Session: Towards Implementations of Materials and Manufacturing Commons: Digital Marketplaces

VIMMP / Semantics in a digital marketplace for materials modelling

UKRI / Silvia Chiacchiera, Martin Thomas Horsch, Michael Seaton and Ilian Todorov

GCL / Gerhard Goldbeck and Daniele Toti

OSTHUS / Rafael Mundim

IFAM / Peter Schiffels and Welchy L. Cavalcanti

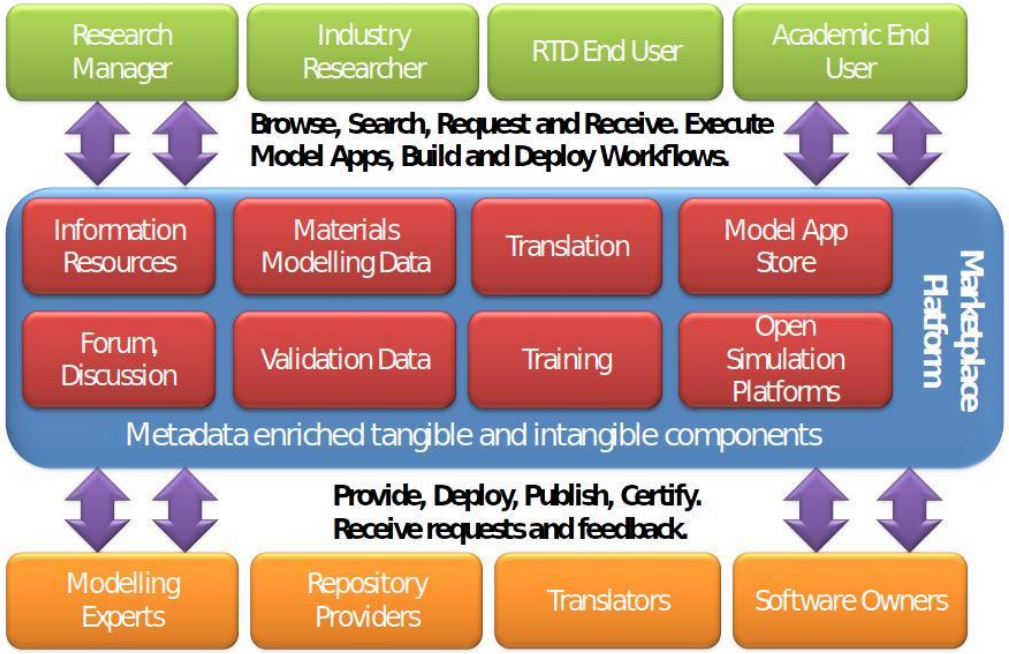
OntoCommons Workshop, April 4th-6th 2023, Fraunhofer Forum Berlin

Towards Materials and Manufacturing Commons - the enablers Digital Marketplaces, FAIR Principles and Ontologies

VIMMP – Virtual Materials MarketPlace

VIMMP is a H2020 project[*] that has developed (Jan 2018-June 2022) a digital marketplace, i.e., a platform to facilitate exchanges between providers and users in the area of materials modelling. Below, we show a graphical summary of the VIMMP concept.

