SIMPHONY FOR ONTOLOGY-BASED MATERIAL EXPLORATION

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At present, the increasing amount of generated data related to computational methods in material science demands for solutions that make this data findable, accessible, interoperable, and reusable (FAIR). Semantic methods, with ontologies at their core, represent a main technology to address this challenge by providing meaning to the existing data. One of their benefits is a human- and machine-readable generic material description based on natural language for the seamless exchange of knowledge between data sources.
The elementary multi-perspective material ontology (EMMO) developed by the European Material Modelling Council (EMMC) is the result of an organised multi-disciplinary effort [1] to create a base for common concepts in the field of materials modelling. In the initiative of several EU Horizon 2020 projects, the stakeholders are continuously contributing to the progress of the EMMO.
A specific EMMO-compliant solution is SimPhoNy (simulation framework for multi-scale phenomena in micro- and nanosystems), an ontology-based open-source Python framework that promotes and enables interoperability between any third-party software tools.
Such tools include the Interoperable Material-to-Device (IM2D) toolbox of the Horizon 2020-funded INTERSECT project, which furnishes semantic interoperability between simulation hub, data hub, and the graphical user interface. This is achieved through SimPhoNy by referencing the generic material science-related concepts of the ontology to the full data provenance in the data hub, while, in parallel, computations are initiated and executed in the simulation hub through AiiDA.
Besides providing semantic interpretation and cataloguing of simulation results, the ontology categorises the parametrisation into different user profiles (persona). Thereby, it gives recommendations related to the users' modelling experience without derogating the usability of the IM2D toolbox for expert users and domain specialists. Moreover, the semantic component of the IM2D toolbox enables coupling of additional workflow and backend solutions and ultimately provides the foundation for exchangeability of data between them.

Keywords
SimPhoNy, Ontology, Semantic Interoperability, IM2D.

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Reference
[1] The European Materials Modelling Council on https://emmc.info/emmo-info/ (15th October 2021).