FAIR Data Management for Designing Sustainable Advanced Materials: A Position Paper

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Abstract

Materials design depends on both conventional experiments such as synthesis and characterization, and theoretical calculations to simulate material structures and properties. However, data generated from these processes often lacks interoperability, hindering integration across the design, experimentation, and production pipeline. In addition, sustainability assessments (e.g., Life Cycle Assessment), which rely on diverse data such as environmental emissions and market prices, are rarely incorporated into materials design. The European Union's Safe and Sustainable by Design initiative has recognized that sustainability is frequently neglected in this context. To address these issues, we first need a methodology for materials design that takes sustainability assessment into account. Addressing this gap requires a design methodology that integrates sustainability assessment from the start of life cycles of production or materials design. Moreover, FAIR (Findable, Accessible, Interoperable, and Reusable) data management is essential for improving semantic interoperability across heterogeneous data sources, to implement such a design methodology. Semantic Web technologies, particularly ontologies, offer promising mechanisms to support this goal by enabling shared vocabularies and semantic-aware data discovery. In this position paper, we present our vision and initial approach to enabling sustainable materials design through semantic-aware data management.

Keywords

Ontology, FAIR Data Management, Sustainability Assessment, Materials Design

1. Introduction

With the rapid emergence of advanced materials, ensuring that their development contributes to a sustainable society has become increasingly important. However, research in this field remains largely focused on technical aspects, often neglecting considerations for sustainability especially at the early stages of materials design [1]. The European Union (EU) has acknowledged this gap through initiatives such as Safe and Sustainable by Design [2] and the Critical Raw Materials Act (Regulation 2024/1252). A major challenge is the lack of clear guidance on integrating sustainability into materials innovation. Beyond technical performance, materials design should also consider environmental, economic, and raw material criticality aspects. Sustainability assessments can serve as a guiding tool by evaluating the implications of raw materials and energy use across the entire life cycle, including extraction, manufacturing, usage, and end-of-life phases. Recent advancements in this field include prospective life cycle assessment (LCA) methodologies addressing design guidelines at the laboratory scale [3, 4]. However, prospective LCA is still in its infancy and has been applied to a limited range of advanced materials. Further advancements are required to extend its applicability, encompassing a broader spectrum of advanced materials thereby already screening those with the least environmental impacts [5]. Additionally, extending these assessments to incorporate economic and raw material

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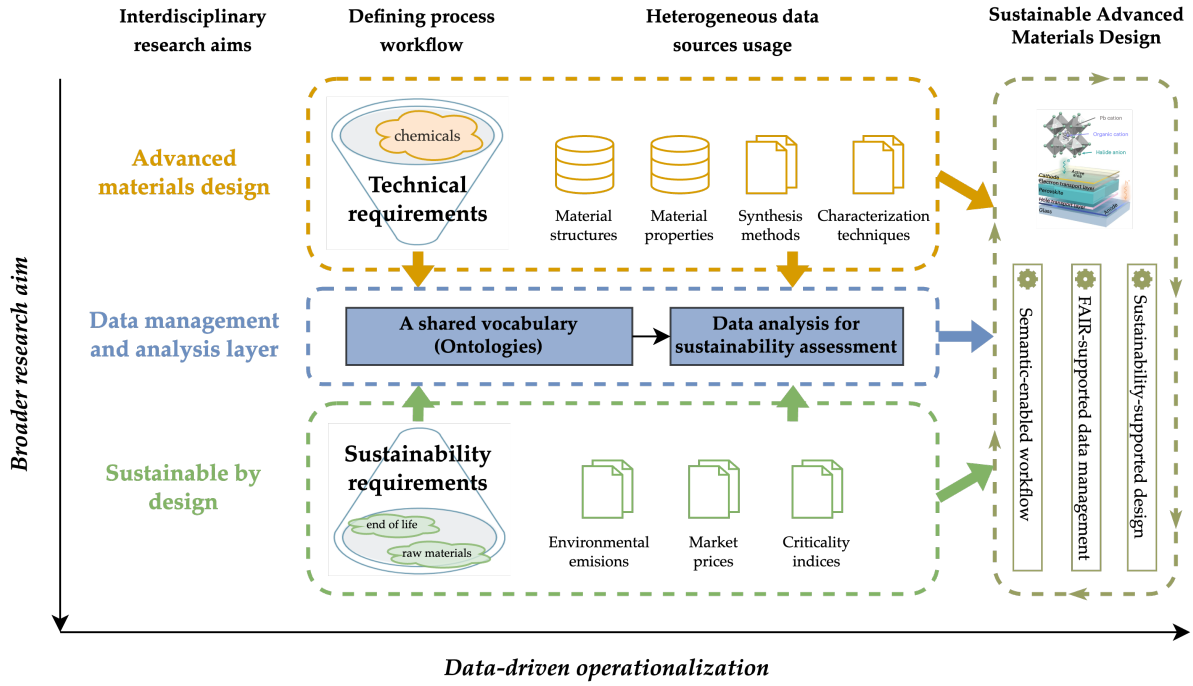

