International Journal on Recent and Innovation Trends in Computing and Communication
ISSN: 2321-8169 Volume: 11 Issue: 1
***Article Received:** 22 November 2022 **Revised:** 30 December 2022 **Accepted:** 12 January 2023*

Constructing a Semantic Data Model for the Field of Material Science through Ontology

[1]T.Kumarasan, [2]Kalpana B, [1]Dr.P.Prabhakaran, [1]C.Franklin, [1]K.Prakash, [1]G.Vinod

[1] Department of Electronics and Communication Engineering, J.J. College of Engineering and Technology, Trichy, Tamilnadu.
[2]Department of Electrical and Electronics Engineering, K.S.Rangasamy College of Technology, Tiruchengode - 637 215. Namakkal Dt. Tamil Nadu. India
[3]Department of Mechanical Engineering Rajalakshmi Institute of Technology, Chennai Tamil Nadu. India
kumarasant@jjcet.ac.in, kalpana@ksrct.ac.in, prabhakaranp@jjcet.ac.in, franklinc@jjcet.ac.in, ramavelm@jjcet.ac.in, vinod.g@ritchennai.edu.in

Abstract:

This research presents a method for constructing a semantic data model for the field of material science based on ontology. The method involves designing the semantic data model and establishing mapping rules between the data model and the ontology. Data semantic analysis and annotation are carried out based on the semantic data model, supporting the integration and efficient retrieval of heterogeneous data in the material science field. Furthermore, the method utilizes the OWL-S technique to describe, issue, and acquire relevant data services, enabling higher-level service semantic synergy in the material science domain. The proposed method effectively enables semantic integration, intelligent inquiry, and personalized services for data in the material science field.

Keywords: Semantic data model, Ontology, Material science, Data integration, Data retrieval, OWL-S

Introduction

In the field of material science, the generation and accumulation of vast amounts of data present both opportunities and challenges. The effective management, integration, and utilization of this data are crucial for advancing research, enabling discoveries, and driving innovation. Traditional data management approaches often fall short in handling the complexity and heterogeneity of material science data, limiting the full potential of valuable information. To address these limitations, the application of semantic technologies and ontologies has gained increasing attention. Ontologies provide a formal representation of knowledge and enable the semantic interpretation of data. By designing a semantic data model based on ontology, it becomes possible to integrate, analyze, and retrieve material science data more effectively, facilitating intelligent inquiry and personalized services (Huang and Cole 2020).

The objective of this research is to propose a method for constructing a semantic data model specifically tailored to the material science field. The method aims to leverage the power of ontologies to enhance data management and analysis in material science. By designing the semantic data model and establishing mapping rules between the data model and the ontology, the research seeks to create a structured framework for organizing and interpreting material science data. Furthermore, the research focuses on data semantic analysis and annotation based on the semantic data model (Khoroshevsky 2019; Trausan-Matu and Neacsu 2008). This step involves analyzing structured, semi-structured, and non-structured data and annotating them with meaningful semantic metadata. The result is the construction of a semantic visual model that provides a comprehensive view of the field data, enabling efficient retrieval and integration of heterogeneous data sources (Deng, Zhang, and Hong 2020; Li, Armiento, and Lambrix 2020).

To support higher-level service semantic synergy in the material science field, the method incorporates the use of OWL-S, an ontology web language for service description. By utilizing OWL-S, relevant data services can be described, issued, and acquired, enabling advanced data-driven applications and facilitating collaboration among researchers and institutions. Overall, the proposed method for constructing a semantic data model based on ontology offers significant potential for the material science field. It provides a foundation for effective semantic integration, intelligent inquiry, and personalized services for material science data (Li, Armiento, and Lambrix 2019). By leveraging semantic technologies and ontologies,

International Journal on Recent and Innovation Trends in Computing and Communication
ISSN: 2321-8169 Volume: 11 Issue: 1
***Article Received:** 22 November 2022 **Revised:** 30 December 2022 **Accepted:** 12 January 2023*

researchers and practitioners can unlock the full value of data, streamline research processes, and drive scientific advancements in the field of material science.

