



Materials Ontology Workshop

29th June, 2018

Brussels, DG RTD, CDMA-SDR-1

EC DG RTD organised a workshop for a wide range of stakeholders to discuss Materials Ontologies. A wide range of experts found in the EC expert database were invited to send input in the form of three slides. Each expert who sent in input was invited to the meeting. Some 130 people expressed an interest and 73 experts from 15 countries got together on 29th June for a full day of presentations and discussions. Stakeholders included:

- EMMC representing academia and industry and all types of modelling
- Characterisation experts
- Processing experts
- Manufacturing experts
- Ontology experts from different communities
- Philosophers

Input contained info on 21 existing taxonomies and 11 existing ontologies for the following domains:

- Cheminformatics
- Nano-safety and toxicology experts
- Characterisation
- Chemical reactions
- Biomass
- Energy management
- Design and manufacturing
- Decision support
- Text mining
- Market Place operations

The workshop provided a unique and probably first-ever opportunity for experts from such a wide range of backgrounds, but sharing a common interest in materials and ontologies, to get together.

Key outcomes of the meeting are:

- The set of presentations given (all shared one week in advance of the workshop on the EMMC website <https://emmc.info/ec-nmbp-workshop-2018-slide-share/>) represent a first compendium of efforts for semantic knowledge systems (keyword lists, taxonomies, ontologies) in the materials space.
- A wide range of reasons for ontologies and benefits of ontologies was gathered including common understanding, data interpretation, source linking, establishing and enforcing rules, inferencing capabilities reasoning also across data sources (hence answer queries that would not otherwise be answered) etc.
- The power of ontologies has been demonstrated in application examples, including data-mining, data-base linking, as well as reasoning example (early AI) and addressing a number of challenges in engineering.

- The need for ontologies to support AI was discussed and clarified: Ontologies support the intermediate structuring and meaningful storage of data, enabling and speeding up AI.
- Currently there are a wide range of efforts and approaches ranging from fundamental ontologies to purely application-oriented ontologies that are not based on fundamental physics/materials science concepts.
- The need for one common ontology across the materials field to enable knowledge extraction and exchange was clearly endorsed by the audience.

The European Materials Modelling Ontology (EMMO) presentation set out some basic features which a common material ontology should have:

- description of materials from a rigorous physics perspective
- formal relations between granularity levels to facilitate multiscale materials description
- definition of material processes to capture the changing and evolution of materials as chain of different states.

Existing ontologies only partially cover these needs. The EMMC found a solution for these needs, and these are incorporated in the EMMO.

Delegates showed a strong interest and motivation to get organised and collaborate on integration. This will include partial integration of ontology modules across domains, e.g. integration of taxonomies into existing ontologies as well as in the longer term achieving a common ontology across the materials field, which requires a deeper agreement on core concepts and upper level ontology.

Delegates received addresses from Peter Dröll, Director NMBP about the importance of Big Data and Artificial Intelligence in NMBP area and H  l  ne Chraye, HoU AM&N about the importance of access in the Materials domain. Peter Dr  ll set the topic of the meeting within the framework of the 2013 European Council decision on the Digital Economy. He gave a clear message for the experts gathered that the status of only about 1% of data generated being used needs to be addressed and that we are called to make data more valuable, i.e to add value by structuring and organising data for their use and for reasoning, i.e. AI. H  l  ne Chraye emphasised the importance of a wide agreement leading to standards.

Margrete Hoffmann-Antenbrink set the materials scene by emphasising the need for a systems approach covering materials research, development and innovation covering materials, technologies, business and social systems. This requires the seamless flow of data and information between systems and along the value chain, which translates into a need for a materials ontology: a systems approach urgently needs a 'common language' between modelling, characterisation, processing and production. Alexandra Simperler picked up on the 'common language' or 'lingua franca' in her excellent introduction to ontologies and provided nice examples and useful applications of ontologies, also illustrating potential pitfalls.

Silvia Chiacchiera and Georg Schmitz presented how ontologies enable the operations of a modelling market place. This market place ties in with the above mentioned 'systems approach', in particular considering how aspects such as training, translation and model validation can be made available via data management.

Other presentations on the agenda presented a range of taxonomies and ontologies as well as ontology use cases. The need for and purpose of ontologies and how the ontologies are represented and implemented were also covered in these contributions.

There were lively discussions throughout the day. Topics included:

- Translation between ontologies
- The contribution of ontologies to big data analysis
- Governance in ontology development
- Provenance of data instances in ontologies and how provenance and accuracy are captured.
- Ontology tools to support working with ontologies.
- Light versus heavy ontologies regarding relations and constraints (to be kept inside or outside of the ontology).
- Reward systems for contributing.

The discussion session already included a number of suggestions on how to work together to gather more detailed information, define use cases, review and document existing ontologies as well as tools, review existing collaborations and collaboration models and integrate all efforts.

As follow up a series of collaborative activities is set up and contain a release of the EMMO in the form of a commented, modular OWL-DL file in September. We will form an Interest Group (IG) that can discuss the modules as well as the relations across. Expressions of interest to take an active part in the International Materials Ontology IG will be solicited in September 2018. The formation and affiliation of IG will be decided in October 2018. The EMMC can host the IG in terms of providing the Forum for discussion etc. A template, called TAXONDA, to collect information on existing list of keywords, taxonomies and ontologies will be shortly send around for comments. Testing on user cases can then be done.

The first possibility to meet again will be the Interoperability workshop in Freiburg on 6-7 November. Details will appear shortly on the EMMC website www.emmc.info.

In conclusion the audience is convinced that data management with ontologies will allow the materials field to harvest the value of data in the eminent digital era.

Anne de Baas and Gerhard Goldbeck

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Agenda

Chair: A.F. de Baas, EC

- 9:00 Importance of Big Data and Artificial Intelligence in NMBP area Peter Dröll, director NMBP
9:15 Importance of access in the Materials domain Hélène Chraye, HoU
AM&N
9:30 Integration in materials domain: a system approach Margrete Hoffmann, *MatSearch*
9:45 Introduction to ontologies Alex Simperler, Simperler consulting
10:15 Status of materials informatics Anne de Baas, PO AM&N
- 10:30 Examples of lists of key words
Starting ontology work for Market Places VIMMP & *Market Place*
Silvia Chiacchiera & *G.Schmitz*
- 10:40 Show case of taxonomies with some relations
SNOMED, a medical taxonomy Alejandro Alija
ALLOTROPE, interface between chemical industry and suppliers Heiner Oberkamp
ENM, a nanotoxicology decision system Egon Willighagen
- 11:10 Existing ontologies
Text mining at Bosch Benedikt Ziebarth
Biomass ontology Nikolaos Trokanas
Energy management Hendro Wicaksono
Characterisation (design and standard protocols) C. Charitidis and Chris Eberl
- 11:50 Show case of the use of ontologies
ONTOKIN, matching chemical reactions and components Amit Bhave
Manufacturing platform for product service design Dimitris Kiritsis
Nuclear reactor operational decisions Dov Dori
Semantic transportation,
decision support and rules expressions for ecolabeling Hedi Karray
- 12:30-13:00 Lunch break**
- 13:00-14:00 European Materials Modelling Ontology (EMMO) Emanuele Ghedini, Univ Bologna
- 14:00-14:30 Purpose of the workshop Gerhard Goldbeck, GCL
Enlarging the EMMO towards the EMO
What are the building blocks?
Modelling, characterisation, processing (and manufacturing)
- 15:00-16:00 Participants comments and Discussion moderator Anne de Baas
- 16:00-16:30 Establishment of Action Plan (bottom-up Working Group)