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NFDI MatWerk Ontology (MWO): A BFO-Compliant Ontology for Research Data Management in Materials Science and Engineering

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The growing complexity and heterogeneity of research data in materials science and engineering (MSE) demand structured and interoperable solutions for effective data management and reuse. To address this challenge, this article introduces the National Research Data Infrastructure (NFDI)-MatWerk Ontology (MWO), as a semantic foundation to standardize metadata, link distributed datasets, and support digital research data management (RDM) in MSE. MWO addresses the need for the structured, standardized, and semantically rich representation of key entities, processes, and resources involved in the generation, sharing, and reuse of MSE research data. Aligned with the Basic Formal Ontology (BFO) , MWO develops as a modular extension of the NFDIcore ontology, and reuses Platform MaterialDigital core ontology (PMDco) MWO offers broad semantic coverage, modeling elements such as researchers, organizations, projects, software, workflows, datasets, metadata schemas, instruments, events, and services. It supports modular, scalable development through ontology design patterns (ODPs) and is maintained via the Ontology Development Kit (ODK) following best practices from the Open Biomedical Ontologies (OBO) Foundry. MWO also serves as the foundation for the MSE Knowledge Graph (MS-KG), which integrates semantically interlinked research data across the NFDI-MatWerk consortium and wider MSE community.

1. Introduction

Research data in Materials Science and Engineering (MSE) are produced in extremely large volumes and are highly heterogeneous due to diverse experimental methods, instruments, and simulation techniques. Most of these data remain unstructured, difficult to find, and often unusable beyond their original context. Digitalization in MSE is therefore crucial to make research data Findable, Accessible, Interoperable, and Reusable (FAIR).[1,2] A key requirement for achieving this is the development and application of ontologies, which are formal, structured representations of domain knowledge that define entities, their properties, and relationships in a machine-interpretable way. Ontologies enable semantic integration of data from multiple sources, improve interoperability across platforms, and support automated reasoning and data-driven discovery.[3] In MSE research, they play a vital role in linking experimental, computational, and materials property data, thus fostering reproducibility and accelerating innovation.[1] To realize these benefits, coordinated initiatives are needed to lead digital research data management (RDM) in MSE, providing shared standards, interoperable ontologies, and collaborative infrastructures that align with the FAIR principles and ensure long-term usability of scientific data.

The National Research Data Infrastructure (NFDI) is a German initiative launched in 2020 to systematically manage and network scientific data across disciplines, both nationally and internationally. Funded by the German Research Foundation (DFG), NFDI comprises 27 consortia, each representing a distinct scientific discipline and working together to build a sustainable infrastructure for RDM across Germany.[4] NFDI-MatWerk (in German: Nationale Forschungsdateninfrastruktur für Materialwissenschaft und Werkstofftechnik) is one of NFDI consortia dedicated to building a digital infrastructure for the MSE community. It focuses on integrating decentralized experimental and simulation data, metadata, workflows, and materials ontologies to improve data interoperability, reproducibility, and reusability. By providing standardized tools and frameworks,

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NFDI-MatWerk supports efficient RDM, long-term accessibility, and fosters collaboration and innovation across the MSE domain.[5] In this context, developing specialized metadata standards that incorporate domain knowledge is essential for improving data management and FAIRness, allowing for consistent descriptions, improved sharing, integration, and long-term use in MSE research. Ontologies support this by defining clear concepts and relationships within the domain, helping to standardize metadata and improve data integration across different systems.[3]

A variety of ontologies have been developed to date in the MSE domain, that can be categorized into below four levels depending on their abstraction and formal detail.[6,7] Top-level ontologies cover broad, general concepts shared across domains and provide a foundation for interoperability. Basic Formal Ontology (BFO)[8] and Elementary Multiperspective Material Ontology (EMMO)[9] are example top-level ontologies that establish semantic standards and incorporate universal and fundamental concepts for developing the ontologies in the MSE domain. Mid-level ontologies add more detailed, modular concepts that connect complex domain ontologies. For example, NFDIcore[10] and Platform MaterialDigital core ontology (PMDco)[11] are mid-level ontologies with the focus on RDM and MSE knowledge, respectively. Domain-level ontologies contain highly specialized expert knowledge specific to a domain, representing detailed concepts, rules, and relations. Materials Science and Engineering Ontology (MSEO),[12] Characterization Methodology Ontology (CHAMEO),[13] Mechanical Testing ontology (MTO),[3] Materials Ontology (MatOnto),[14] and Tribology Ontology (tribAIn),[15] are example domain-level ontologies in MSE domain. Eventually, application-level ontologies provide highly detailed semantics for specific domains.[16,17] For example, in the domain of materials mechanical properties testing, several application ontologies have been developed so far, including the Tensile Testing Ontology (TTO),[3,18] Fatigue Testing Ontology (FTO),[19] Vickers Testing Ontology (VTO),[20] and Tensile Stress Relaxation Ontology (TSRO).[21]

A critical barrier for effectively reusing the existing MSE ontologies is their very low level of interoperability. Interoperability refers to the capacity of ontologies to support consistent data representation, enable reuse across different systems, and facilitate semantic integration in diverse application contexts. Limited interoperability undermines data consistency, restricts scalability, and impedes collaboration across domains.[3,6] As a result, the efficiency and usability of ontologies in supporting comprehensive data integration and advancing interdisciplinary research are significantly compromised, highlighting the need for more coherent and integrative approaches to ontology development in MSE. Ensuring ontology interoperability requires adherence to a common foundational framework and shared formal standards. The ISO/IEC 21838-2:2021 standard establishes such criteria by specifying the use of BFO as a top-level ontology.[22] Developing ontologies in accordance with BFO principles promotes semantic coherence, enables integration with a wide range of ontologies, and supports high levels of interoperability across diverse domains.

The NFDI-MatWerk Ontology (MWO) is introduced in this article as a solution for developing a highly interoperable ontology through RDM-in-MSE domain. MWO aims to provide a structured, standardized, and semantically rich representation of concepts, processes, and resources involved in the generation, curation, sharing, and reuse of MSE research data. It formalizes key RDM-in-MSE elements (such as datasets, instruments, software, standards, and roles) while aligning with the BFO framework and existing standards to establish a highly interoperable and consistent ontological framework. Furthermore, MWO has been developed as a modular extension for NFDIcore and as such serves the same purpose as other NFDIcore module extensions like NFDI4Culture ontology (CTO)[23] and NFDI4DS ontology (nfdi4dso).[24] MWO enhances metadata quality through standardized metadata representation and improves data traceability, enabling more efficient data discovery. It facilitates the integration and interoperability of materials data across heterogeneous sources, supporting the seamless integration and reuse of decentralized data across platforms and research activities. By aligning with FAIR principles, MWO strengthens interoperability and reproducibility in MSE research, while promoting data sharing and collaboration across projects and institutions. Ultimately, it serves as a building block for the OneNFDI vision of enabling interoperability of research data across (all) disciplines.

To support these goals, MWO (v3.0.0) introduces several key features that enable consistent semantic representation, cross-source integration, and alignment with community standards, as outlined below: 1) Conforming to the ISO/IEC 21 838-2:2021 standard,[22] MWO is built upon BFO as the top-level ontology, developed as a modular extension of NFDIcore (a mid-level ontology for RDM concepts within NFDI consortia),[10] and integrates with PMDco (a BFO-aligned mid-level ontology in the MSE domain).[11] In addition, MWO incorporates entities from various other ontologies, including Information Artifact Ontology (IAO),[25] Software Ontology (SWO),[26] and Data Catalog Vocabulary (DCAT),[27] ensuring broad applicability and cross-domain connectivity. Through this standards-based alignment, MWO achieves high interoperability, enabling a high degree of reusability and extensibility. MWO currently serves as the foundation for several MSE-specific application ontologies. 2) MWO offers high semantic coverage and richness, providing the necessary expressiveness and depth to effectively capture the complex requirements of RDM-in-MSE. It models key aspects of MSE research, including community structures, projects, researchers, and organizations, as well as essential RDM resources such as software, workflows, ontologies, publications, datasets, metadata schemas, instruments, facilities, and educational materials. Furthermore, MWO represents academic events, training courses, international collaborations, and other community services, supporting a comprehensive and semantically coherent view of the MSE research ecosystem. 3) MWO is developed and released using the Ontology Development Kit (ODK),[28] which ensures a standardized workflow aligned with best practices from the Open Biomedical Ontologies (OBO) Foundry.[29] ODK supports automated quality control to enhance consistency, streamlines versioning, and release management, and standardizes ontology maintenance and documentation processes. 4) MWO's capacity for scalable, reusable, and semantically robust knowledge representation is strengthened through the use of MWO-aligned ontology design patterns (ODPs). ODPs provide standardized templates for tasks such as hierarchy modeling, semantic relationship management, and data source integration, enabling the development of technically sound and adaptable ontology structures.[30] Their application supports consistent, efficient, and extensible semantics, as demonstrated in several practical RDM-in-MSE use cases. 5) MWO provides the foundational framework for the design of the MSE Knowledge Graph (MSE-KG).[31] The MSE-KG is a structured digital resource that integrates heterogeneous research data through graph-based representations of entities and their relationships, enabling advanced querying, semantic understanding, and unified access to distributed data across the NFDI-MatWerk consortium and the broader MSE community. As the backbone of the MSE-KG, MWO substantially enhances data integration and retrieval, promotes interdisciplinary collaboration (especially with knowledge graphs from other NFDI consortia, like NFDI4Culture KG),[32] supports the digital transformation of materials research, and drives innovation through improved data discoverability, reusability, and semantic interoperability.