Related Work

The concept of ontology originates from the field of philosophy and is defined as a systematic description of entities in the world. However, in the field of computer and information science, ontology refers to a formal and detailed explanation system for shared ideas. It provides a shared vocabulary for describing specific domains, including object types, concepts, attributes, and their relationships (Huang and Cole 2020).

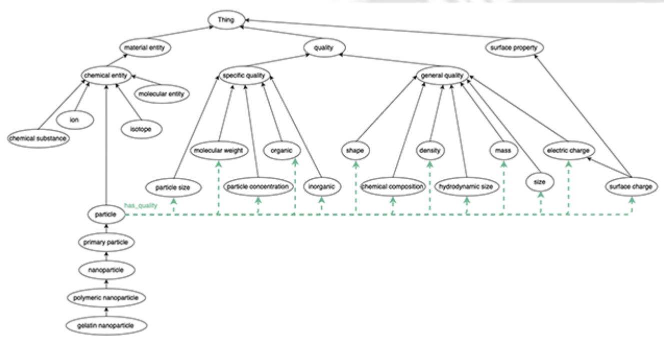

Figure 1. Example from NanoParticle Ontology

The NanoParticle Ontology encompasses various elements such as particle dimensions, molecular mass, particle density, concentration, organic and inorganic nature, shape, chemical composition, hydrodynamic dimensions, mass, size, and electric charge. Additionally, particles possess inherent qualities, which are depicted by an axiom establishing a connection between the concepts of particle and quality through the "has quality" relation (**illustrated by green dashed arrows in Figure 1**). Properties represented by relations are inherited within the is-a hierarchy, thereby extending the relationship between sub concepts of particles and associated qualities.

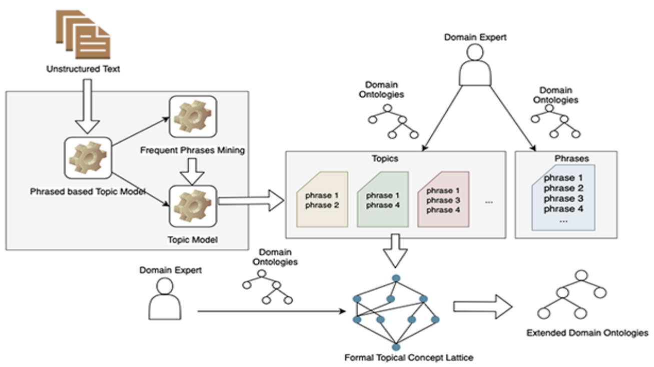

Figure 2. Methodology for enhancing ontologies

Essentially, ontology formalizes the expression and relationships of concepts within a specific domain. Ontology is a specific type of terminology with structured features, making it highly suitable for use in computer systems (Li et al. 2019). Its purpose is to obtain domain knowledge, determine commonly accepted vocabulary in the target domain, and provide clear and formal definitions of the relationships between these terms. By using ontology to provide formal descriptions for specific domains, it encompasses the formal representation of knowledge, precise definitions of field-specific terms, and semantemes.

Methodology: The top section of the diagram (**Figure 2**) illustrates the construction of a phrase-centric topic model, utilizing unstructured text as input and producing phrases and topics as output. The bottom section demonstrates the application of formal topical concept analysis, taking topics as input and generating a topical concept lattice as output. In both sections, the outcomes are verified and interpreted by a subject matter specialist.

The formal nature of ontology enables machine-accessible semantic descriptions, facilitating interaction between humans and machines, and supporting reasoning to uncover implicit domain knowledge and provide value-added information services to users (Himanen et al. 2019). In recent years, ontology has found widespread applications in various fields such as scientific data sharing, intelligent information retrieval, digital libraries, knowledge engineering, artificial intelligence, and information system integration. The research on data integration based on ontology has achieved significant progress, and the use of ontology to solve semantic heterogeneity issues between data sources has become a commonly adopted method for integrating heterogeneous data sources.

