RDA/CODATA Materials Data, Infrastructure & Interoperability IG

Formation of a Materials Ontologies Task Group

Proposed Co-chairs

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Background

Ontologies provide a way of expressing our understanding of the world, or specific domains in a way that enables interoperability based on semantics and logics rather than just formats and agreed metadata. Ontologies also have an important role to play in making data FAIR. There have been developments in ontologies in the materials domain for many years, in particular in applications that support the integration of data, see for example MatSeek [1], the work by Ashino [2], a recent review paper [3] and a recent example [4]. Current efforts also include the development of the European Materials Modelling Ontology in the framework of the European Materials Modelling Council [5].

There is also an interest from engineering and manufacturing to connect to materials ontologies, see for example the Industrial Ontologies Foundry [6].

International collaboration on materials ontologies are a means to enabling the exchange of data and knowledge with impact on the many research and industrial domains that draw on and benefit from materials technologies.

Format of the initiative

Within the structure of RDA, the form of a Task Group provides a means for a group of interested people to get together in a rather informal manner. The Task Group will pursue certain objectives but does not target a formal deliverable or report as a Working Group would.

Objectives of the Task Group:

Once formed, the Task Group will discuss its objectives and prioritisation. The following is a first attempt at expressing some of the topics for discussion. The items are roughly ordered in terms of starting with items aimed at building a community. It is not meant to reflect the importance of the items.

- Establish improved communication between groups involved in materials ontologies around the world. Ensure clear definitions so that we know we talk about the same thing. Map the field in terms of
    - Who are those groups?
    - What are they involved with?
- Check and communicate relevant existing RDA recommendations/reports in the ontologies field. Put together relevant definitions/explanations of what we mean by ontologies.
- Collection of use cases and requirements for materials ontologies
    - Set up online means for collection (e.g. github).
    - Create problem statements and sample instance graph related to use case; instance diagrams showing how to solve problem using different ontologies/implementations. Consider SHACL queries associated with these. Also datasets (open materials data) linked to use case.

- Determine together with Semantic Assets Task Group about recommended repositories for Materials Ontologies (e.g. Bioportal). Making ontologies FAIR.
- Develop recommendations on a governance system for materials ontology development, including domain branches. Investigate the governance model proposed by Industrial Ontologies Foundry.
- Discuss upper level ontologies in the context of materials science needs.
- Develop recommendations regarding interoperability of materials ontology developments.
- Discuss and develop recommendations for ontology alignment. Topics include using different languages, e.g. interoperability when same concepts have been expressed in different languages; how to bring ontologies with different perspectives together around concepts described in both ("cross-perspective" interoperability and integration). Bringing ontologies with the same (in principle) perspective together so that a machine can operate on both (same perspective interoperability across different ontologies/languages).
- Discuss how best to work and interface with other domains e.g. engineering ontologies.

How the group will operate

The Task Group will operate informally working via regular online meetings and reporting updates via the IG. It will use a simple communication and collaboration tools such as google docs/sites to share information. Anyone with an interest in materials ontologies is welcome to join.

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References

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[2] Ashino, T., 2010. Materials ontology: an infrastructure for exchanging materials information and knowledge. Data Science Journal 9, 54–61.

[3] Zhang, X., Zhao, C., Wang, X., 2015. A survey on knowledge representation in materials science and engineering: An ontological perspective. Computers in Industry 73, 8–22.

[4] Takahashi, L., Miyazato, I., Takahashi, K., 2018. Redesigning the Materials and Catalysts Database Construction Process Using Ontologies. Journal of Chemical Information and Modeling 58, 1742–1754.

[5] https://emmc.info/taxonda/emmo-european-materials-modelling-ontology/

[6] https://sites.google.com/view/industrialontologies/home