Ontology-based semantic interoperability on the Virtual Materials Marketplace[⋆]

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Abstract. The marketplace-level domain ontologies from the Virtual Materials Marketplace (VIMMP) project are presented. It is discussed

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how a two-step ontology alignment approach can be employed for aligning the domain ontologies with the European Materials and Modelling Ontology (EMMO), the top-level ontology used by VIMMP. This is illustrated by an example from molecular modelling and simulation.

Keywords: Computational molecular engineering · Semantic interoperability · Process data technology · European Materials and Modelling Ontology.

Digitalization of industrial process and product design and the uptake of industry 4.0 driven manufacturing methods is closely tied to innovations in process data technology. In this context, semantic interoperability can facilitate the integration of data with a heterogeneous provenance into a coherent framework [5].

The Virtual Materials Marketplace (VIMMP), which is under development in an ongoing Horizon 2020 project, will be an open two-sided marketplace platform, supporting the provision and acquisition of services and tools in materials modelling. For purposes of data management, ingest, and retrieval, VIMMP develops and employs a system of marketplace-level domain ontologies [7]. Thereby, knowledge representation is formalized for computational resources (domain ontology MACRO), materials modelling translation (MMTO), simulation workflows (OSMO), training (OTRAS), communication (VICO), simulation software (VISO), validation (VIVO), and model variables (VOV). An overview over this system of ontologies is given in previous work [7]; for a thorough exposition we refer to the documentation [8] and to articles that introduce the marketplace-level domain ontologies MMTO, OSMO, and VISO specifically [6, 9].

The European Materials and Modelling Ontology (EMMO), cf. Goldbeck et al. [4], is used as a top-level ontology to facilitate interoperability between platforms. The VIMMP ontologies have been released recently [8], and for the EMMO, the full (alpha) version [2] and a simplified version (EMMO1s) used by VIMMP [8] have been made openly accessible. In Figs. 1 and 2, a knowledge graph describing a molecular model for acetylene is shown as an example. JSON-LD serializations of knowledge graphs can be exchanged between VIMMP and other platforms to communicate data and metadata in a well-defined way; e.g., prospectively with the MolMod DB [10] and Bottled SAFT [3] model databases.

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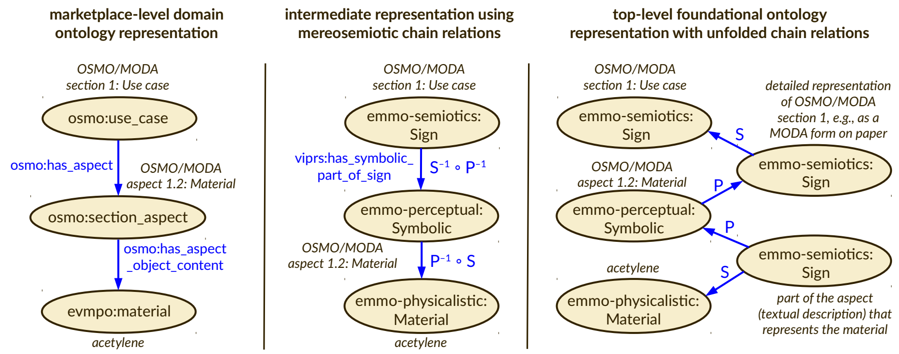

Fig. 1. Correspondences between the domain and top levels; example: Description of a materials modelling use case following MODA [1] and OSMO [9]. Ellipses denote individuals (i.e., objects), labelled by the concept names from the respective ontologies (EVMPO, OSMO, and multiple EMMO modules), and arrows denote relations; P and S stand for the main mereotopological and semiotic relations "is proper part of" and "is sign for," respectively. At the intermediate stage, mereosemiotic chain relations from the VIPRS ontology (VIMMP Primitives) are used to support the alignment [8].