However, there is still a need for further research on the application of ontology for material science data integration. This is because material science data presents unique challenges that require specific solutions in the following aspects: First, there is a high demand for handling large amounts of data in material science applications, requiring support for managing extensive material science data. Second, material science data is heterogeneous, distributed, mixed, and often disorganized, with complex structural associations (Pauwels et al. 2015; Porotto 2015). Third, achieving semantic interoperability between material data sources is challenging, as the configuration of isomeric data models is complex and subject to change, requiring improved access efficiency. Fourth, scientists often need to access required material science data from multiple autonomous systems, and manually extracting the necessary

International Journal on Recent and Innovation Trends in Computing and Communication
ISSN: 2321-8169 Volume: 11 Issue: 1
***Article Received:** 22 November 2022 **Revised:** 30 December 2022 **Accepted:** 12 January 2023*

services can be time-consuming and labor-intensive. Addressing these challenges and expanding the use of ontology for material science data integration is an important area of research. By developing methods and techniques that leverage ontology to overcome semantic heterogeneity, manage extensive data, and support efficient access and retrieval, researchers can enhance the integration and utilization of material science data, enabling advancements in the field and facilitating scientific discoveries and innovations.

Research Objective:

The main objective of this research is to create a method for building a semantic data model specifically tailored for the field of material science, using the concept of ontology. The aim is to develop a comprehensive framework that facilitates effective semantic integration, intelligent inquiry, and personalized services for data in the material science domain. To achieve this objective, the research focuses on several key aspects. Firstly, the data model itself is designed, taking into consideration the specific requirements and characteristics of material science. This involves defining the concepts, attributes, and relationships that accurately represent the domain knowledge in a structured manner.

Secondly, mapping rules are established to connect different data patterns (structured, semi-structured, and unstructured) with the ontology. These rules ensure that data from diverse sources and formats can be aligned with the predefined concepts and relationships in the ontology.

Thirdly, data semantic analysis and annotation are conducted based on the semantic data model. This process involves analyzing the meaning and context of the data, identifying important concepts, and adding semantic tags or labels to the data elements. It enables a deeper understanding of the data and enhances its searchability and interpretability.

Furthermore, a semantic visual model is constructed using the annotated data. This visual model provides a comprehensive representation of the material science data, enabling researchers to efficiently integrate and retrieve heterogeneous data. It supports better data exploration, knowledge discovery, and decision-making in the material science field. Lastly, the research leverages OWL-S technology (Ontology Web Language for Services) to describe, publish, and acquire relevant data services. OWL-S enables the higher-level semantic collaboration of services in the material science domain. By utilizing OWL-S, researchers can access and utilize a wide range of data services, such as data retrieval, analysis, and inference engines, which enhance the overall capabilities and intelligence of the system.

By accomplishing these objectives, the research aims to provide material scientists with a powerful tool for effectively integrating, analyzing, and utilizing data in the material science field. It enables researchers to leverage the semantic knowledge captured in the ontology, facilitating advanced data exploration, decision-making, and personalized services tailored to the specific needs of material science research.

Constructing a Semantic Data Model for the Field of Material Science through Ontology

A Method for Building a Semantic Data Model in Material Science using Ontology. This research presents a method for constructing a semantic data model in the field of material science based on ontology. The method consists of the following steps:

Step 1: Designing a material science semantic data model using ontology and establishing a mapping rule between different data patterns and ontology.

- In this step, a semantic data model is created specifically for the field of material science. This model is designed based on the principles of ontology, which involves defining a set of shared concepts, attributes, and relationships that accurately represent the domain of material science. Additionally, a mapping rule is established to connect different data patterns (such as structured, semi-structured, and unstructured data) to the ontology. This mapping rule ensures that data in various formats can be aligned with the concepts and relationships defined in the ontology.

Step 2: Performing data semantic analysis and annotation for structured, semi-structured, and unstructured data in material science.

- Once the semantic data model is established, it is used to analyze and annotate data in the field of material science. This analysis involves understanding the meaning and context of the data, identifying key concepts, and assigning semantic tags or labels to the data elements. This process is performed for structured data (organized in a specific format), semi-structured data (partially organized or annotated), and unstructured data (lacking a specific format or organization). The outcome of this step is the creation of a semantic visual model, which provides a comprehensive representation of the data and enables efficient integration and retrieval of heterogeneous data in the material science field.