Figure 1: The concept for FAIR data management for designing sustainable advanced materials.

criticality dimensions is crucial for steering material science innovation toward holistic sustainability considerations.

Although extending sustainability assessments is conceptually straightforward, the challenge lies in operationalizing these efforts, particularly given the vast amounts of data that must be managed from diverse sources. Taking sustainability assessment as an example, although datasets for environmental, economic, and material criticality assessments are available, they are often handled manually and exist in disparate formats, making integration difficult. This lack of standardization hinders direct comparison and analysis, making comprehensive sustainability assessments for advanced materials a tedious and resource-intensive process [6]. Moreover, advanced materials design also relies on material experiments and theoretical calculations taking various data from material properties, calculation methods, synthesis methods into account. Similarly, data generated from experimental and simulation tools in materials research are typically stored in various repositories with different metadata, further hindering reuse and interoperability. An example of such issue is that data about a material is stored in various databases (such as materials properties and structures from theoretical calculations, synthesis and characterization data from experiments).

The FAIR (Findable, Accessible, Interoperable, Reusable) data principles [7] provide a foundation for addressing these challenges. As illustrated in Figure 1, we envision a FAIR data management approach that enables consistent modeling and integration of sustainability-related information throughout the materials design process. Semantic Web technologies, particularly ontologies and knowledge graphs, can facilitate this by providing shared, standardized vocabularies and supporting semantic-aware data retrieval across domains. Previous work has applied ontologies to materials science [8] and the circular economy [9], but sustainability-specific ontologies remain underdeveloped. To enable integrated assessments in advanced materials design, it is essential to establish interoperability across existing ontologies for materials, LCA, and sustainability. Figure 2 presents a conceptual architecture for such an ontology-driven data infrastructure.

In the following sections, we present survey results on relevant ontologies and standards and illustrate a use case on FAIR data management for semiconductor materials.

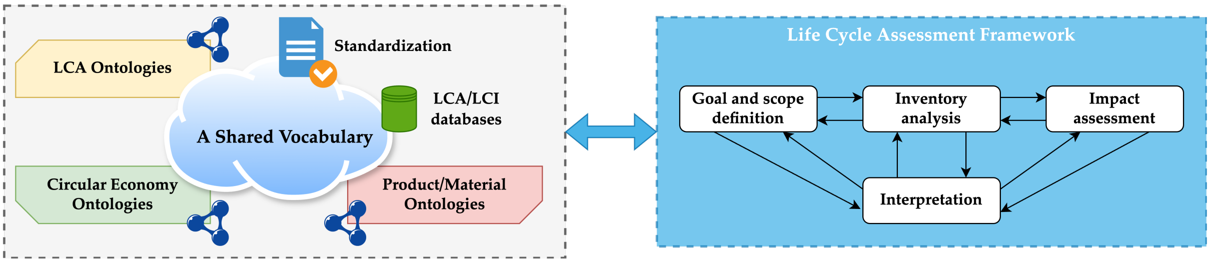

Figure 2: Conceptual illustration of ontology architecture with foundation on LCA framework.

2. Related Ontologies

To enable a FAIR data infrastructure for sustainable materials design and to define a shared vocabulary as illustrated in Figure 2, it is essential to first examine existing vocabularies or ontologies in relevant domains. Therefore, we conducted a survey of ontologies in the domains of sustainability, life cycle assessment (LCA), circular economy and materials, focusing on their applicability to sustainable assessment and materials design. In Table 1, we show example terms from these surveyed ontologies.

2.1. Ontologies related to Sustainability and LCA

From the survey, we identified six ontologies in total that address aspects of sustainability or LCA, respectively: the BONSAI-core ontology [10] from the BONSAI project,[1] the Environment Ontology (ENVO) [11], the Sustainable Development Goals Interface Ontology (SDGIO) [12], the Life Cycle Asset Information Management (LCAIM) ontology [13], the Life Cycle Cost Analysis Ontology (LCCA-Onto) [14], the Life Cycle Engineering Ontology (LCEO) [15].