Users

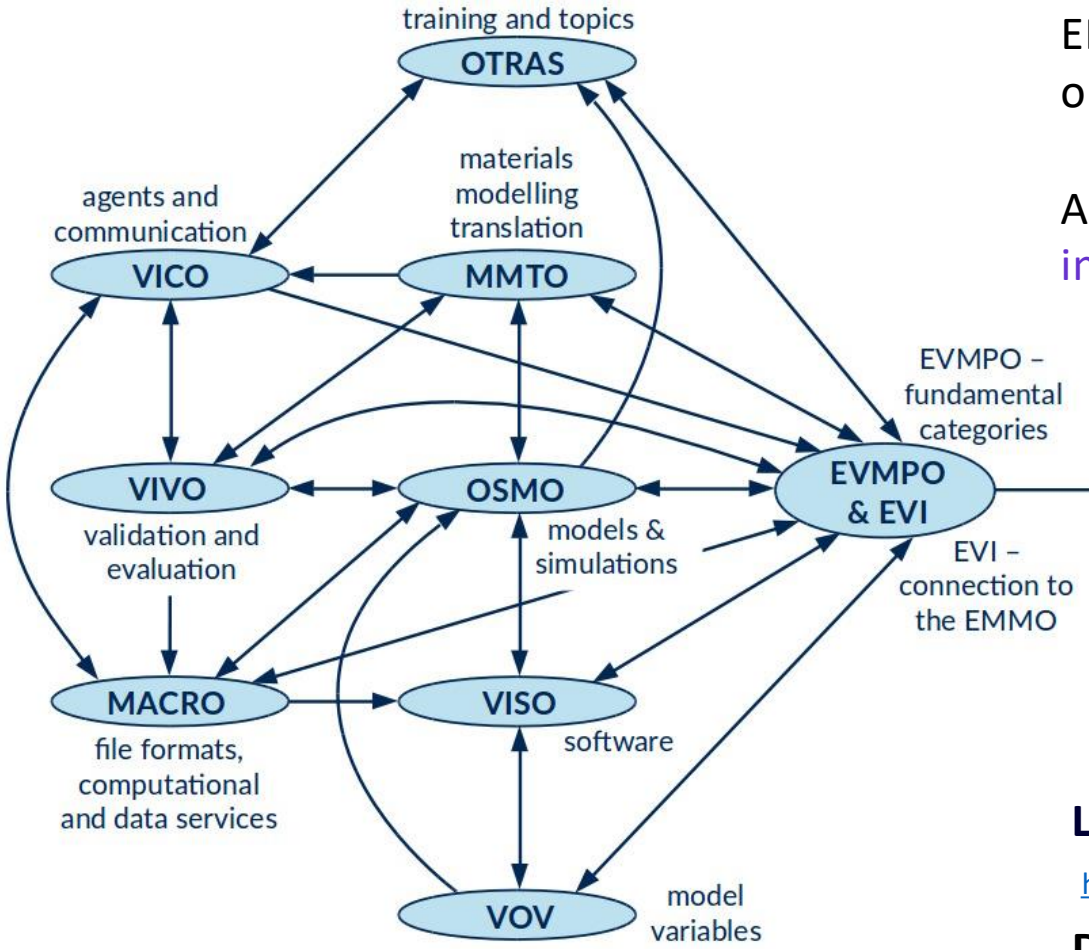


Providers

An open platform. The interoperability of components relies on semantic standards (i.e., **a set of ontologies**).

[*] The project site is: https://www.vimmp.eu/ . Project coordinator: W. L. Cavalcanti (Fraunhofer IFAM). Consortium of 17 partners. System architect: OSTHUS. Metadata and standardization: STFC/UKRI.

The VIMMP ontologies



We have developed a system of ontologies, aligned with the EMMO, providing a framework to organize knowledge on virtual material marketplaces.

Are used as metadata in the VIMMP platform, for data ingest, storage, search and browsing.