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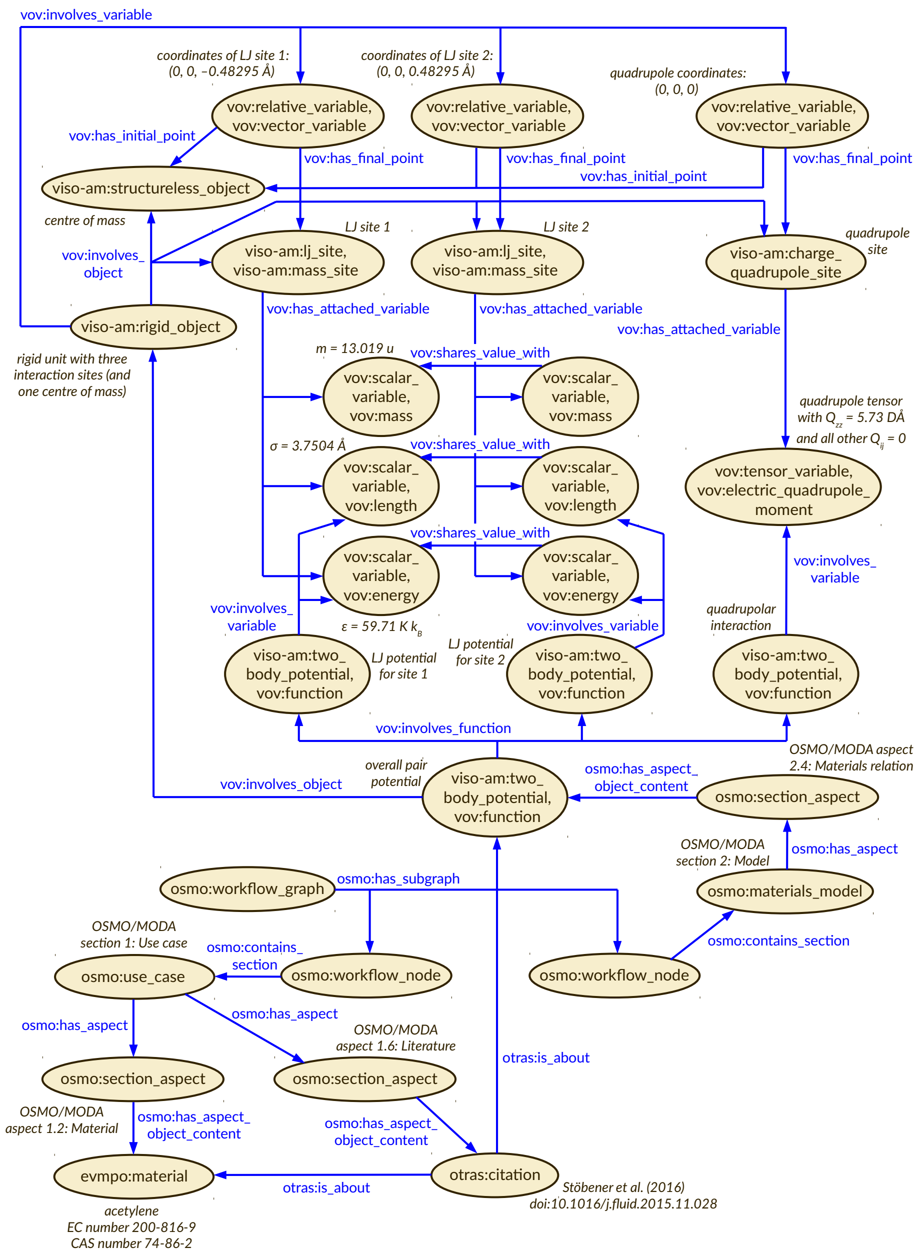

Fig. 2. Knowledge graph representing a two-centre Lennard-Jones plus point quadrupole model for acetylene by Stöbener et al. [11], i.e., model ID 97 (C_2H_2 III) from the MolMod DB [10]. The graph from Fig. 1 is included in the bottom left corner.