Step 3: Utilizing OWL-S technology to describe, publish, and acquire relevant data services for higher-level semantic collaboration.

- In this step, OWL-S technology (Ontology Web Language for Services) is used to describe, publish, and acquire data services that support higher-level semantic collaboration in material science. OWL-S provides a standardized way to describe the functionalities and capabilities of data services, allowing them to be easily discovered, accessed, and integrated into the material science ecosystem. These data services can range from data retrieval and analysis tools to advanced semantic reasoning engines. By utilizing OWL-S, material scientists can benefit from a wide range of data services that enable collaboration, knowledge sharing, and advanced data-driven insights in the field of material science.

The integration of heterogeneous data in material science involves several steps. It includes integrating the semantic annotations of structured and semi-structured material data, tagging and organizing unstructured material data for retrieval purposes, and creating a semantic visual representation that supports multi-lingual environments.

The data retrieval and semantic visualization step in a multi-lingual environment involves the following:

- Establishing a mapping mechanism using Semantic Web Technology to enable the semantic mapping of implicit knowledge in material science data.
- Utilizing clustering, classification, and association analysis techniques to analyze data from multiple sources and different granularities and dimensions. This helps create a real-time mining model for the intrinsic characteristics of data semantics in a multi-lingual environment, facilitating collaborative inference and evolution.
- Employing information visualization techniques to build a data semantic visualization model in an interactive multi-lingual environment. This model enables the merging of various application services based on semantics and supports decision-making processes.

By implementing this method, material scientists can effectively integrate, query, and analyze data in the field of material science, leading to improved research outcomes and decision support.

Conclusion

The proposed method for constructing a semantic data model based on ontology offers significant advantages for the material science field. It enables effective semantic integration, intelligent inquiry, and personalized services for data. The semantic data model facilitates structured, semi-structured, and non-structured data analysis and annotation, leading to the construction of a semantic visual model for efficient data retrieval. By utilizing OWL-S, relevant data services can be described, issued, and acquired, promoting higher-level service semantic synergy. Overall, this research contributes to realizing the full potential of data in the material science field, improving research efficiency, and supporting advanced data-driven applications in the domain.

References:

1. Deng, Shiqi, Zhen Zhang, and Liang Hong. 2020. “Domain Ontology Construction for Intelligent Anti-Telephone-Fraud Applications.” Pp. 200–210 in.
2. Himanen, Lauri, A. Geurts, Adam Foster, and Patrick Rinke. 2019. “Data-Driven Materials Science: Status, Challenges, and Perspectives.” *Advanced Science* 6. doi: 10.1002/advs.201900808.
3. Huang, Shu, and Jacqueline Cole. 2020. “A Database of Battery Materials Auto-Generated Using ChemDataExtractor.” *Scientific Data* 7. doi: 10.1038/s41597-020-00602-2.
4. Khoroshevsky, Vladimir. 2019. “ONTOLOGY DRIVEN SOFTWARE ENGINEERING: MODELS, METHODS, IMPLEMENTATIONS.” *Ontology of Designing* 9:30–49. doi: 10.18287/2223-9537-2019-9-4-429-448.
5. Li, Huanyu, Rickard Armiento, and Patrick Lambrix. 2019. “A Method for Extending Ontologies with Application to the Materials Science Domain.” *Data Science Journal* 18:50:1-50:21. doi: 10.5334/dsj-2019-050.
6. Li, Huanyu, Rickard Armiento, and Patrick Lambrix. 2020. *An Ontology for the Materials Design Domain*.
7. Pauwels, Pieter, Seppo Törmä, Jakob Beetz, Matthias Weise, and T. Liebich. 2015. “Linked Data in Architecture and Construction.” *Automation in Construction* 57:175–77. doi: 10.1016/j.autcon.2015.06.007.
8. Porotto, Alessandro. 2015. *Urbanity and Construction of the City*.
9. Trausan-Matu, Stefan, and Anca Neacsu. 2008. “An Ontology-Based Intelligent Information System for Urbanism and Civil Engineering Data.” Pp. 85–92 in.