Note: new EMMO logo and name

European Materials and Modelling Ontology

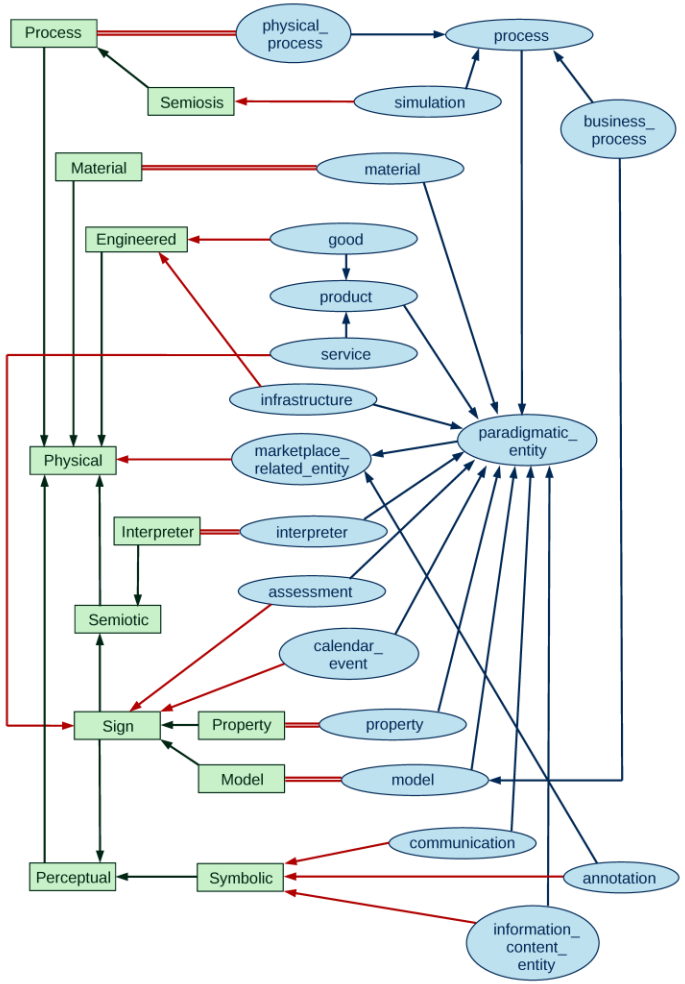
Elementary Multiperspective Material Ontology

License: LGPL-v3. Ontology repository:

https://gitlab.com/vimmp-semantics/vimmp-ontologies

Documentation: see "References" slide

EVMPO: European Virtual MarketPlace Ontology



EMMO ← EVI — EVMPO

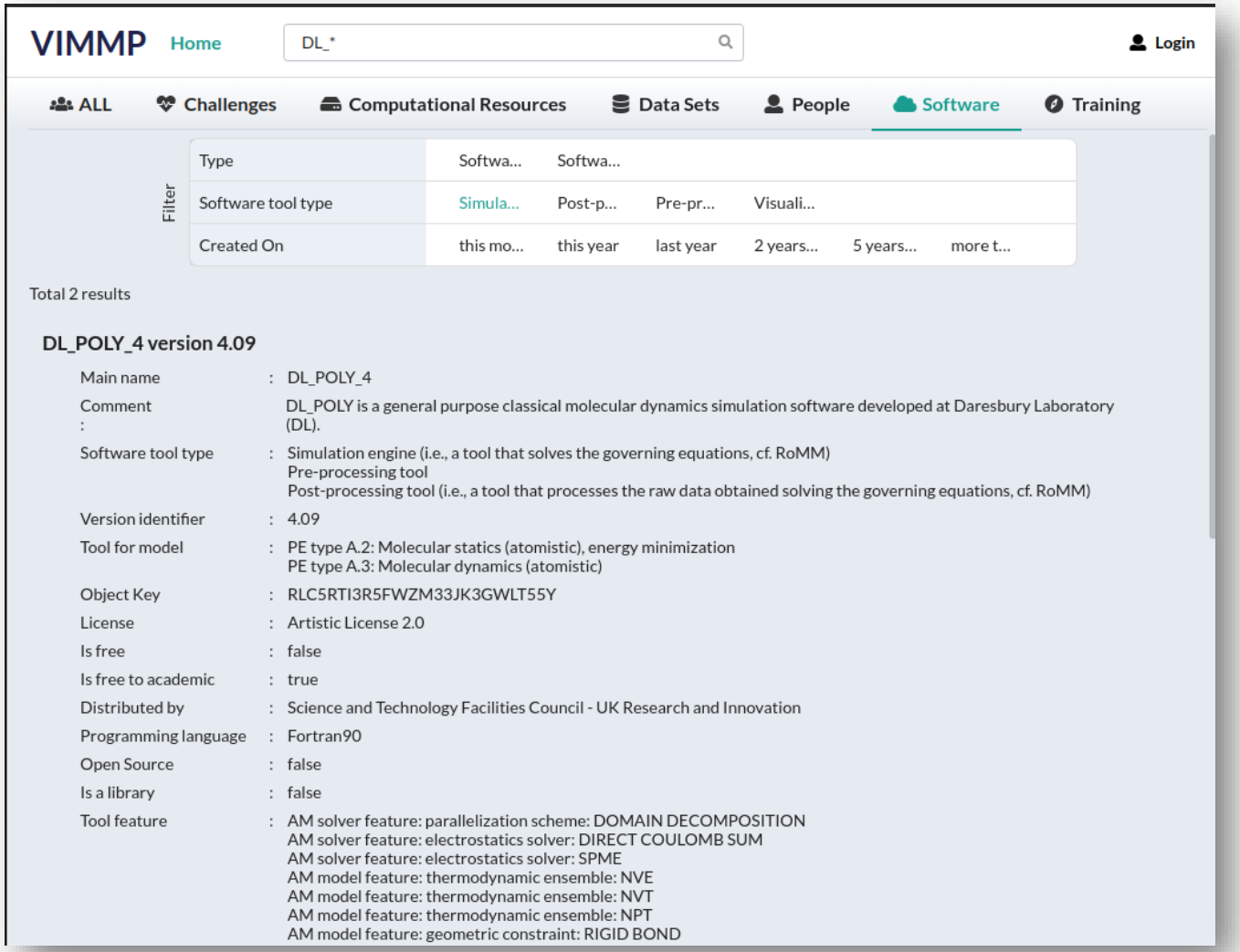
VIMMP VIRTUAL MATERIALS MARKETPLACE

EMMC

MarketPlace

(0) annotation (non-paradigmatic fundamental category), i.e., anything in the knowledge graph that is not under (1) – (11)
(1) assessment, i.e., a proposition on accuracy or performance or an expression of trust
(2) calendar_event, i.e., a meeting or activity that is scheduled or can be scheduled; from W3C iCal ontology
(3) communication, i.e., a message or part of a message (e.g., an attachment) that is communicated
(4) information_content_entity from the Information Artifact Ontology; e.g., a journal article, a data set, or a graph
(5) infrastructure, i.e., a digital platform infrastructure, e.g., data access, hardware, or software
(6) interpreter, i.e., an item that can carry out a semiosis, as formalized by Peirce & the EMMO, creating an interpretant
(7) material, i.e., an amount of substance & part of an object
(8) model, i.e., a representamen that represents an object by direct similitude or within a mathematical framework
(9) process, i.e., temporal evolution of one or multiple entities
(10) product, i.e., a good or service that can be traded
(11) property, i.e., a representamen that is determined as an interpretant by observation, involving a specific observer

MM software on VIMMP platform



A snapshot of the VIMMP **metadata-enriched platform**, showing an entry for **Materials Modelling (MM) Software.**