2. Competency Questions and Ontology Scope

Competency questions define the knowledge an ontology must capture, acting as functional requirements while helping to scope and delimit the represented domain. They guide ontology development by clarifying what content is essential and relevant. Designed by domain experts, these questions reflect real-world needs, ensuring the ontology supports intended use cases and aligns with community practices and expectations. In the context of MWO, a wide range of competency questions were provided by the NFDI-MatWerk community,[33] covering various key aspects of RDM-in-MSE. They emerged from a series of meetings within the MatWerk community and MSE domain experts. The process involved iterative discussion, consolidation, and refinement, where redundant questions were merged and the most relevant ones were prioritized. This ensured that the final set of questions reflected both community perspectives and practical applicability for ontology development. Examples of these competency questions are listed below: 1) What are the research projects associated to consortium/institution X1? Who is working there on project X2? 2) Who is the contact point (author, creator, contributor, etc.) for resource (project, software, dataset, publication, etc.) X? 3) List all roles of person/organization X? 4) List all available ontologies/workflow environments in subject area X? 5) List electronic lab notebooks (ELNs) used in project/organization X, including their type (commercial or open-source), name, provider, license, and data output format. 6) Where I can find instrument X1? list all institutions, addresses, contact points, and X2 characteristics of all available instruments. 7) What are the available educational resources for subject area X? 8) Which software or service tools were used by project X, including their name, type, version, and accessibility information? 9) Which software were provided by project X? What is the version, license, programming language, and repository URL of each software? 10) What are the reference/experimental/simulation datasets of process/material X? 11) List publications related to the project/software/dataset X. 12) Which training/educational services provided by person/organization/project X? 13) List all events related to subject area X.

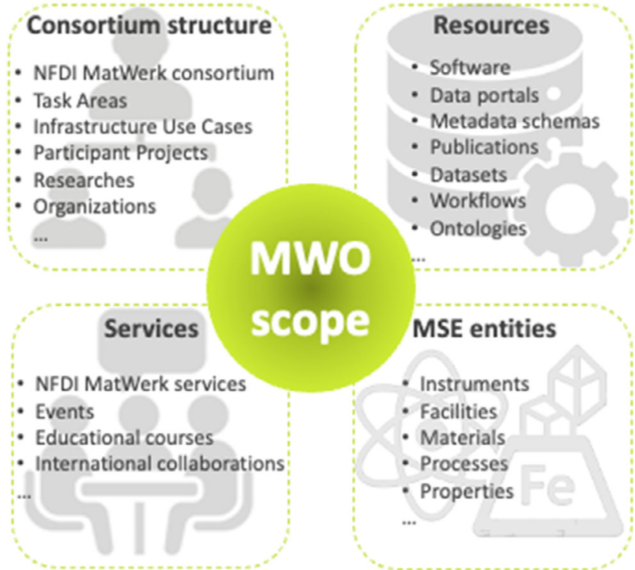

Figure 1. Key aspects of NFDI-MatWerk Ontology (MWO) scope.

To ensure that the desired ontology remains focused, relevant, and aligned with user and domain-specific requirements, the MWO scope has been formulated by analyzing the content and intent of aforementioned competency questions, which reveal the key concepts, relationships, and use cases the ontology must support. Accordingly, as also illustrated in **Figure 1**, the scope of MWO has been structured around the following key aspects: 1) Consortium structure: NFDI-MatWerk consortium, its structures (Task Areas (TAs), Infrastructure Use Cases (IUCs), and Participant Projects (PPs)), researches, and organizations, 2) NFDI resources: software, data portals, metadata schemas, scientific publications, datasets, workflows, and ontologies, 3) NFDI-MatWerk services, events, educational courses, and international collaborations, and 4) MSE-related instruments, facilities, materials, processes, and properties.

3. MWO Development

3.1. Collecting Ontology Key Concepts (terminology)

To ensure that the ontology effectively addresses the needs and priorities of the MSE community, a community-driven ontology development process was undertaken. In alignment with the defined competency questions and the overall scope of the ontology, key concepts in MWO were identified and refined through targeted surveys and expert consultations within the NFDI-MatWerk community. As a result, the ontology's terminology was shaped by inputs from community-driven competency questions, the requirements for representing diverse MSE research metadata, and the demands of MSE-KG development. Each collected term was carefully evaluated to determine whether it qualifies as an ontology entity, considering factors such as domain relevance, conceptual clarity, reusability, and semantic stability. This process culminated in the creation of the MWO terminology glossary, featuring precise labels and clear, community-aligned definitions for each entity.

3.2. Graphical Semantics Modeling

The visual representation of ontology entities was developed using the OntoPanel tool,[34] a graphical plugin for diagrams.net[35] which leverages a customizable shapes library and an integrated entity manager to simplify ontology modeling and visualization for domain experts. Within this framework, the ontology's terminological components were structured by organizing entities according to the hierarchy defined by desired top- and mid-level ontologies (see Section 4). This classification process was supported by extensive discussions with expert ontologists and guided by resources such as the BFO 2020 decision tree[36] and well-established OBO Foundry ontologies[37] to ensure consistent and accurate categorization. Likewise, ODPs and assertional component use cases were graphically modeled by identifying representative individuals and the semantic relationships between them. In line with OBO Foundry principles,[38] MWO introduced as few new object properties as necessary; instead, existing BFO 2020 properties were reused to represent most semantic relations, ensuring interoperability and adherence to established standards.

3.3. Ontology Development Kit (ODK)

MWO was developed collaboratively using GitHub-based workflows, supported by ODK. ODK is a toolkit designed to support the creation, maintenance, and release of ontologies, especially those aligned with OBO Foundry principles.[28,38] It provides templates, automation scripts, and workflows for tasks like editing in ROBOT,[39] quality control, format conversion, dependency management, and release packaging. By streamlining these processes, ODK helps ontology developers maintain consistency, ensure compliance with best practices, and reduce manual effort throughout the ontology lifecycle. The MWO GitHub repository configuration was managed in an mwo-odk.yaml file.[40] The file configures the ontology project setup for MWO, including metadata, GitHub repository details, release formats, imported ontologies, documentation settings, and quality control rules for ODK-based development. The ODK generated MWO repository[40] consists of "release files" that form the official ontology used by the community, "imports" which are external ontology subsets reused but not part of the base product, and "components" that are native ontology parts fully included in the base and managed internally, often used for automated or complex ontology segments. With ODK, ontology imports in MWO can be efficiently managed and updated using standardized commands that download, filter, and merge external ontologies based on the configuration specified in the mwo-odk.yaml file.

3.4. Collaborative MWO Editing Workflow

The MWO editing process followed a structured and collaborative workflow. Ontology developers edited the central ontology file (mwo-edit.owl) using the Protégé[41] tool in their local environments. Editing activities included creating new classes, properties, and individuals; structuring them hierarchically in alignment with reused top- and mid-level ontologies; adding rich annotations for new entities (such as definitions, references, examples, and editorial notes), defining logical axioms and property constraints (e.g., domain and range), and including comprehensive ontology annotation metadata (e.g., title, label, description, creators, contributors, version info, previous versions, license, and citation). Once local changes were made, they were committed to individual Git branches, pushed upstream to GitHub, and submitted via pull requests.

