: Use reliable and FAIR-aligned repositories for publishing data

Description: Publish your data using reliable repositories that ensure long-term accessibility and adherence to FAIR principles. Examples include platforms such as Zenodo, Figshare, and institutional repositories, which provide persistent identifiers (e.g., DOIs) and facilitate data citation.

Why: Reliable repositories make datasets easily discoverable, citable, and accessible, encouraging reuse and collaboration. Persistent identifiers ensure that data can always be referenced accurately, even if moved to a different server.

How: Select an appropriate open repository based on your institution or community preferences. During the upload process, attach an open license, such as Creative Commons Attribution (CC BY 4.0), to clearly define reuse terms. Ensure that datasets are uploaded in structured formats, such as CSV, JSON, or HDF5, and avoid proprietary formats like Excel unless strictly necessary.

Example: A dataset detailing charge-discharge cycling tests for a lithium-ion battery is published on Zenodo with a DOI, an open-access license, and associated metadata describing the conditions of the experiment.

3.2 Best Practice: Prioritize Non-Proprietary, Widely Supported Data Formats

Description: Structure datasets using standardized formats to ensure they are easily interpretable and interoperable across platforms and tools. Widely used tabular formats like CSV or XLSX and hierarchical formats like JSON or XML provide flexible options for different data types. For long-term usability, prioritize non-proprietary formats over proprietary ones.

Why: Non-proprietary formats like CSV, JSON-LD, or HDF5 ensure compatibility with a broad range of tools and software, avoiding potential issues associated with proprietary formats such as Excel. These formats enhance data sharing, integration, and reuse, making them suitable for collaborative and multidisciplinary research.

How: When preparing datasets, assess the intended use cases and select formats that offer both flexibility and accessibility. Avoid proprietary formats unless they are essential for specific workflows. Convert data stored in Excel or similar tools into open formats like CSV for tabular data or JSON-LD for structured linked data. Ensure the format supports the metadata and data structures required for long-term storage and sharing.

Example: A dataset containing voltage and current measurements from battery cycling tests is saved as a CSV file, with clearly labelled columns and metadata provided in a corresponding README file. The CSV format ensures the dataset can be opened and processed by a wide range of tools, both now and in the future.

3.3 Best Practice: Provide machine-readable and human-readable metadata

Description: Provide both machine-readable and human-readable metadata to enhance the usability and understanding of your datasets. Include fields that describe the dataset's title, description, creator, keywords, and creation date.

Why: Metadata ensures datasets are discoverable, interpretable, and reusable. Machine-readable metadata supports automated processes and integration with software tools, while human-readable metadata provides clarity for researchers unfamiliar with the dataset.

How: Use standards such as DCAT or Schema.org for structuring machine-readable metadata. For human-readable metadata, include a README file with contextual descriptions of the dataset, such as experimental setup, data collection methods, and any pre-processing steps. Ensure metadata describes units, variables, and any assumptions.

Example: A dataset of electrochemical impedance spectroscopy measurements includes metadata fields such as the creator (e.g., SINTEF), date (e.g., 2024-10-31), and dataset description (e.g., "Electrochemical impedance data for lithium-ion batteries at various frequencies and temperatures"). The README explains how the data was collected, its structure, and how to interpret it.

3.4 Best Practice: Validate datasets using controlled vocabularies and ontologies

Description: Validate your datasets by using controlled vocabularies and ontologies, such as the Battery Domain Ontology or the Elementary Multi-perspective Materials Ontology (EMMO). Perform periodic reviews to maintain alignment with evolving standards.

Why: Controlled vocabularies and ontologies provide consistent terminology and definitions, improving dataset accuracy and interoperability. Regular updates ensure that datasets remain relevant and usable as new technologies and standards emerge.

How: Integrate ontology terms into your data descriptions using tools like rdflib or EMMOntoPy. Periodically review datasets to identify inconsistencies or outdated terminology. Align datasets with the latest ontology versions and community standards, leveraging Python libraries for version control and updates.

Example: A dataset describing a cathode material uses ontology terms such as "particle size distribution" and "electrical conductivity" from the Battery Domain Ontology. The dataset is updated annually to ensure compatibility with new ontology releases.

3.5 Best Practice: Link datasets to external resources using RDF and URIs

Description: Link your datasets to external resources using RDF vocabularies and assign unique URIs to entities to enhance integration and interoperability.

