



# The European Materials Modelling Council

## EMMC Workshop on Interoperability in Materials Modelling

### Interoperability Discussion and Action Plan

*EMMC-CSA project has received funding from the European Union's Horizon 2020 research and innovation programme, under Grant Agreement No.723867*



## Objective

- Demonstrate the efficiency and practicality of a semantic approach to improving communication, curation, integration and interoperability.



## Approach

1. Establish a standard for terminology and classification of materials modelling, and for the documentation of simulations: CWA!
2. BFO based Materials Modelling Ontology.

A semantic reference for the specifications of file-based schema (“data formats”) such as the hierarchy and keywords in HDF5.

3. Agree on open standards for interoperability





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## Discussion Points

- How can materials modelling build on the success of ontologies in other fields, e.g. life sciences, chemical engineering etc?
- What “lessons learnt” should be taken into account?



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## Discussion Points

EMMO is designed to provide the semantic framework for software vendors to build interoperable solutions.

- What are the software owner needs?
- What collaborations can be put in place to further the common goals?
- What can we learn from industry initiatives such as Allotrope.



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## Discussion Points

EMMO should support industry in managing and utilising models and data better as 'digital assets'; facilitate the integration of materials modelling with other digitalisation efforts.

- What are industry requirements?
- How can collaborations with industry be built to ensure this goal is achieved?
- What efforts are needed to make this happen in an efficient and effective manner?



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## Discussion Points

EMMO success requires commitment from the whole community to endorse it and use it.

- What are the potential bottlenecks and barriers for a wide endorsement and use?
- What governance structure should be put in place of the EMMO?



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## Workshop etiquette

- Interact and discuss in an open and courteous manner
- Be respectful of the considerations expressed by others.
- Since the agenda is dense, attention to and respect of the time frame is crucial.





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## Thanks to our sponsors



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## Marketplaces



**Cross domain or semantic interoperability requires ontology, but this is usually used to annotate data, while data repositories and marketplace need to cater for the curation and utilisation of data.**

- Is this sufficient to achieve interoperability and linking between repositories?
- Do we need an ontology of “operations, methods, and actions” on data, in terms of post, pre-processing, and accessibility? (these can be manifested, e.g., by ontology of application programming interfaces (API's))



### **Marketplaces contain much more than data, also models, workflows, and other “social networking” components**

- Does the interoperability between marketplaces require necessary an auxiliary ontology (perhaps from existing ones) for workflows? Should this be part of the EMMO?
- Are there ontologies out there already for workflows that we can use?