The BONSAI-core ontology [10] was developed in the BONSAI project to support structured knowledge representation for life cycle sustainability assessments. Its primary focus is to model product footprints and support comparative assessments and decision-making. For instance, it represents life cycle activities in terms of their inputs and outputs and has been used to annotate databases such as EXIOBASE[2] [16] and YSTAFDB[3] [17], which are widely used in sustainability studies. For instance, EXIOBASE, including data from multiple industries and countries, can be used for tracking emissions, resource use, and other environmental pressures along global supply chains [16]. YSTAFDB contains data that describes material cycles, criticality, and recycling covering 62 elements and various engineering materials [17].

An important aspect in sustainability assessment is to consider impacts for the environment. ENVO [11] specifies a number of essential environment types that could be useful for annotating biological data. Moreover, it defines basic concepts such as environmental materials and processes, which are relevant for modeling environmental impacts and linking materials to ecosystems in LCA. SDGIO [12] aims to represent knowledge related to the sustainable development goals [18] including their targets and indicators, which is particularly useful for embedding sustainability policy considerations into assessment frameworks as illustrated in Figure 2. Additionally, SDGIO reuses a number of existing ontologies from different domains such as ENVO as introduced above.

Several LCA-related ontologies have been developed, each targeting specific perspectives or application domains. The LCAIM ontology [13] represents LCA assets in terms of costs, resources, and conditions. It is particularly useful in the scope definition and inventory analysis phases, where it supports data structuring and standardization. LCCA-Onto [14] focuses on cost analysis for maintenance and repair processes in the construction domain, especially for building facilities and Internet of Things (IoT) applications. LCEO [15] supports life cycle engineering (LCE) analysis at the product level by modeling LCE processes and properties from technical, ecological, and economic perspectives.

[1]BONSAI project: https://bonsai.uno
[2]EXIOBASE database: https://www.exiobase.eu
[3]YSTAFDB database: https://zenodo.org/records/2561882

Table 1
Related Ontologies and Example Terms.

Domains	Ontologies	Example terms
sustainability, CE, LCA	BONSAI-core [10]	balanceable property, person-time, activity
sustainability	ENVO [11]	environmental material, environmental variability, environmental system, environmental role
sustainability	SDGIO [12]	environmental monitoring, environmental pollution, sustainable development process
LCA	LCCA-Onto [14]	life cycle cost, inflation rate, labor rate, price
LCA	LCAIM [13]	condition, energy use, cost, asset
LCA	LCEO [15]	process, technological properties, ecological properties, economic properties, material, product
CE	CEON [9]	product, process, energy, material, chemical entity, resource, resource property, resource quality
CE	CAMO, CEO [19]	biological material, technological material, biological activity, technological activity, resource, product
CE	BiOnto [20]	process, material, energy, chemical substance
materials, simulation	MDO [21]	material, material structure, material property, calculation
materials	MATONTO [22]	material, material quality, material property
materials, measurement	MPO [23]	material, material layer, measurement, material property
materials, simulation, experiment	MAMBO [24]	material, simulation, experiment, experimental method
materials science and engineering	PMDco [25]	material, simulation, property, process, energy

2.2. Ontologies related to Circular Economy

In the Onto-DESIDE project,[4] we developed a Circular Economy Ontology Network (CEON) [9].[5] CEON contains key semantics for the circular economy, including actors, processes across the life cycle of resources, and their roles within circular value networks. These concepts and relationships are also relevant for sustainability assessment. Before developing CEON, we conducted a survey [26] of existing CE-related ontologies. This identified the Circular Materials and Activities Ontology (CAMO) [19], the Circular Exchange Ontology (CEO) [19], and BiOnto [20] from the BIOVOICES project[6] and BONSAI-core (as mentioned above). BiOnto and CEON share many concepts, including chemical entities, materials, and energy-related terms. CEO and CAMO also contain core CE concepts such as materials, resources, and products, but are more focused on the construction domain.