Why: Linking data to external resources enriches the dataset's context and value, enabling cross-domain analysis and collaboration. Unique URIs prevent ambiguity and allow seamless integration into global knowledge graphs.

How: Use RDF vocabularies like DCAT or domain-specific ontologies to describe data components and their relationships. Assign URIs to entities (e.g., materials, processes) and establish connections to relevant external datasets, such as material property databases or lifecycle assessment tools.

Example: A dataset on battery cycling performance links to external material property data for the electrode composition using RDF. The cycling performance data is represented in a knowledge graph, enabling researchers to query relationships between material properties and performance metrics.

4 DATA SHARING IN PRACTICE

Effective data sharing is essential to accelerate innovation, foster collaboration, and ensure the long-term usability of research data. The BIG-MAP data infrastructure provides a robust framework for data sharing, integrating tools that enable compliance with FAIR principles while addressing security and interoperability challenges. This section explores the practical implementation of data sharing through the BIG-MAP infrastructure and offers a checklist for researchers to optimize their data sharing practices.

4.1 The BIG-MAP data infrastructure

The BIG-MAP data platform comprises four main tools, namely:

- the archive (<https://archive.big-map.eu>),
- the electronic lab notebooks (<http://big-map-notebook.eu>),
- the app store (<https://big-map.github.io/big-map-registry>), and
- the battery ontology (<https://github.com/BIG-MAP/BattINFO>).

All of these contribute to the FAIR'ification of data in different ways, from providing a platform to store the data and code (archive and app store) to standardise and automate experiments (notebook) and creating a battery vocabulary (ontology).

To comply with the requirements of data security and protection, the data archive has recently been upgraded to ensure that each project in Battery 2030+ has a dedicated workspace to store data and share it only among the project participants (Figure 1). This is done with three levels of openness. At the lowest tier, data are shared only among the individual project participants. At a higher tier, the project can decide to share data between all the Battery 2030+ partners. At the highest tier, the project can decide to make the data available to the public (full open source).

By using one dedicated data infrastructure for all Battery 2030+ projects, we ensure interoperability and homogenisation of the data. This concept is being further explored by integrating ontology concepts into data and metadata, making (meta)data machine readable. We are continuously demonstrating how to use of the BIG-MAP infrastructure with Battery 2030+ project in large workshops or 1:1 dedicated meetings.

4.1.1 Towards the creation on a EUnified battery data space

Over the past two years, approximately 10 projects have joined the Battery 2030+ initiative. A key milestone in building a unified battery data space was a three-day workshop (January 29–31, 2024), where 50 participants engaged in hands-on demonstrations of the BIG-MAP tools. As can be seen in the figure below, the workshop consisted of presentations on the data infrastructure followed by practical demonstrations where all participants could try all the presented tools. Furthermore, round table discussions have been organised to plan how to further develop the synergy between projects on data.

Monday, January 29, 2024	
Free arrival – Optional activities/excursions Official check-in time 16:00 (earlier if room available) 17:00 Opening session: BIG-MAP and Battery 2030+ Tejs Vegge • Kristina Edström 17:20 Opening session: all project leads/representatives Quentin Bigouraux • Ivano Castelli • Gerhard Domann • Simon Clark • Joris de Hoog • Martin Thomas Horsch • Samson Yuxiu Lai • Kourosh Malek 18:20 Presentations by BIG-MAP prize winners Eibar Flores • Fuzhan Rahmanian • Laura Hannemose Rieger • Tushar Thakur • Monika Vogler 19:30 End of talks 19:45 Dinner	13:30 Demo desk: hands-on sessions (in parallel) – Hands-on session: uploading your data to the BIG-MAP Archive Valeria Granata – Hands-on session: FINALES and remote experiments Johan Carlsson • Matthias Albert Popp • Simon Steensen • Simon Stier • Monika Vogler – Hands-on session: Sharing ontologized scientific data through the BIG-MAP notebook Fernando Caro • Lukas Gold 15:00 Big picture session: panel discussion What are the special data requirements, formats, and quantities. What do we generate, what will we need in terms of data? Digital Materials and AI for Science in EU Ivano Castelli • Kristina Edström • Gerhard Goldbeck • Nicola Marzari • Giovanni Pizzi • Gian-Marco Rignanesi • Tejs Vegge 16:00 Coffee break 16:30 Demo session on BIG-MAP App Store Tushar Thakur 16:45 Demo session on BIG-MAP Apps: AiIDAlab Quantum ESPRESSO app Xing Wang 17:15 Demo on PANOSC search API in large-scale facilities Majid Ounsy 17:45 Follow-up/wrap-up Q&A 18:15 End of talks 19:00 Dinner 20:30 Socializing evening
Tuesday, January 30, 2024	
08:00 Breakfast 09:00 Data management plan for BIG-MAP Ivano Castelli 09:30 Demo session on BIG-MAP Archive Valeria Granata 10:00 Demo session on ELNs and semantic data annotations Fernando Caro • Lukas Gold • Simon Stier 10:30 Coffee break 11:00 Demo session on FINALES and remote experiments Johan Carlsson • Matthias Albert Popp • Simon Steensen • Simon Stier • Monika Vogler 12:00 Follow-up/wrap-up Q&A 12:30 Lunch	Wednesday, January 31, 2024 08:00 Breakfast 09:00 Big picture session: Introduction to EMMO, EMMC, Optimade Emanuele Ghedini • Gerhard Goldbeck • Gian-Marco Rignanesi 10:30 Coffee break 11:00 Demo session on integration with BATTINFO Simon Clark 11:30 Demo session on AURORA Edan Bainglass • Corsin Battaglia 12:00 Conclusions 12:30 Lunch