3.5. Ontology Evaluation and Testing Workflow

During the MWO development, reasoning tools such as HermiT and Pellet[42] were actively used within Protégé for ontology validation. These tools supported consistency checking, helped infer class hierarchies and instance classifications, and identified potential redundancies or modeling issues early in the editing process. This reasoning-driven validation ensured the logical soundness of the ontology as it evolved. In addition, after submitting a pull request for ontology edits, ODK automatically triggered a series of evaluation and testing workflows through GitHub Actions Continuous Integration. These workflows, powered by ROBOT, performed automated quality control to validate the ontology's structure, syntax, annotation completeness, and logical consistency.[28] Ontology evaluation was also supported using tools like OOPS! (Ontology Pitfall Scanner!), which automatically analyzes the ontology for common modeling pitfalls, structural issues, and best-practice violations.[43] In parallel, expert reviews and regular collaborative meetings with the community were held to assess the ontology's structure, resolve modeling issues, and ensure that it remained aligned with shared goals and quality standards.

3.6. Ontology Release

The MWO release process was streamlined using ODK's automated workflow, which follows these steps: running the release with ODK, reviewing the output, merging changes into the main branch, and creating a GitHub release. The ontology is distributed in three variants, available in both Web Ontology Language (.owl) and Turtle serializations (.ttl): The "full release" includes all logical axioms along with merged imports and components to represent the complete intended ontology with inferred subsumptions; the "base file" contains only the ontology's core entities, their public metadata, and classification hierarchy; and the "simple" artifact provides a minimal existential graph of essential classes without imports or complex logical definitions. Additionally, ODK supports robust version control for MWO on GitHub, ensuring thorough documentation of changes in each release, management of previous versions, and clear tracking of the ontology's evolution over time.

3.7. MWO Documentation, Publishing, and Maintaining

MWO was documented using two approaches: first with the Widoco template, a documentation generator for ontologies that automatically produces human-readable HTML documentation including metadata, hierarchies of classes, properties, and annotations;[44,45] and second, through the MkDocs documentation system, which uses a "docs" directory and "mkdocs.yaml" file to produce structured, user-friendly web documentation covering best practices, examples, and usage guidelines for MWO.[46,47] Additionally, MWO has been published in public repositories such as BioPortal[48] and MatPortal,[49] enhancing its accessibility. To support ongoing development and transparency, the GitHub issue tracker is actively used to gather community feedback and coordinate collaborative MWO improvements.

4. Reused Top- and Mid-Level Ontologies

MWO was designed to ensure interoperability with existing semantic resources developed within and beyond the NFDI ecosystem. To achieve this, MWO reuses and extends upper- and mid-level ontologies that provide stable conceptual foundations and domain-specific coverage, including BFO, IAO, NFDIcore, and PMDco ontologies. Each of these ontologies contributes to a different layer of the semantic framework; BFO offers a top-level formal structure for all entities and processes, IAO defines information-related concepts, NFDIcore represents organizational and infrastructural aspects across NFDI, and PMDco bridges general ontology design with MSE concepts. Together, these ontologies ensure consistent semantic modeling and interoperability across MSE data. By reusing established frameworks, MWO ensures consistent semantic modeling and interoperability across MSE data, promoting modularity, reusability, and alignment of standardized, well-defined entities and relationships across the materials science research landscape.

Figure 2 presents the graphical design of a subset of MWO classes, created by reusing various top- and mid-level ontologies. The structural design of MWO primarily draws on the following ontologies (partially reused ontologies and vocabularies such as SWO,[26] DCAT,[27] and the schema.org vocabulary[50] are not depicted in this figure).

4.1. BFO 2020

Following the OBO Foundry principles, BFO provides a domain-neutral foundation for building interoperable ontologies.[51] Its latest version, BFO 2020, is part of the ISO/IEC 21 838-2:2021 standard for semantic interoperability.[22] BFO divides all entities into two main categories: occurrents (things that happen over time, such as experiments or processes) and continuants (things that persist over time, such as materials or instruments). Furthermore, "continuants" are divided into 1) "independent continuants" including "material entities" (e.g., specimens, instruments) and "immaterial entities" (e.g., surfaces, boundaries) that exist on their own, 2) "specifically dependent continuants" which depend on particular bearers and include "qualities" (e.g., mass, temperature) and "realizable entities" (e.g., roles, dispositions, and functions), and 3) "generally

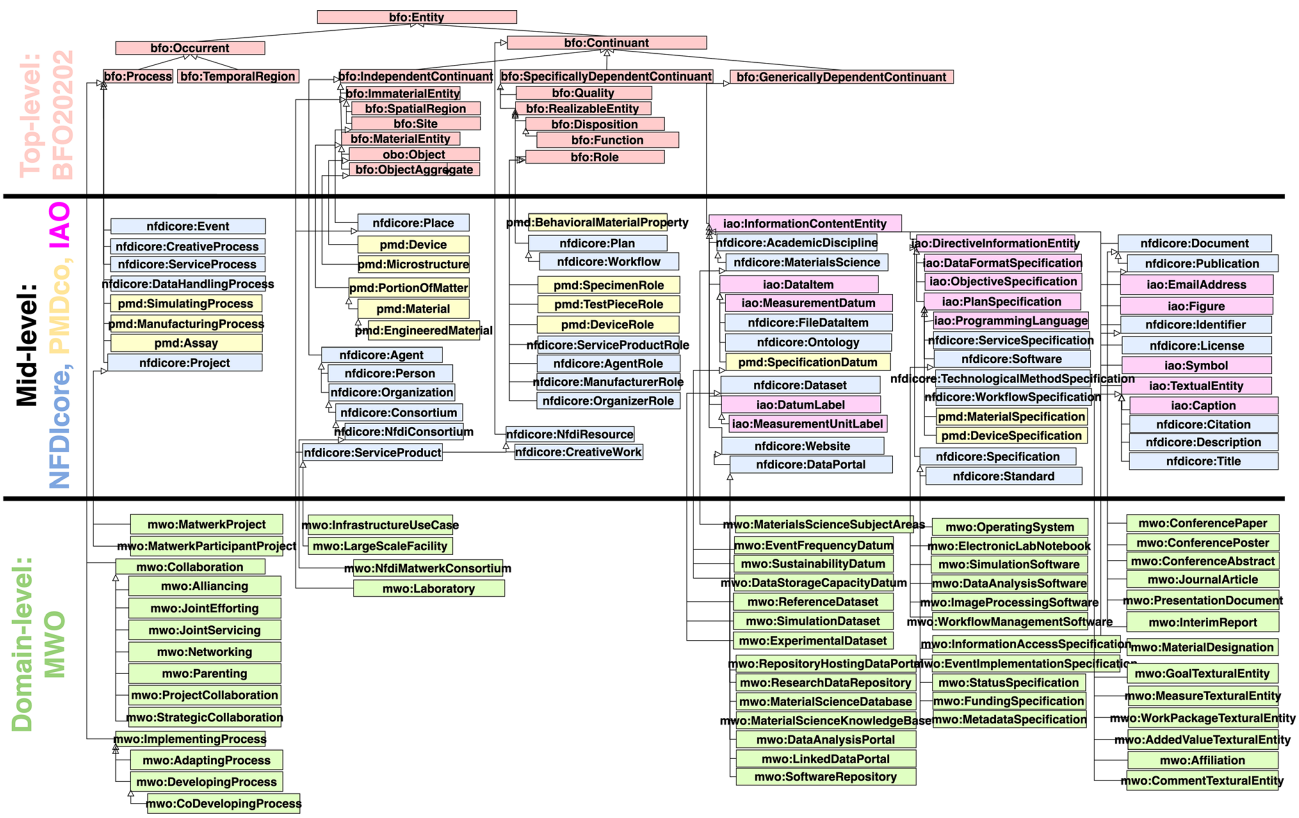

Figure 2. Partial structure of MWO classes (green) mapped onto the class hierarchies of top-level BFO2020 (red), and mid-level IAO (purple), NFDIcore (blue), and PMDco (yellow) ontologies.

dependent continuants" that depend on other entities but can exist across multiple bearers; typical examples are digital files or textual content.[36,52] This structure helps organize scientific information consistently and supports automated reasoning for checking logical correctness. MWO adopts BFO as its top-level ontology because it offers a stable and widely accepted framework that ensures semantic coherence and interoperability with other scientific ontologies.[37]

4.2. IAO (2022 Release)

IAO is a mid-level ontology originally derived by work by the Ontology for Biomedical Investigations (OBI) for the representation of information entities.[53,54] IAO is used in MWO to describe all kinds of informational artifacts that appear in materials research, ensuring that data and metadata are consistently represented and linked. As can be seen in Figure 2, at the heart of IAO is the "Information Content Entity (ICE)" class (subclass of bfo:GenerallyDependentContinuant) that includes entities like data item, measurement datum, labels, symbol, figure, textual entity, and plan/objective specification.

