




FAIRLinked: Data FAIRification Tools for Materials Data Science

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

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Software

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Summary

FAIRLinked is a software package created to support the FAIRification of materials science data, ensuring proper alignment with FAIR principles: Findable, Accessible, Interoperable, and Reusable (Wilkinson et al., 2016). It is built to be compatible with MDS-Onto, an ontology designed to capture the semantics of various types of materials data, enabling integration and sharing across different research workflows (Rajamohan et al., 2025). The package is subdivided into three subpackages: InterfaceMDS, RDFTableConversion, and QBWorkflow. The first subpackage, InterfaceMDS allows users to search for terms using either string search or various filters, explore different domains and subdomains, and add terms to MDS-Onto. RDFTableConversion is used for serialization and deserialization of data from CSV into JSON-LDs and vice versa in a way that captures the semantics of the data using MDS-Onto. Lastly, QBWorkflow is a serialization and deserialization workflow that incorporates RDF Data Cube vocabulary, useful for working with multidimensional datasets. By offering these packages, FAIRLinked lowers the barrier of creating FAIR, machine-actionable data for researchers in the materials science community.

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Statement of Need

Modern materials science research generates data from a wide range of experimental techniques (e.g., synchrotron X-ray diffraction, IV measurements, Suns-Voc, pyrometry, spectroscopy, degradation measurements) spanning multiple application domains like photovoltaics, advanced manufacturing, and electronic components. These experiments produce measurements of various material properties under a multitude of environmental conditions.

The heterogeneity of these data sources introduces the well-known “3V” challenges of big data: volume, velocity, and variety (Laney, 2001). Materials science datasets can also be multimodal, consisting of numerical tables, images, time-series measurements, and other formats. Additionally, different research groups often use inconsistent terminologies, abbreviations, or naming conventions for the same quantities, instruments, or experimental procedures. This inconsistency creates substantial barriers to integrating datasets across laboratories and domains, thereby reducing interoperability and increasing the effort required to reuse data (Dernek et al., 2025; Tran et al., 2025).

To minimize the effort required to process and reuse historical materials data, these datasets must be machine-actionable. The FAIR principles, which stand for Findable, Accessible, Interoperable, and Reusable, offer a widely recognized framework for achieving this objective (Brinson et al., 2024; Hernandez et al., 2024; Huerta et al., 2023; Scheffler et al., 2022). Rather than prescribing specific technical standards, these principles define the qualities a dataset should possess to minimize human intervention and enable automated processing. One widely adopted approach to realize FAIR is through the Resource Description Framework (RDF), which represents knowledge as subject–predicate–object triples within a graph structure (Allenmang et al., 2020). RDF facilitates semantic interoperability by linking data to shared vocabularies and ontologies, enabling better integration and reuse across diverse experimental sources and terminological variations.

There exists a notable lack of dedicated software packages designed specifically to support materials research scientists in FAIRifying their data according to these guidelines. There are multiple tools designed to transform tabular data into linked data, like Virtuoso (Virtuoso, 2025) and morph-kgc (Arenas-Guerrero et al., 2024), but they require using R2RML Mapping Language (Das et al., 2012). This mapping language requires a good understanding of both relational databases and the RDF data model, making it difficult for many materials researchers to use these packages. FAIRLinked is created to be a dedicated simple package that enables both lightweight and RDF Data Cube-based FAIRification in materials data science by providing practical workflows and tools that transform terminologically inconsistent materials data into RDF-based, machine-actionable formats fully compliant with the FAIR principles.

Materials Data Science Ontology (MDS-Onto)

The Materials Data Science Ontology (MDS-Onto) was developed to support the FAIRification of materials science data by providing consistent vocabularies and abbreviations for a wide range of experimental contexts (Rajamohan et al., 2025). Materials science research produces data from diverse facilities, experimental techniques, and analysis workflows, resulting in highly variable vocabulary and inconsistent terminology. Differences in naming conventions and the omission of critical metadata, such as instrument details, pose challenges for data sharing and reuse. MDS-Onto addresses these issues by providing a standardized semantic framework that improves clarity, ensures contextual completeness of shared datasets, and facilitates interoperability across research groups. This common data model advances the goal of machine-actionable materials data science.

Terms in MDS-Onto are categorized using three attributes: domain, subdomain, and study stage. Domains and subdomains categorize different types of data within materials science, while study stages represent generic procedural steps in a study protocol. By embedding ontology terms with these attributes, MDS-Onto enables targeted term retrieval, allowing users to filter vocabulary based on research needs. For instance, a researcher focusing on photovoltaic cells can easily access only the terms tagged with the “PV-Cell” subdomain. This structured organization improves discoverability and ensures researchers can quickly identify the most relevant vocabulary for their work.

