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Sommario/riassunto

This open access book discusses advances in semantic interoperability for materials modelling, aiming at integrating data obtained from different methods and sources into common frameworks, and facilitating the development of platforms where simulation services in computational molecular engineering can be provided as well as coupled and linked to each other in a standardized and reliable way. The Virtual Materials Marketplace (VIMMP), which is open to all service providers and clients, provides a framework for offering and accessing such services, assisting the uptake of novel modelling and simulation approaches by SMEs, consultants, and industrial R&D end users. Semantic assets presented include the EngMeta metadata schema for research data infrastructures in simulation-based engineering and the collection of ontologies from VIMMP, including the ontology for simulation, modelling, and optimization (OSMO) and the VIMMP software ontology (VISO).