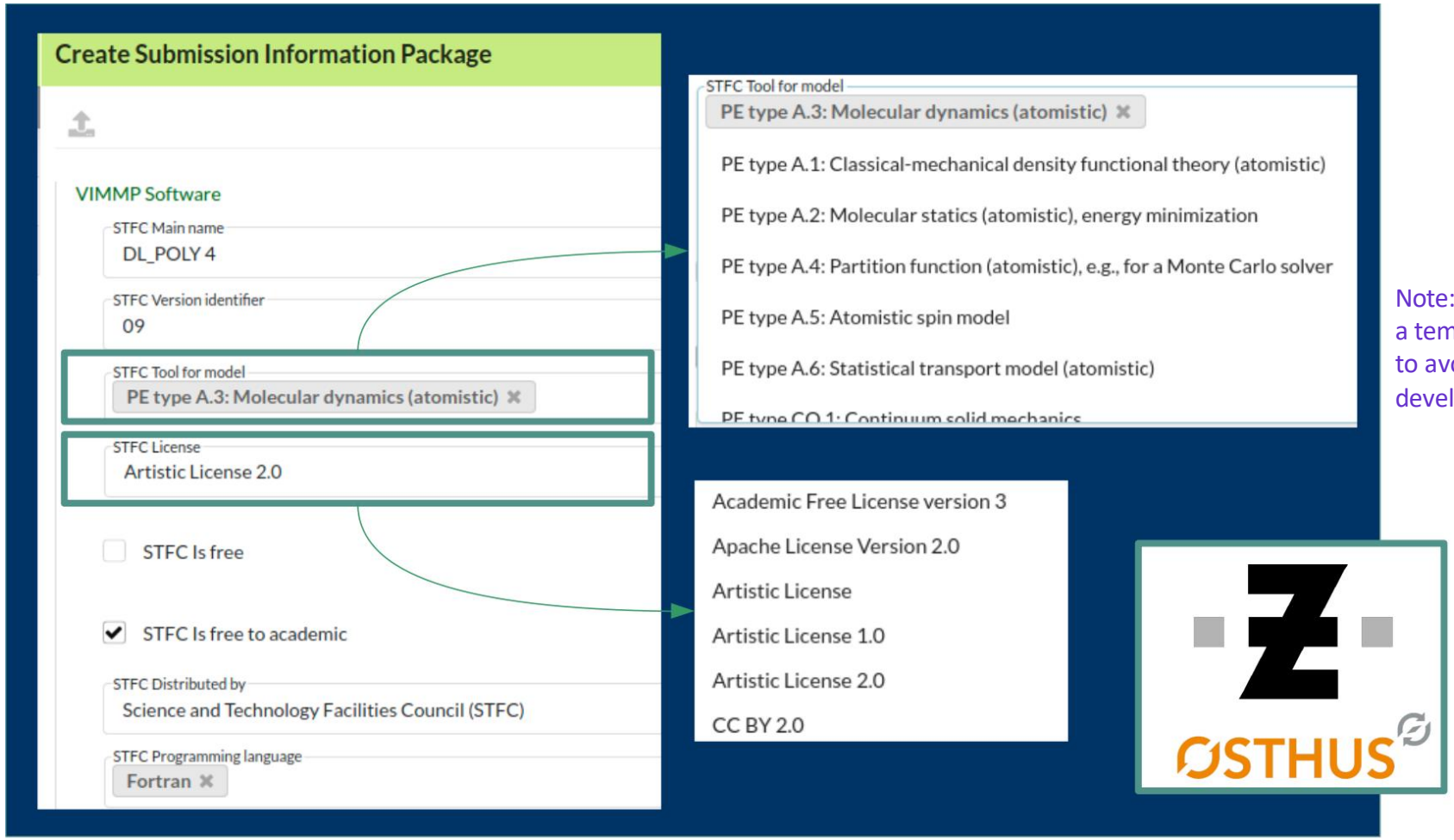
VIMMP ontologies are used, mainly VISO and OSMO in this case.

Other top categories beside Software: Challenges, Computational Resources, Data Sets, People, Training.

The VIMMP platform (based on Zontal Space), its UI and API were run by OSTHUS, the VIMMP platform architect.

Metadata-enriched platform: Ingest example

Creating a record for a “software” on the VIMMP backend (run by Osthus, based on Zontal Space).
Fields (left) and dropdowns (right) are related to the VIMMP ontologies.



Note: here “STFC” was a temporary tag in names, to avoid name clash in the development phase

The VIMMP ontologies in use on Zontal

Software

Preferred Label	Definition	Group	Information ...	Lifecycle Sta...	Properties	Property Cla...	Default Value	Minimum Co...	Maximum C...
Main name	Software main name	VIMMP Soft...						1	1
Dissemination Policy	Dissemination Policy	Access Rights				Disseminati...		0	1
Comment	Comment, brief description of the resource	VIMMP Pro...						0	1
Software tool type	Points to the types(s) of tool (e.g., simulation engine or p...	VIMMP Soft...				software_to...		0	6
Version identifier	Software version identifier	VIMMP Soft...						1	1
Tool for model	Physics equation type of the model addressed by the tool	VIMMP Soft...				physical_equ...		1	25
Object Key	The object key uniquely identifies the object in the S3 bu...	Reference P...						0	1
License	Software license	VIMMP Soft...				license		1	1

@hasLicense

Property Name	@hasLicense
Property Type	Code List
Preferred Label	License
Definition	Software license
Path	https://purl.vimmp.eu/semantics/viso/viso-general.ttl#has_license

License

Property Class
https://purl.vimmp.eu/semantics/viso/viso-general.ttl#license

URIs for properties and for classes for dropdown menus.