Key Features

The FAIRLinked package comprises three subpackages: InterfaceMDS, RDFTableConversion, and QBWorkflow, each addressing distinct aspects of FAIRification based on MDS-Onto.

- InterfaceMDS: Searching, filtering, and adding terms to MDS-Onto.
- RDFTableConversion: Create FAIR Linked data (JSON-LD).
- QBWorkflow: Create FAIR Linked data compliant with the RDF Data Cube Vocabulary.

Interfacing with MDS-Onto (InterfaceMDS)

The InterfaceMDS subpackage streamlines access to the large MDS-Onto by providing functions for:

- Retrieving the latest version of MDS-Onto,
- Searching ontology terms by string,
- Filtering terms by domain,
- Listing available domains and subdomains, and
- Adding new terms to a local ontology file.

These features make it easier for users to explore and discover relevant vocabulary without manually inspecting the ontology file.

FAIRLinked Core Workflow (RDFTableConversion)

The RDFTableConversion subpackage implements the core FAIRification workflow by guiding users through metadata template preparation, converting tabular datasets into JSON-LD, and enabling deserialization back into CSVs with relevant metadata. Each row of a CSV is transformed into an individual JSON-LD file with unique names created based on the study stages present in the data. Within these JSON-LDs, data are also linked with standardized QUDT units ([QUDT, 2022](#)) and ontology-backed terminology and definition. The workflow also supports iterative updates, allowing researchers to update JSON-LDs with new data obtained from analysis. Compared to the more complex RDF Data Cube approach, this provides a simpler path to making datasets FAIR and reusable but does not provide as many statistical contexts as QBWorkflow.

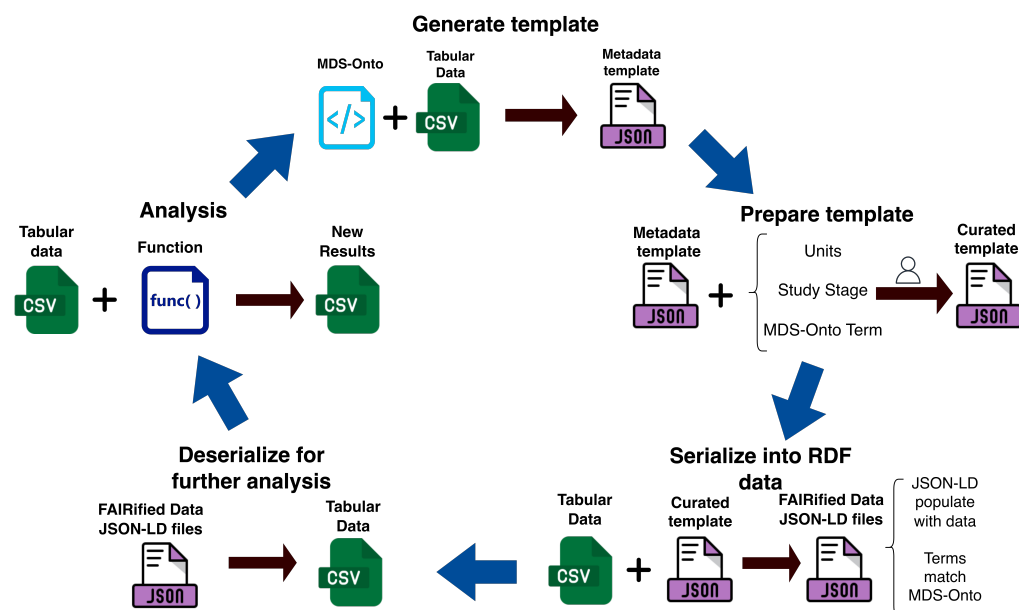


Figure 1: FAIRification Workflow for materials science data, which includes four steps: metadata template generation, conversion to ontology-compliant JSON-LD files, deserialization back to CSV, and iterative data analysis and update.

RDF Data Cube Workflow (QBWorkflow)

For users who wish to add richer metadata to their dataset, FAIRLinked provides the QBWorkflow subpackage, which utilizes the RDF Data Cube vocabulary to capture the structure of multidimensional data into a linked data format ([RDF Data Cube Vocabulary | DCC, 2024](#)).

Code Availability

The source code for FAIRLinked can be retrieved [from PyPi](#) or in the [GitHub repository](#).