2.3. Ontologies related to Materials

In our prior work [21, 27], we also investigated existing ontologies related to the materials science domain. While this domain is relatively well-covered, challenges remain in modeling materials at

[4]Onto-DESIDE project: https://ontodeside.eu. The project aims to support acceleration of the digital and green transitions, automating the discovery and formation of new collaborations in the circular economy.
[5]Circular Economy Ontology Network: http://w3id.org/CEON
[6]BIOVOICES project: https://www.biovoices.eu

the granularity for different application domains such as circular economy and sustainability. As illustrated in Figure 1, advanced materials design needs to integrate data from both experiments (e.g., synthesis and characterization) and simulations (material structures and properties). Thus, we examined ontologies addressing both perspectives: the MDO (Materials Design Ontology) [8], Material Ontology (MATONTO) [22], Material properties ontology (MPO) [23], Materials and Molecules Basic Ontology (MAMBO) [24], and Platform Material Digital Ontology (PMDco) [25]. MDO [8] contains a structure module describing composition information of materials, as well as material calculations focusing on representing simulation data. A semantic search application based on MDO is presented in [28]. Both MATONTO and MPO represent general knowledge in the materials science domain, where MPO focuses more on properties and measurements. MAMBO intended to represent both simulation and experiment domain knowledge but remained at an abstract level. PMDco is a mid-level ontology, developed based on the Basic Formal Ontology (BFO)[7] that focuses on modelling workflows in materials science and engineering.

3. Standards related to Sustainability and LCA

To develop high-quality ontologies and reliable approaches for sustainable materials design approaches, it is necessary to consider standardization at both global and EU levels. Therefore, we reviewed existing and ongoing standardization initiatives related to sustainability and LCA. We identified several relevant standards developed by ISO (International Organization for Standardization),[8] ASTM (Advancing Standards Transforming Markets),[9] and the European Union through EUR-Lex[10] as summarized in Table 2. Collectively, these standards will not only guide the development of methodologies for sustainable materials design but also offer essential terminology and guidelines necessary for creating a shared vocabulary (ontologies) to enhance semantic interoperability and support the envisioned methodology for designing sustainable advanced materials.

3.1. Global-level Standards

Among the standards as listed in Table 2, ISO14040:2006 and ISO14044:2006 are two foundational works that provide a framework and guidelines for LCA. Specifically, ISO 14040:2006 [29] provides an LCA framework consisting of four core steps: goal and scope definition, inventory analysis, impact assessment, and interpretation (see Figure 2). ISO 14044:2006 [30] further elaborates on these procedures. Both standards are recognized at the EU level and adopted nationally, such as by Sweden. Additionally, ISO/TS 14074:2006 [31] details guidelines for normalization, weighting, and scoring in LCA, while ISO/TS 14048:2002 [32] specifies data documentation procedures for Life Cycle Assessment and Life Cycle Inventory.

The global standards organization ASTM provides three relevant sustainability standards [33, 34, 35], detailed in Table 2. These standards include terminology for sustainability and guidelines addressing sustainable manufacturing processes and chemical selection.

3.2. EU-level Standards

The European Union Commission has also established regulations and recommended frameworks for sustainable product design. For instance, the EU taxonomy for sustainable activities [36] is a regulation established in 2020 to classify economic activities by their environmental sustainability. Ecodesign for Sustainable Production Regulation (ESPR) [37] expands the existing Ecodesign Directive which defines environmental performance criteria that are mandatory for products to be satisfied before being placed on the EU market. More recently, the European Union introduced the Safe and Sustainable

[7] BFO: https://basic-formal-ontology.org
[8] International Organization for Standardization: https://www.iso.org
[9] Advancing Standards Transforming Markets: https://www.astm.org
[10] EU law: https://eur-lex.europa.eu/

Table 2
Relevant Standards, Regulations and Policies.