4.3. NFDIcore v3.0.0

The NFDIcore ontology provides a shared semantic backbone for RDM within the NFDI consortia.[10] NFDIcore is fully aligned with BFO 2020 and IAO (blue classes in mid part of Figure 2), offering structured classes for organizations, people, projects, and research outputs such as datasets, software, publications, and standards.[55] Its modular design makes it suitable for representing the interdisciplinary nature of NFDI projects, including MatWerk. It should also be noted that NFDIcore is continuously evolving through the incorporation of multidisciplinary entities from various NFDI modular extensions. For instance, a significant portion of its current classes originates from the MWO prerelease and earlier versions.

4.4. PMDco v3.0.0-Alpha

Developed within the MaterialDigital initiative, PMDco is a mid-level ontology for describing experiments, simulations, materials, and devices in MSE. It connects general BFO concepts with application-specific MSE knowledge, enabling detailed and traceable representation of manufacturing, characterization, and computational processes. For MWO, only a few high-level PMDco classes were imported to demonstrate interoperability and prepare for future integration of more detailed MSE ontologies.[56] PMDco and MWO together form a semantic bridge between top-level frameworks and domain-specific applications in digital materials research.

5. MWO Structure

5.1. MWO Semantics Metrics

MWO is more than a taxonomy, it is a formal ontology that not only organizes terminology hierarchically, but also provides a rich, relational structure to represent and retrieve RDM-in-MSE knowledge through well-defined classes, properties, and semantic rules. **Table 1** summarizes the quantitative characteristics of the MWO, including its axiom count, semantic richness, reuse level, and overall complexity metrics. These semantic metrics not only reflect the structural richness of MWO but also indicate how comprehensively materials-related entities, such as specimens, instruments, and processes, can be described and linked within real MSE research workflows.

Table 1. Overview of MWO semantic metrics.

Semantic richness metrics	
Axioms	3799
Logical axioms count	743
Class count	335
Object property count	121
Data property count	10
Annotation property count	83
Total individuals count	77
Reusing imported ontologies metrics	
Reused classes	81%
Reused object properties	89%
Reused data properties	80%
Reused annotation properties	100%
Reused individuals	95%
Complexity metrics	
Absolute cardinality (Root/Leaf/Sibling)	1/189/251
Depth (Absolute/Average/Maximal)	1452/5.8/9
Breath (Absolute/Average/Maximal)	251/4/19
Tangledness	0.10

MWO comprises a set of semantic elements (including classes, properties, and individuals) most of which are derived from reused top- and mid-level ontologies such as BFO, PMDco, NFDIcore, and IAO. For instance, out of a total of 335 classes and 121 object properties defined in MWO, ≈81% of the classes and 89% of the object properties originate from these reused ontologies (recall that a considerable number of current NFDIcore classes were adopted from the MWO prerelease and prior versions). The high reuse metrics shown in Table 1 reflect MWO's strong alignment with established semantic standards and demonstrate that the selected combination of candidate ontologies sufficiently covers the scope of MWO. By reusing the mentioned ontologies, MWO promotes semantic interoperability and consistency across the MSE and NFDI ecosystems, while also reducing redundancy, improving maintainability, and accelerating development. Only a small number of domain-specific entities were added, resulting in a conceptually coherent and extensible ontology. This reuse-driven approach also enhances trust in the ontology's structure and supports its integration with other ontologies.

Table 1 also presents a detailed analysis of the various structural complexity metrics characterizing the MWO structure. These metrics were measured using the OntoMetric tool,[57] and include absolute cardinality, depth, breadth, and tangledness, each offering insights into different aspects of the ontology's structure. Absolute cardinality refers to the count of key structural elements such as roots, leaves, and siblings. The root is the topmost node in a hierarchy, leaves are terminal nodes without children, and siblings are nodes sharing the same parent. A low number of roots indicates a cohesive and unified structure, while the high counts of leaves and siblings reflect both the granularity of the ontology (enhancing specificity and coverage) and its organizational clarity, with many concepts grouped under common parent classes. Depth measures the number of hierarchy levels and, in the case of MWO, a high depth score points to a well-layered ontology with a clearly defined conceptual hierarchy. Conversely, low breadth and low tangledness scores suggest that MWO avoids excessive complexity, such as wide branching or multiple inheritances, thereby improving ontology readability, usability, and computational performance.[6]

5.2. MWO Classes

A selection of the MWO's main classes is shown at the bottom of Figure 2, highlighted in green and marked with the "mwo" prefix. The complete list of MWO classes, along with their hierarchical structure, is available in the MWO documentation.[45] As seen in Figure 2, most MWO extensions falling under the bfo:GenericallyDependentContinuant/iao:InformationContentEntity class indicate a strong focus on representing information and knowledge artifacts rather than physical entities. This highlights MWO's emphasis on modeling data, metadata, and conceptual structures essential for RDM-in-MSE, ensuring that the ontology effectively captures the informational content necessary for interoperability and semantic clarity.

Concerning the ontology's scope, the key concepts in MWO v3.0.0 are organized into below four primary categories:

5.2.1. Consortium Structure

These classes help represent the organizational context of MSE research, linking projects, institutions, and contributors involved in generating and managing materials data. Example classes for this category are for representing the structure of the NFDI-MatWerk consortium, encompassing TAs, IUCs, PPs, and the associated persons and organizations involved. 1) NFDI-MatWerk Consortium (subclass of bfo:Independent Continuant/.../nfdicore:NFDIConsortium): NFDI-MatWerk will focus on the research areas of materials science and materials engineering. The key challenges in these fields are the digital mapping of materials and their process and loading parameters. This process touches core aspects of scientific ways of working starting with scientific exchange, data handling and the resulting technological possibilities. The digital transformation of materials science and materials engineering is an opportunity to promote, structure, and optimize this exchange—provided that transparent communication standards are created. This fundamental change is therefore being tackled in a joint effort by the consortium and the specialist community. 2) MatWerk Project (subclass of bfo:Process/nfdicore:Project): A MatWerk project is a project within the NFDI-MatWerk consortium that involves coordinated research, development, or infrastructure activities aimed at advancing MSE through data-driven methodologies and digitalization. 3) MatWerk PP (subclass of mwo:MatwerkProject): PPs are projects by NFDI-MatWerk partners that address specific scientific and technological challenges, providing practical examples and feedback for the development and validation of the infrastructure. 4) Furthermore, a variety of agents (person and organization) and related roles were created in subclasses of nfdicore:Agent and nfdicore:AgentRole.

5.2.2. NFDI Resources

By describing MSE subject areas and MSE-related digital resources such as data portals, workflows, and ontologies, MWO enables researchers to connect their experimental or simulation data with shared infrastructures for data publication and reuse. Example classes in NFDI resource category are: 1) Materials science subject areas (subclass of iao:InformationContentEntity/nfdicore:AcademicDiscipline) classified in ten groups of computational materials science, data-driven material science, materials characterization, materials deformation processes, materials design, materials mechanical behavior, materials microstructural, materials processing, materials surface science, and materials thermodynamics. 2) nfdicore:Dataset includes some MWO subclasses like experimental dataset (a dataset that contains measured or observed data collected from laboratory experiments, physical tests, or scientific investigations), simulation dataset (a dataset that contains data generated from computational models, numerical simulations, or digital twin environments to predict material behavior, properties, and interactions), and reference dataset (a dataset that serves as a benchmark or standardized collection of data used for validation, comparison, and reproducibility in scientific research and engineering applications). 3) nfdicore:Document subclasses like presentation document, interim report, conference abstract, conference paper, conference poster, and journal article. 4) Metadata specification, a detailed document that describes metadata structures, guidelines, and usage policies for standardization and adoption. 5) nfdicore:DataPortal subclasses of data analysis portal, linked data portal, material science database, material science knowledge base, repository hosting data portal, research data repository, and software repository. 6) iao:TextualEntity subclasses like affiliation, added value textual entity, goal textual entity, and measure textual entity. 7) pmd:SpecificationDatum subclasses like data storage capacity datum.