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References

- Allenmang, D., Hendler, J., & Gandon, F. (2020). *Semantic Web for the Working Ontologist: Effective Modeling for Linked Data, RDFS, and OWL* (3rd ed.). Association for Computing Machinery. ISBN: 978-1-4503-7614-3
- Arenas-Guerrero, J., Chaves-Fraga, D., Toledo, J., Pérez, M. S., & Corcho, O. (2024). Morph-KGC: Scalable knowledge graph materialization with mapping partitions. *Semantic Web*, 15(1), 1–20. <https://doi.org/10.3233/SW-223135>
- Brinson, L. C., Bartolo, L. M., Blaiszik, B., Elbert, D., Foster, I., Strachan, A., & Voorhees, P. W. (2024). Community action on FAIR data will fuel a revolution in materials research. *MRS Bulletin*, 49(1), 12–16. <https://doi.org/10.1557/s43577-023-00498-4>
- Das, S., Sundara, S., & Cyganiak, R. (2012). *R2RML: RDB to RDF Mapping Language*. <https://www.w3.org/TR/r2rml/>
- Dernek, O., Mehdi, R., Yue, W., Bachman, J. A., Holt, F. R., Ponon, G. O., Tripathi, P. K., Willard, M. A., Ernst, F., & French, R. H. (2025). A Perspective on Synchrotron Data Science. *Interdisciplinary Information Sciences*, 31(1), 83–88. <https://doi.org/10.4036/iis.2025.A.08>
- Hernandez, K. J., Barcelos, E. I., Jimenez, J. C., Nihar, A., Tripathi, P. K., Giera, B., French, R. H., & Bruckman, L. S. (2024). A data integration framework of additive manufacturing based on FAIR principles. *MRS Advances*, 9(10), 844–851. <https://doi.org/10.1557/s43580-024-00874-5>
- Huerta, E. A., Blaiszik, B., Brinson, L. C., Bouchard, K. E., Diaz, D., Doglioni, C., Duarte, J. M., Emani, M., Foster, I., Fox, G., Harris, P., Heinrich, L., Jha, S., Katz, D. S., Kindratenko, V., Kirkpatrick, C. R., Lassila-Perini, K., Madduri, R. K., Neubauer, M. S., ... Zhu, R. (2023). FAIR for AI: An interdisciplinary and international community building perspective. *Scientific Data*, 10(1), 487. <https://doi.org/10.1038/s41597-023-02298-6>
- Laney, D. (2001). *3D data management: Controlling data volume, velocity and variety*. META group research note.
- QUDT. (2022). <https://www.qudt.org/>
- Rajamohan, B. P., Bradley, A. C. H., Tran, V. D., Gordon, J. E., Caldwell, H. W., Mehdi, R., Ponon, G., Tran, Q. D., Dernek, O., Kaltenbaugh, J., Pierce, B. G., Wieser, R., Yue, W., Lin, K., Kambo, J., Lopez, C., Nihar, A., Savage, D. J., Brown, D. W., ... French, R. H. (2025). Materials Data Science Ontology(MDS-Onto): Unifying Domain Knowledge in Materials and Applied Data Science. *Scientific Data*, 12, 628. <https://doi.org/10.1038/s41597-025-04938-5>

RDF Data Cube Vocabulary | DCC. (2024). <https://www.dcc.ac.uk/resources/metadata-standards/rdf-data-cube-vocabulary>

Scheffler, M., Aeschlimann, M., Albrecht, M., Bereau, T., Bungartz, H.-J., Felser, C., Greiner, M., Groß, A., Koch, C. T., Kremer, K., Nagel, W. E., Scheidgen, M., Wöll, C., & Draxl, C. (2022). FAIR data enabling new horizons for materials research. *Nature*, *604*(7907), 635–642. <https://doi.org/10.1038/s41586-022-04501-x>

SDMX User Guides | *SDMX – Statistical Data and Metadata eXchange*. (2025). <https://sdmx.org/user-guide/>

Tran, Q. D., Barcelos, E. I., & Bruckman, L. S. (2025). Designing Data-Centric Study Protocols Guided by FAIR Principles. *Interdisciplinary Information Sciences*, *31*(1), 75–82. <https://doi.org/10.4036/iis.2025.A.07>

Virtuoso. (2025). OpenLink Software. <https://vos.openlinksw.com/owiki/wiki/VOS>

Wilkinson, M. D., Dumontier, M., Aalbersberg, I. J., Appleton, G., Axton, M., Baak, A., Blomberg, N., Boiten, J.-W., Da Silva Santos, L. B., Bourne, P. E., Bouwman, J., Brookes, A. J., Clark, T., Crosas, M., Dillo, I., Dumon, O., Edmunds, S., Evelo, C. T., Finkers, R., ... Mons, B. (2016). The FAIR Guiding Principles for scientific data management and stewardship. *Scientific Data*, *3*(1). <https://doi.org/10.1038/sdata.2016.18>