

Modelling and characterisation as knowledge sources in a digital materials ecosystem: activities of EMMC, EMCC and related projects

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Materials modelling and characterisation are distinct yet strongly intertwined approaches to understanding, determining and predicting the behaviour of materials. Their interconnectedness comes into focus even more strongly in the era of Industry 5.0, relating to:

- (1) Digitalisation of materials, i.e. not just machine readable but also interoperable information on which new decisions can be based.
- (2) A human centric approach, i.e. better ways of integrating stakeholder knowledge
- (3) Developing sustainable materials, i.e. a complex range of criteria must be met.

Meeting these challenges requires a deep integration of all types of 'knowledge sources': expert knowledge as well as knowledge gained from multi-disciplinary, multi-scale modelling and characterisation protocols.

EMMC¹ and EMCC² represent modelling and characterisation communities, with a shared objective of overcoming barriers in communication and industrial deployment of advanced methods. They developed widely agreed schema known as MODA (Modelling Data) and CHADA (Characterisation Data) (each documented in CEN Workshop Agreements³), for harmonised documentation of simulations and characterisation experiments, including complex workflows. Building on these, EMMC and EMCC support further integration of modelling and characterisation in terms of data, workflows and knowledge. A foundation is the development of EMMO⁴ ontology as a framework that enables machine-readable, integrated representation of materials knowledge.

In this context, the presentation will present current developments from a number of EMMC and EMCC related projects including OntoCommons, OntoTrans, OpenModel and NanoMECommons, that share the objective of building an interconnected knowledge systems of materials. Such interoperable and meaningful data combined with ML/AI will become a powerful resource for materials scientists to extract and act upon complex information. Future directions will also be discussed, in particular the EMMC and EMCC contributions to the Materials 2030 Roadmap.⁵

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¹ <https://emmc.eu/>

² <http://characterisation.eu/>

³ https://www.cencenelec.eu/media/CEN-CENELEC/CWAs/RI/cwa17284_2018.pdf
<https://www.cencenelec.eu/media/CEN-CENELEC/CWAs/ICT/cwa17815.pdf>

⁴ <https://github.com/emmo-repo/EMMO>

⁵ <https://emmc.eu/news/materials-2030-roadmap-draft-published/>