5.2.3. Service, Events, Educational Coerces, and Collaborations

These category captures activities like workshops, training sessions, and collaborative projects, supporting traceability of community interactions and knowledge exchange in MSE research. Some of MWO classes in this category include: 1) IUC (subclass of bfo:ImmaterialEntity/nfdicore:ServiceProduct): a service product that defines a specific application scenario, requirement, or implementation of research infrastructure, demonstrating its functionality, benefits, and impact in a given scientific or industrial domain. 2) Collaboration: a bfo:Process in which multiple entities, such as individuals, organizations, or institutions, work together toward shared goals, contributing resources, expertise, or services to achieve mutual benefits. The collaboration subclasses within MWO include alliancing, joint efforting, joint servicing, networking, parenting, project collaboration, and strategic collaboration. 3) Event frequency datum: describes how often an event occurs within a given time interval. 4) Sustainability datum: represents the duration or persistence of a process, system, or resource over time. It defines how long an entity is expected to remain viable or functional.

5.2.4. Specification of MSE-Related Materials, Instruments, and Facilities

While most of MSE-related concepts in MWO are derived from the PMDco ontologies, additional domain-specific entities have been included in MWO to facilitate the detailed description of materials, instruments, and research facilities. Such entities enable materials scientists to link data from characterization experiments (e.g., tensile or fatigue testing) directly with processing and simulation workflows, supporting integrated analysis and reuse of research data. Example classes in this category are: 1) Large-scale facility (subclass of bfo:ImmaterialEntity/nfdicore:ServiceProduct): A large-scale facility is a service product that provides specialized, high-capacity infrastructure for scientific research, engineering, or computational purposes, supporting large-scale experiments, simulations, and data analysis in various domains. 2) Laboratory (subclass of bfo:Site/nfdicore:Place): A place that provides a controlled environment equipped with specialized instruments and facilities for conducting scientific research, experiments, measurements, and testing across various disciplines. 3) Material designation (subclass of iao:InformationContentEntity/nfdicore:Identifier): Material designation is an identifier assigned to a material to specify its name, Id, classification, composition, or standardized reference in scientific, engineering, or industrial contexts.

5.3. MWO Object Properties

Figure 3 demonstrates parts of the hierarchies for MWO classes, object properties, data properties, and individuals as visualized in Protégé. Similar to the reuse approach applied to classes, Figure 3 also shows that most object properties in MWO are derived from reused top- and mid-level ontologies. As the foundational top-level ontology, all 64 object properties defined in BFO 2020 have been imported into MWO. Notable examples include: "concretizes", "has participant", "continuant/occurrent part of", "specifically/generically depends on", "has location", "occurs in", "exists at", "occupies temporal region", "realizes", and "bearer of". In addition, all object properties from the NFDIcore ontology have been integrated, such as "has agent", "has input/output", and "is subject of", along with its subproperties like "has license", "has dataset", "has software", "has standard", and "has subject area". MWO also partially reuses selected object properties from IAO (e.g., "is about", "denotes", and "is quality measurement of") and PMDco (e.g., "has value specification", and "simulated by").

In alignment with the principles of the OBO Foundry,[38] BFO-based ontologies are primarily extended through the addition of domain-specific classes, while significant alterations to object properties are generally discouraged to maintain semantic consistency and ensure interoperability across ontologies. Accordingly, only a minimal number of new object properties were introduced in MWO, aimed at simplifying the representation of semantic relationships specific to the domain. Examples of object properties defined within MWO include: 1) "implemented by": The property relates an entity to an agent that has adapted or developed the entity for a specific purpose and actively uses it within a particular context (inverse of: mwo:implements, domain: nfdicore:NFDIResource, and range: bfo:IndependentContinuant). This object property was created on request of NFDI-MatWerk community to respond to competency questions like which tools are "developed", "codeveloped", or "adopted" by specific agents (e.g., NFDI-MatWerk TA/IUC/PP organizations). Actually, this property is a shortcut for expressing the relation when nfdicore:NFDIResource is output of some mwo:ImplementingProcess which has participant of bfo:IndependentContinuant. 2) "has applicant organization": The property relates a project to the organization that applied for that (subproperty of: bfo:hasParticipant, inverse of: mwo:applicantOrganizationOf, domain: nfdicore:Project, and range: nfdicore:Organization). 3) "has measurement datum": The property is a relation between an entity and a measurement datum (subproperty of nfdicore:isSubjectOf, inverse of: mwo:measurementDatumOf, and range: iao:MeasurementDatum). 4) "has measurement unit label": The property is a relation between an entity and a measurement unit label. (subproperty of nfdicore:isSubjectOf, inverse of: mwo:measurementUnitLabelOf).

In conclusion, following the best ontology development practices defined by the OBO Foundry principles, MWO avoids creating highly domain-specific object properties that could reduce semantic reusability and increase redundancy. Instead, it emphasizes the reuse of generic BFO-based relations to ensure high interoperability and semantic consistency across ontologies. Consistent with this approach, even mid-level BFO-compliant ontologies in the MSE domain, such as PMDco, rely on BFO relations for representing MSE semantics. Accordingly, MWO introduces only a minimal number of new properties, added solely when existing ones were insufficient or when shortcut relations improved query efficiency. The four examples presented in this section reflect these modeling principles, illustrating how MWO extends BFO, NFDIcore, and IAO to support domain-independent but RDM-relevant relations.

5.4. MWO Data and Annotation Properties

Since BFO 2020 does not define any data properties, all seven data properties from the NFDIcore ontology (such as "has value", "has URL", and "file extension") were imported into MWO. Additionally, MWO defines two domain-specific data properties: "mwo:hasAcronym", representing a relation between an ICE and its specific acronym, and "mwo:hasID", indicating a relation between an ICE and its unique identifier.

On the other hand, Table 1 shows that by directly importing the BFO and NFDIcore ontologies into MWO, all necessary annotation properties (originating from established vocabularies

