EMMC Task Group Report:
Characterisation Methodology Domain Ontology

Duration

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Task Group Leaders, Members, Contributors

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Goals

The goal of the task group was to support and coordinate the development of an EMMO domain ontology capturing materials characterisation methodologies.

The ontology should serve as a common framework for applications in all areas of materials characterisation, supporting harmonization and interoperability and FAIR data documentation. The starting points of the development are the CHADA CWA 17815, EMMO Top and Middle Level ontologies as well as initial ontology work carried out in European projects.

Objectives and planned outcomes

Community agreement on the representation of CHADA (concepts and workflows) in an ontology.

Agreed taxonomies for key CHADA entities, in particular of characterisation methods. Collaborate with other relevant Task Groups on these taxonomies.

Guidelines to support consistent subdomain and application developments based on the characterization domain ontology.

Group Activities

The group met regularly online and there is a track of the meetings in the EMMC Forum: https://emmc.eu/forum?view=topic&id=154

A wide range of topics related to the Task Group came up and here are some key resources that were noted:

- https://gitlab.cc-asp.fraunhofer.de/EMI_datamanagement/bwmd_ontology/ has sample preparation and various materials testing concepts in BFO based ontology
- https://bioportal.bioontology.org/ontologies/ENM/ has microscopy instruments etc
- https://bioportal.bioontology.org/ontologies/NPO/ also has various analytical methods

- Vibrational Spectroscopy Ontology (VIBSO) https://github.com/NFDI4Chem/VibrationalSpectroscopyOntology
- https://nfdi4chem.github.io/VibrationalSpectroscopyOntology/

Taxonomies and classification

- NIST https://datascience.codata.org/articles/10.5334/dsj-2021-018/
- Instead of a fixed taxonomy, we should define methods as concepts with different dimensions (probe, signal, data dimension, 'in-situ/ex-situ/etc (see https://iupac.org/projects/project-details/?project_nr=2021-009-2-500
- EM Glossary as a good approach and resource https://gitlab.hzdr.de/em_glossary/em_glossary
- Glossary of methods and terms used in analytical spectroscopy https://www.degruyter.com/document/doi/10.1515/pac-2019-0203/html

Properties

- https://paulingfile.com/index.php?p=physical%20properties#list%20of%20properties
- Pauling file properties tab added to the shared spreadsheet https://docs.google.com/spreadsheets/d/1WbdFaAh1s2l5_CVOfnvMOPcB5rL2--ms/edit#gid=34329318
- Madices: https://madices.github.io/. Highlight: https://terminology.nfdi4chem.de/ts/index,
- RAMAN spectroscopy is to use Wikidata: https://wiki.charisma.ideaconsult.net/wiki/Project:About

Semantic Wiki

- Semantic wikimedia for collaboration, e.g. KIproBatt Wiki (Simon Stier - Fraunhofer ISC) https://kiprobatt.de/wiki/Main_Page
- See also Onto-Wiki https://onto-wiki.eu/wiki/Main_Page
- https://demo.open-semantic-lab.org/wiki/Main_Page

BPMN

- List of BPMN tools
- http://bpmn-miwg.github.io/bpmn-miwg-tools/
- https://bpmn.io/ Web-based tooling for BPMN, DMN, CMMN, and Forms | bpmn.io

Outcomes

The main outcomes of the Task Group are the CHAMEO ontology as well as specific method ontologies for nanoindentation and FIB-DIC, all supported by NanoMECommons.

CHAMEO was developed as an ontological, i.e. machine-readable representation of the CEN Workshop Agreement on Materials characterisation – Terminology, metadata and classification (CWA 17815:2021). Revising all of the conceptualisations and using the EMMO as a top and middle level ontology, CHAMEO was updated and extended. The eventual CHAMEO version then informed an updated CEN Workshop Agreement on Materials characterization - Terminology and structured documentation.

For further information, please see the CHAMEO documentation.

Associated research projects and acknowledgements

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