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MODA AND CHADA: STANDARDIZATION AND DIGITALIZATION OF SIMULATION AND CHARACTERIZATION DATA IN MATERIALS SCIENCE

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Following the new paradigm of materials development, design, and optimization, digitalization is the In the landscape of materials science, achieving standardization is a key enabler for an efficient management of simulation and characterization data. This presentation introduces the MODA (Modeling Data) and CHADA (Characterization Data) frameworks, products of European initiatives, that were specifically developed for the documentation of simulation processes and materials characterization experiments in a standard and machine-readable manner. CHADA focuses on the documentation of laboratory characterization experiments, while MODA is dedicated to capturing the essentials of simulation processes. The standardization effort includes the creation of their semantic representation that is grounded in the Characterisation Methodology Domain Ontology (CHAMEO), which relates to the Elementary Multi-perspective Material Ontology (EMMO).

Accompanied by a supporting ecosystem, engineers and material scientists can create, via a friendly user interface, digital objects for the procedures, protocols and the settings that were involved in the workflow. These objects are stored in a purpose-built dataspace in which they can be found and queried. A complementing data integration pipeline can be configured by users to link input and output data and process parameters to the CHADA and MODA objects.

In a vision where digital twins of materials are stored in a dataspace, in which the semantics of data is directly understood by the system, MODA and CHADA will play a key role for outlying the ways in which materials data has been acquired and produced, including steps such as sample preparation, mathematical models, and post processing.