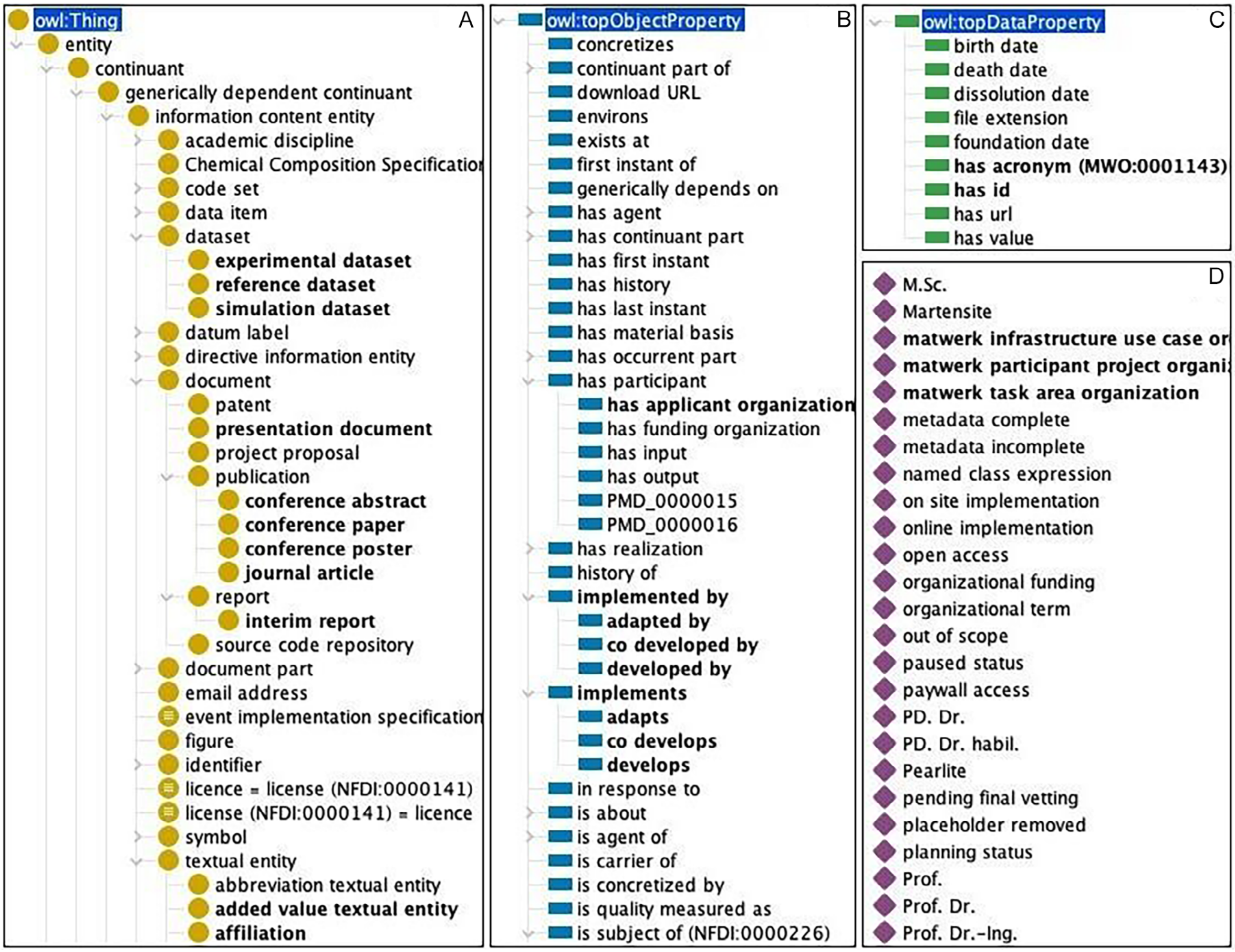

Figure 3. Visualization of selected MWO components in Protégé, including A) hierarchies of classes, B) object properties, C) data properties, and D) individuals. Entries in bold indicate items newly created in MWO, while nonbold entries represent reused or imported items from reference ontologies like BFO, NFDIcore, and PMDco.

such as dc, dcterms, rdfs, owl, and skos)[58] were made available without the need to define any additional annotation properties within MWO. This comprehensive coverage includes properties for labeling, documentation, provenance, and classification, ensuring that the ontology remains semantically rich and well-documented.

These data and annotation properties enable materials scientists to describe experimental parameters, link measurement values to specimens and instruments, and record contextual metadata in a standardized way.

These findings highlight that the reuse of top- and mid-level ontologies provided a robust foundational framework, significantly simplifying the construction of the domain ontology while maintaining interoperability and adherence to semantic web standards.

5.5. MWO Individuals

In practical MSE use cases, individuals represent real-world entities such as specific materials, samples, instruments, or experiments, linking ontology concepts directly to experimental data. As a backbone for MSE-KG, MWO does not define application-specific instances by default but instead provides a flexible framework that allows users to instantiate individuals relevant to their specific use cases. The current set of individuals present in MWO (as seen in Figure 3) primarily results from the full import of the NFDIcore ontology and the partial import of selected PMDco entities along with their associated axioms. In addition to these reused individuals, a minimal number of domain-relevant instances, such as those representing components of the NFDI-MatWerk consortium (e.g., TAs, PPs, and IUCs), were defined within MWO as illustrative examples. These example instantiations serve to demonstrate how MWO can be applied and extended in real-world RDM contexts.

6. Ontology Design Patterns (ODPs)

ODPs are modular, reusable components that capture best practices for solving recurring challenges in ontology development.[30] They provide standardized templates for common modeling tasks such as defining hierarchies, managing semantic relationships, and integrating diverse data sources. In practical MSE workflows, such patterns enable uniform representation of experiments, such as connecting a specimen to its processing steps, testing methods, and measured properties. By promoting clarity and consistency, ODPs enable developers and domain experts to build efficient, extensible, and technically robust ontologies. They are especially valuable for ensuring uniform representation of relationships between entities and instances, which enhances interoperability across systems. ODPs can also support constraint modeling through SHACL shapes,[59] allowing for precise validation of data within knowledge graphs. Overall, by using ODPs, ontology users and developers benefit from a scalable, adaptable framework that streamlines development while addressing complex, evolving domain needs.[30,60]

As part of the MWO development, a series of MWO-based ODPs were designed to help domain experts more effectively create structured semantic knowledge representations. These ODPs were tailored to address both foundational and domain-specific modeling needs within the MSE community. The pattern list includes semantic representation of: 1) process-agent-role, 2) service, 3) resource contact point, 4) resource implementation agent, 5) resource description, 6) value specification, 7) temporal region, and 8) material entity description. Each pattern serves a specific modeling purpose, supporting consistent and reusable representations of concepts and their interrelations. Detailed descriptions and visualizations of all patterns are available in the ontology documentation repository.[47] In this section, we present just three examples to illustrate the use of structural, content-based, and presentation ODPs, demonstrating how they establish core entity arrangements, encapsulate domain-relevant semantics, and enhance usability and clarity for ontology users.

6.1. Pattern 1-Resource Contact Point

Figure 4 presents the OntoPanel visualization of the pattern specifically developed to semantically model the contact information of a resource (such as a service, dataset, software, publication, or data portal). The primary purpose of this pattern is to ensure that each resource (NfdiResource-X) is properly linked to a responsible contact agent (ContactPoint_X) through a clearly defined role (ContactPointRole_X) and supported by accessible communication channels like name, email address, or website.

The semantic structure of the pattern is built upon key object properties, including bfo:has_participant, bfo:participates_in, bfo:realizes, bfo:bearer_of, bfo:is_concretized_by, iao:denoted_by, and nfdicore:hasContactPoint. According to this structure, NfdiResource_X can be any instance for mwo:NfdiResource (bfo:Continuant) which participates in Process_X (instance of bfo:Process), has contact point of ContactPoint_X (instance of nfdicore:Agent), and is concretized by ContactPointRole_X (instance of nfdicore:ContactPointRole). Here, Process_X has participant of ContactPoint_X and realizes ContactPointRole_X, while ContactPoint_X also bearers of ContactPointRole_X. In this regard, ContactPoint_X and ContactPointRole_X can be denoted by generally dependent continuants like ContactPoint Name_X, EmailAddress_X, and ContactPointWebsite_X.

This pattern is highly applicable for a range of use cases, such as linking a dataset to a responsible researcher, assigning a support team to a software tool, or defining contact details for a service or event. For example, a scientific dataset in an NFDI repository can be linked to a dedicated expert with their name and email, enabling better communication and accountability. By adopting this ODP, ontology developers and domain experts can ensure consistent, clear, and reusable representations of contact information, ultimately improving the transparency, usability, and trustworthiness of NFDI services and digital research infrastructures.

6.2. Pattern 2-Resource Implementation Agent

Similar to the resource contact point ODP, the resource implementation pattern of **Figure 5** aims to provide a structured semantic representation of how a given resource (e.g., dataset, ontology, software, or service) is linked to the agent responsible for its development, codevelopment, or adaptation. The core goal of this pattern is to ensure that each mwo:NfdiResource_X is properly connected to an independent continuant using the

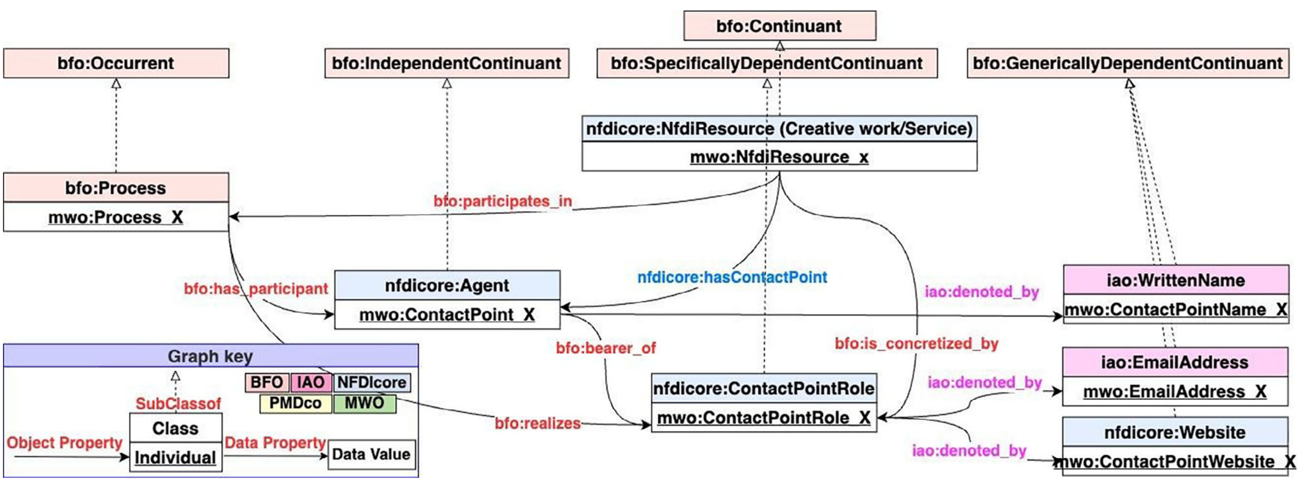

Figure 4. Ontology design pattern for representing a resource contact point.