FIGURE 1: AGENDA OF THE EUNIFIED BATTERY DATA SPACE WORKSHOP

4.2 Practical Checklist for Data Sharing

To streamline data sharing, the following checklist provides researchers with actionable steps:

Publishing Data

- ✓ Use secure, FAIR-compliant repositories such as BIG-MAP Archive or Zenodo.
- ✓ Determine appropriate access levels (project-specific, consortium-wide, public).
- ✓ Assign persistent identifiers (e.g., DOIs) for datasets.

Data Formats

- ✓ Use structured, non-proprietary formats (e.g., CSV, JSON-LD, HDF5).
- ✓ Avoid proprietary formats like Excel unless necessary.

Metadata and Documentation

- ✓ Provide metadata compliant with standards like DCAT or Schema.org.
- ✓ Include comprehensive metadata and a README file for human-readable context.

Data Quality

- ✓ Validate data with controlled vocabularies and ontologies (e.g., EMMO, BattINFO).
- ✓ Regularly review datasets to maintain consistency with evolving standards.

Data Linking and Interoperability

- ✓ Use RDF vocabularies and URIs to link datasets to external resources.
- ✓ Incorporate ontological terms to ensure machine-readability and interoperability.

5 CONCLUSION

In this deliverable, we have detailed our progress toward implementing guidelines for data sharing within the Battery 2030+ initiative. Central to these efforts has been the enhancement and deployment of the BIG-MAP data infrastructure, a unified platform designed to support data sharing, interoperability, and FAIR compliance across multiple projects. The infrastructure now accommodates three tiers of openness, allowing projects to tailor data access based on their specific requirements—ranging from internal project sharing to full public availability.

The rollout of this infrastructure has been accompanied by comprehensive outreach efforts, including workshops and hands-on demonstrations, to ensure its effective adoption across all participating projects. These workshops have not only introduced the BIG-MAP tools to researchers but also fostered discussions about the broader vision of a unified battery data space. As a result, all projects within Battery 2030+ now have access to the BIG-MAP platform and have committed to uploading their newly generated data into this centralized repository.

However, the journey toward full data sharing and seamless interoperability is ongoing. While significant strides have been made, a closer integration between data, metadata, and the battery ontology (as outlined in Deliverable D3.1) remains a critical next step. Such integration will ensure that datasets are not only accessible but also interoperable and machine-readable, further enhancing their utility across disciplines and research objectives.

Looking ahead, several key challenges and opportunities will shape the path forward. Ensuring that metadata standards are uniformly applied across projects will require sustained effort, as will the task of continuously updating and aligning ontologies with emerging data types and research needs. Moreover, ongoing engagement with researchers through training and feedback will be essential to refine the tools and practices developed thus far.

In conclusion, the progress reported here underscores the potential of a unified, ontology-driven approach to data sharing in battery research. By addressing remaining challenges and deepening the integration of data and metadata with ontology frameworks, the Battery 2030+ initiative is well-positioned to set a new standard for collaborative and data-driven research. The steps taken so far lay a solid foundation for future advancements, ensuring that the shared data ecosystem supports innovation, reproducibility, and the broader goals of the scientific community.

6 REFERENCES

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