Level	Name	Description
Global Level	ISO 14040:2006 Environmental management — Life cycle assessment — Principles and framework [29]	This standard presents a methodological LCA framework including principles, phases and key features of LCA. It is a EU level and Swedish national standard.
	ISO 14044:2006 Environmental management — Life cycle assessment — Requirements and guidelines [30]	This standard provides more detailed guidelines on LCA framework. It is a EU level and Swedish national standard.
	ISO/TS 14074:2006 Environmental management — Life cycle assessment — Principles, requirements and guidelines for normalization, weighting and interpretation [31]	This standard addresses for instance the use of normalization, weighting, scoring of LCA in addition to ISO 14040:2006 and ISO 14044:2006.
	ISO/TS 14048:2002 Environmental management — Life cycle assessment — Data documentation format [32]	This standard introduces a data documentation format for reporting Life Cycle Inventory analysis data.
	ASTM E2114-23, Standard Terminology for Sustainability [33]	A terminology explains terms related to the sustainability domain.
	ASTM E3027-18a, Standard Guide for Making Sustainability-Related Chemical Selection Decisions in the Life-Cycle of Products [34]	A guide outlines sustainability factors into which manufacturers take account for choosing chemicals or ingredients through a product's life cycle.
	ASTM E2986-22, Standard Guide for Evaluation of Environmental Aspects of Sustainability of Manufacturing Processes [35]	A guide provides guidelines for evaluating sustainability in manufacturing processes.
EU Level	EU taxonomy for sustainable activities [36]	The regulation classifies economic activities in terms of environmentally sustainable.
	Ecodesign for Sustainable Products Regulation (ESPR) [37]	This regulation extends a previous Ecodesign directive to set up a framework to define ecodesign requirements for specific product groups. It entered into force on 18 July 2024.
	Safe and sustainable by design [38]	This is a framework as a voluntary approach to guide the innovation process for chemicals and materials. It is a commission recommendation by EU.
	European Critical Raw Materials Act [39]	This regulation aims to secure a sustainable supply of critical raw materials for the EU.
	EU Critical Raw Materials List [40]	The list contains 34 raw materials that should be considered critical.

by Design (SSbD) [38] as a policy concept promoting the development of chemicals, materials, and products that are both: Safe for human health and the environment, and Sustainable throughout their life cycle (from raw materials extraction to end-of-life scenarios such as disposal or reuse). SSbD represents a preventive strategy, embedding safety and sustainability considerations early in innovation and product design rather than managing risks after market entry. Moreover, the European Critical Raw Materials Act [39] intends to make the supply chain of critical materials secure and sustainable while enhancing overall circularity and sustainability. The related EU regulation proposal, [40] includes a list of critical raw materials such as lithium and nickel. These materials are essential for cutting-edge technologies, including semiconductors. However, their use poses challenges related to supply risks, environmental impacts, and end-of-life recovery. Therefore, the design of materials involving such critical raw materials should receive greater attention.

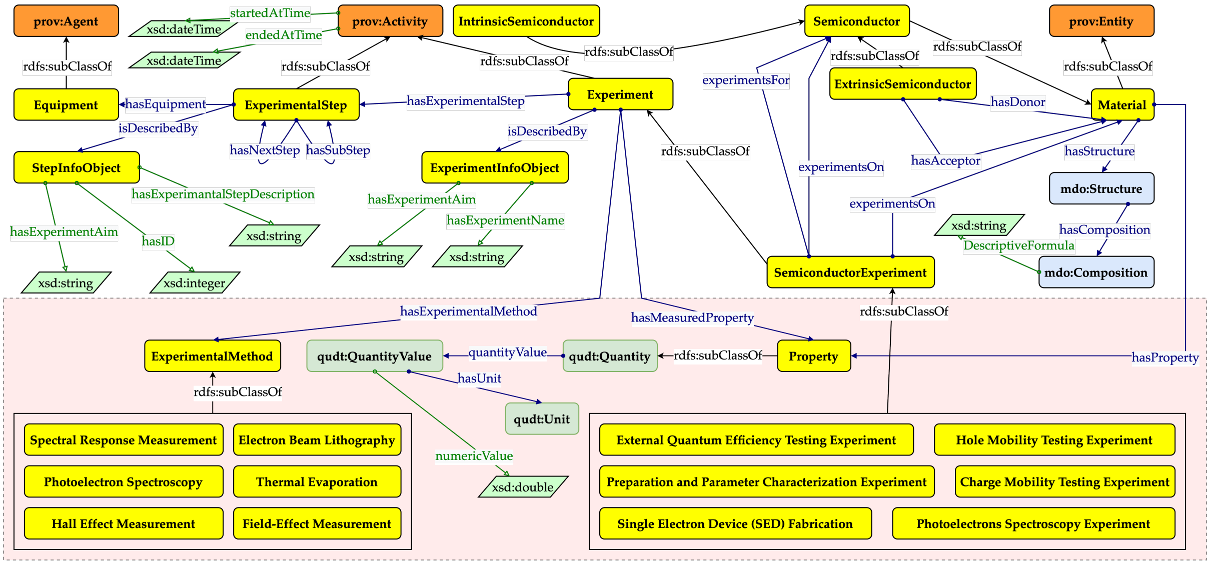

Figure 3: The semiconductor ontology, with latest extensions in the dashed box at bottom [43, 44].