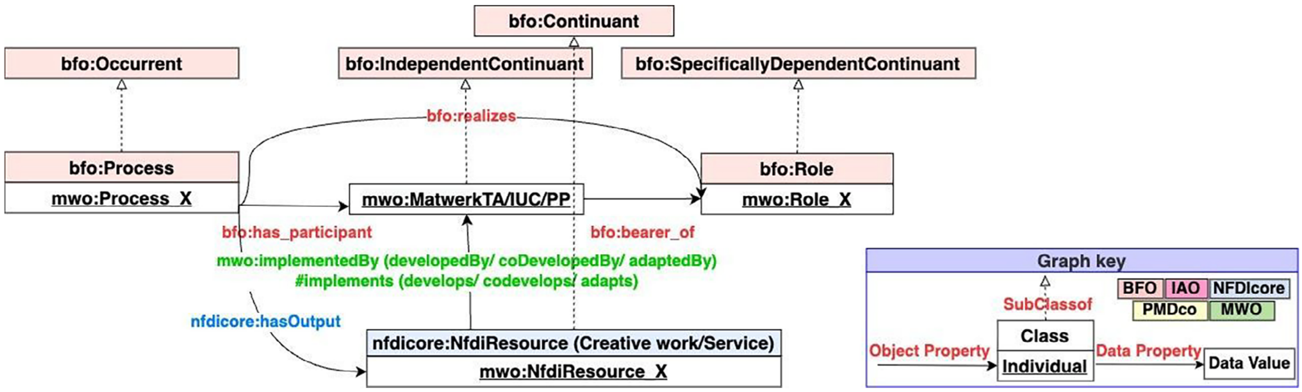

Figure 5. Resource implementation ODP for linking each resource to its responsible agent via mwo:implementedBy and its related subproperties.

property mwo:implementedBy, which extends to mwo:developedBy, mwo:coDevelopedBy, and mwo:adaptedBy.

The contributing object properties of this pattern included bfo:has_participant, bfo:realizes, bfo:bearer_of, nfdicore:hasOutput, and mwo:implementedBy. In this pattern, the NfdiResource_X is an output of Process_X and has participant of an independent continuant (like a MatWerk TA, IUC, or PP agent). The property mwo:implementedBy provides a shortcut for linking the NfdiResource_X to the independent continuant that implemented it, simplifying the tracking of tools, services, and digital outputs within the NFDI-MatWerk consortium.

Use cases of this pattern include representing which working group, institution, or individual developed a specific tool, codeveloped a software library, or adapted an ontology. For instance, a data portal developed by a specific task area, or a workflow adapted by a participant project, can be clearly linked to its agent. This pattern helps to address competency questions such as: Which resources were implemented by Agent X? or Who developed Resource Y?

6.3. Pattern 3-Material Entity Description

Figure 6 visualizes the material entity description ODP, designed to semantically represent material entities such as devices, instruments, or materials used in research. Its goal is to provide a structured way to describe MaterialEntity_X along with key metadata like name, related processes and projects, responsible agents, locations, functions, roles, dispositions, and specifications. MaterialEntity_X can be any instance for bfo:Material Entity which participates in mwo:Process_X, and is output of Project_X. MaterialEntity_X may have an agent (like Agent_X), located in Place_X and has continuant part(s) like MaterialEntity_Y. Connecting such material entities to specifically dependent continuants (like function, role, and disposition)

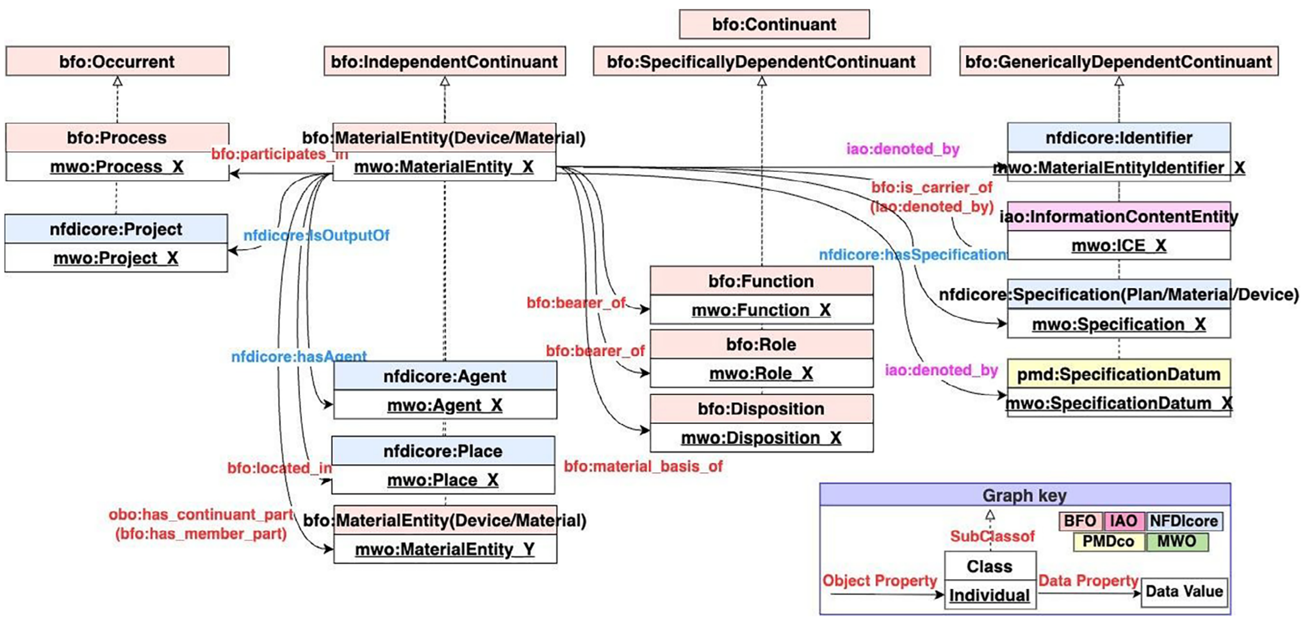

Figure 6. Material entity description ODP for semantically representing research-related devices, instruments, and materials with key metadata.

can be expressed with object properties like bfo:bearer_of and bfo:material_basis_of. MaterialEntity_X can be denoted by instances of nfdicore:Identifier or pmd:SpecificationDatum classes, and specifies with some iao:DirectiveInformationEntity instances like mwo:MateriaDesignation.

As example use cases for this pattern, one can mention modeling metadata for a tensile test machine, capturing its name, subcomponents, operating organization, location, operational status, and technical specifications. Another example could be a heat-treated steel specimen, where information such as its unique identifier, the heat-treatment process applied, the originating project, the responsible agent, and associated specifications are semantically structured for retrieval and reasoning. This pattern plays a critical role in enhancing the findability, reusability, and interoperability of physical object data within research ecosystems. By annotating devices and materials with rich,

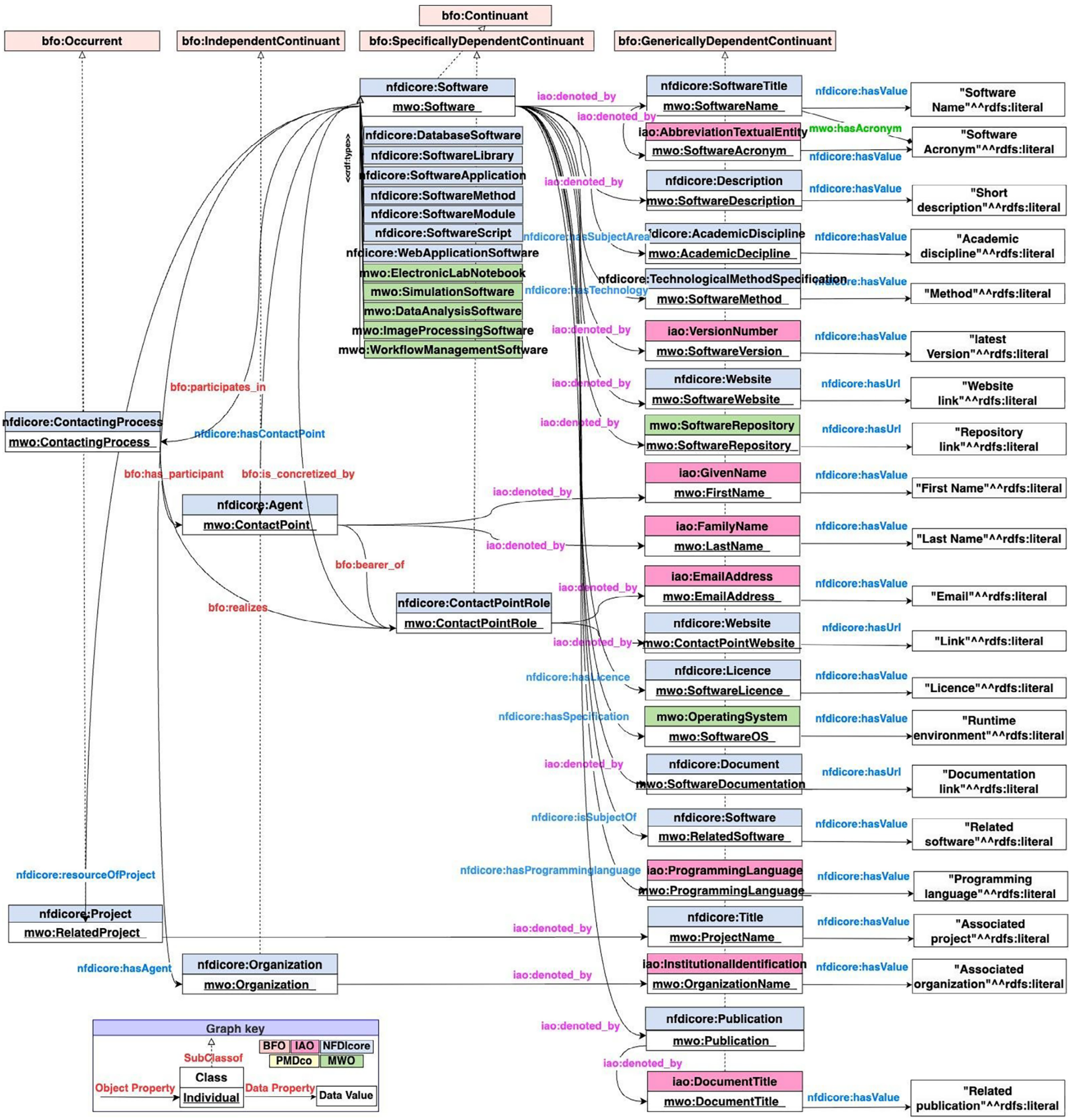

Figure 7. Example MSE-KG semantic graph for describing software resource metadata using MWO-based patterns.

standardized metadata, researchers can more easily compare equipment, track provenance, manage experimental assets, and integrate material-related data across systems and projects.

7. MWO use Cases

In real MSE research, the NFDI-MWO enables scientists to semantically link materials, experiments, instruments, and results within a unified digital framework. By describing these research components in a standardized and machine-readable way, MWO helps organize experimental data, trace relationships between processes and properties, and integrate results across laboratories and projects. This ensures that materials data become more comparable, interoperable, and reusable throughout the research lifecycle.

MWO currently serves as the foundation for the development of several application ontologies in the RDM-in-MSE domain, as well as for the MSE-KG.[31] The MSE-KG is a curated, machine-readable graph that integrates data from diverse sources within the NFDI-MatWerk ecosystem. It represents entities and their relationships using graph structures, enabling semantic search, metadata-based retrieval, and advanced querying. By unifying access to distributed research data across the MSE community, the MSE-KG transforms isolated data silos into a shared semantic infrastructure. This fosters data interoperability, supports automated reasoning, and empowers data-driven decision making, thus accelerating research, enhancing collaboration, and driving innovation in MSE.

In alignment with MWO scope, the current version of MSE-KG (v2.0) includes structured descriptions of resources across four main categories: A) consortium structure, covering the NFDI-MatWerk consortium along with its TAs, IUCs, PPs, people, and organizations; B) NFDI resources, including tools, software, publications, datasets, data portals, and metadata items; C) featuring services, events, educational courses, and international collaborations; and D) instruments and large-scale research facilities. The graph representing all mentioned categories was semantically modeled using MWO and its well-structured ODPs. For example, the software description graph of **Figure 7** utilized some MWO-based patterns including resource description, resource contact point, value specification, and material entity description. This figure illustrates a typical semantic graph structure within MSE-KG for describing metadata of a software resource (nfdicore:Software). It captures details such as software type, name, and acronym, its description, subject area, version, license, website or repository, runtime environment, programming language, documentation link, and contact point information (including name, email address, and website). Additionally, the graph connects software resources to related entities like documents, projects, organizations, and publications. By interlinking these elements, the MSE-KG enables seamless integration with other graphs, such as those describing people, organizations, or publications, supporting advanced semantic search, data reuse, and knowledge discovery across the NFDI-MatWerk ecosystem. The graph representations of other MSE-KG elements can also be found in the MWO documentation repository.[47]

8. Conclusion

This article presented the NFDI-MWO as a comprehensive, BFO-compliant semantic framework for advancing the RDM-in-MSE domain. Designed to meet the complex requirements of interoperability, reusability, and semantic clarity, MWO formalizes core RDM concepts (such as datasets, software, instruments, metadata, and organizational structures) by aligning with established ontologies including BFO, IAO, NFDIcore, and PMDco.

MWO v3.0.0 introduces extensive semantic coverage, modular architecture, and rich ODPs that support reusable and scalable modeling of key MSE resources and processes. Developed using ODK and released through a FAIR-compliant workflow, MWO ensures standardized documentation, quality control, and long-term maintainability.

The ontology's scope encompasses four main areas: consortium structure, NFDI resources, community services and collaborations, and domain-specific instruments and materials. Structurally, MWO emphasizes a lightweight but expressive description logic (AL), maximizing reasoning efficiency while preserving semantic richness. Its high reuse of mid- and top-level ontologies promotes consistency across domains and supports seamless integration with external data sources.

As demonstrated in practical use cases, MWO provides the foundation for several application ontologies and the MSE-KG. The MSE-KG leverages MWO's semantic backbone to represent distributed, interconnected research data, enabling advanced querying, semantic search, and automated reasoning. Together, MWO and MSE-KG foster cross-institutional collaboration, accelerate data-driven innovation, and support the digital transformation of MSE research through a shared semantic infrastructure.

Future work will focus on the continuous extension of MWO through the development of MSE-specific application ontologies and their integration into the MSE-KG. Further efforts will also address ontology alignment and interoperability across NFDI consortia, as well as the implementation of automated validation tools to ensure ontology quality and consistency. Additionally, the development of user-oriented interfaces and annotation tools is planned to facilitate the adoption and practical use of MWO within the MSE community.

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Conflict of Interest

The authors declare no conflict of interest.

Data Availability Statement

MWO and its related resources can be accessed via the MWO GitHub repository,[40] Widoco documentation,[45] and the ODK-based MkDocs documentation.[47] Additionally, MWO is published on BioPortal[48] and MatPortal[49] for enhanced discoverability. The MSE Knowledge Graph (MSE-KG),[31] built upon MWO, is also available for exploration and reuse.

Keywords

knowledge graph, materials science and engineering, ontology, ontology design pattern, research data management

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