4. Use Case - Semiconductor Materials

Our initial use case focuses on FAIR data management for sustainable semiconductor materials primarily for perovskite-based structures such as Perovskite Solar Cells (PSCs) and Perovskite Light-Emitting Diodes (PeLEDs). They have gained significant interest due to their low production costs and high power conversion efficiencies (PCEs) [41, 42]. For instance, some PSCs and PeLEDs have reached more than 20% PCE [41, 42]. These properties qualify them as ideal candidates for building-integrated photovoltaics (BIPV) and many mobility applications such as in vehicles, boats, and airplanes, where traditional silicon solar cells are unsuitable. In the following sections, we describe our initial work on sustainable PeLEDs design and the implementation of FAIR data management practices for semiconductor experiments.

4.1. Sustainability Analysis for PeLEDs

In [6], we conducted a comprehensive cradle-to-grave LCA and techno-economic analysis of 18 state-of-the-art PeLED devices. We evaluated environmental impacts and economic costs across all phases: raw material extraction, manufacturing, distribution, usage, and end-of-life. Furthermore, we introduced a novel metric Relative Impact Mitigation Time (RIMT)—the minimum operational lifespan required to offset manufacturing impacts. However, this work does not provide a direct method or workflow for integrating LCA results into materials design decisions at the lab level from the beginning. Future work will investigate how to integrate such LCA results into materials design, via Semantic Web-based technologies.

4.2. FAIR Data Management for Semiconductor Experiments

We have begun investigating FAIR data management principles for designing semiconductor-based materials. The design of semiconductor materials such as PSCs and PeLEDs with desired properties requires semiconductor experiments involving various perovskite compositions, different synthesis methods and a range of characterization techniques (e.g., microscopy for microstructure investigation and analysis). These experiments generate extensive experimental data which is crucial for advancing semiconductor applications. For instance, experimental parameters can influence material properties, potentially making them suitable for a range of applications. Visualization or diagrammatic analysis of experimental data can highlight insights that are not immediately apparent in raw data. Furthermore, machine learning can leverage these datasets to predict material behaviors under conditions difficult to reproduce experimentally, such as extreme temperatures or pressures. Integrating experimental data with simulation results from computational methods like Density Functional Theory further enriches the understanding of semiconductor materials [45].

In previous work, we initially explored how to represent semiconductor domain knowledge in ontologies by developing a semiconductor ontology, SemicONTO as shown in Figure 3. The initial version, SemicONTO v0.1, demonstrated the ability to represent basic experimental information such as objectives, procedures, and detailed descriptions [43]. In the ongoing work [44], we extend SemicONTO by incorporating additional concepts and relationships specific to semiconductor experiments, particularly focusing on experimental methods and material properties observed during experiments. In addition, the ontology includes taxonomies of semiconductor experiments and experimental methods, respectively. Figure 3 illustrates the ontology with its latest extensions. Using this extended ontology, we have developed SemicKG, a knowledge graph representing semiconductor experimental data. SemicKG is publicly accessible through the ontology's documentation page,[11] and a SPARQL endpoint is available for users to query and access the knowledge graph.

5. Summary and Outlook

Materials science is undergoing a transformation, with growing emphasis on sustainability assessment. This shift poses a new challenge for data-driven materials design: integrating and managing data from diverse sources, including experimental results, simulations, and sustainability evaluations. In this position paper, we outline our vision for sustainable advanced materials design, emphasizing the role of Semantic Web technologies in enhancing interoperability throughout the materials design workflow. These technologies enable machine-readable, semantically rich data representations, which facilitate efficient data sharing, reuse, and analysis.

To support this vision, we first survey existing ontologies related to sustainability, life cycle assessment, circular economy and materials, identifying opportunities for alignment and extension within these relevant domains. Furthermore, we review existing global and EU standards on LCA and sustainability, which will offer valuable guidelines for developing materials design methodologies that incorporate sustainability considerations. We then present a semiconductor materials use case, demonstrating how experimental data can be semantically annotated and how sustainability considerations can be incorporated into the design process.

Subsequently, we aim to establish interdisciplinary collaborations to further develop, test, and validate the concepts in our vision. Future work will extend the approach to additional use cases in both materials and product design, with a particular focus on sustainable materials development guided by FAIR principles and supported by Semantic Web technologies.

Declaration on Generative AI

During the preparation of this work, the authors used GPT-4-turbo in order to grammar and spell check, and improve the text readability. After using the tool, the authors reviewed and edited the content as needed to take full responsibility for the publication's content.

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