Tools, ontologies, benefits

- Which tools/platforms and ontologies have you been using?
  - **Tools:** Protégé, OntoFox [1], Owlready2 [2] (for ontologies); Zontal Space [3] (for data and metadata management); Widoco, Matportal and GitLab (documentation and development).
  - **Ontologies**:
    - EMMO (TLO, applied sciences)
    - EVMPO (MLO, digital marketplaces)
    - VIMMP Ontologies (set of DOs, digital marketplaces for materials modelling)
    - Re-use of multiple semantic artefacts (both generic, as SKOS, and specific as SWO)
- What benefits did you observe from use of semantic technologies in your use case?
  - Better knowledge organization, metadata handling

[1] https://ontofox.hegroup.org/
[2] https://pypi.org/project/Owlready2/
[3] https://www.zontal.io/

TLO = Top-level ontology
MLO = Mid-level ontology
DO = Domain ontology

FAIRness, access rights and governance

- **FAIRness and Interoperability** (Syntactic, semantic; both within VIMMP and with the wider landscape):
  - Ontologies in OWL, TTL format.
  - RESTful APIs for the marketplace (for ingest, search, download) exchanging data as JSON-LD.
  - Reuse of multiple semantic artefacts (e.g., IAO, SWO) and formalization of knowledge sources (e.g., MODA and concepts from RoMM -> OSMO). Alignment with EMMO. Co-developed EVMPO (with Marketplace project, also used within DOME 4.0).
- **Data space:**
  - The marketplace has a "data space", with UI and API; entries can be metadata only or have attachments
  - **Access levels** to records from the UI: public (open to all) and restricted (visible after login only). Possibility to create private collaborative spaces between users (e.g., to exchange data).
  - **How does your system deal with ontology updates?** A workflow for metadata governance was designed (cf. VIMMP D1.6 "Taxonomy editor")

Challenges / difficulties

- Using new technologies without missing out on existing previous approaches and a plethora of available tools
- Finding a right balance between expressivity and usability
- Identifying suitable levels of detail for the descriptions
- Many choices need to be made during ontology development: impossible to combine consensus with wider field and development time constraints
- Finding and evaluating suitability of existing artefacts before re-use, then harmonizing them

Lessons learnt and suggestions

- **Interoperability:** Semantics is an important part of the solution, but not the whole story. Syntatics does matter too (e.g., concrete/technical implementations and the constraints they carry).
- **Human factor:** user-facing components (e.g., dropdown menus) need to be navigable and friendly; annotation and alignment are personnel-intensive (tools welcome, can give partial support).
- Importance of **sharing** own ontologies (also in early development stages) and **getting feedback** (from peers, end-users, developers of components using the ontologies).
- Importance of in-depth **documentation** of semantic assets (including alignments).

References

- **Development:** on GitLab.com [1]
- **Releases:** on [1] and also on matportal.org [2]
- **Documentation:** Springer Brief [3], KI paper [4], Zenodo technical report [5]
- **VIMMP Project overview:** website [6] and CORDIS (including deliverables) [7]

[1] https://gitlab.com/vimmp-semantics/vimmp-ontologies/

[2] https://matportal.org/ontologies/VIMMP_ONTOLOGIES

[3] M. T. Horsch, S. Chiacchiera, W. L. Cavalcanti, B. Schembera, Data Technology in Materials Modelling, Springer, 2021. (open access, https://doi.org/10.1007/978-3-030-68597-3 , ISBN: 978-3-03068596-6)

[4] M. Horsch et al, Ontologies for the Virtual Materials Marketplace, KI – Künstliche Intelligenz 34(3), 423–428, 2020 . (https://doi.org/10.1007/s13218-020-00648-9)

[5] M. Horsch et al, Introduction to the VIMMP Ontologies, 2021 (https://doi.org/10.5281/zenodo.3936795)

[6] VIMMP project website: https://www.vimmp.eu/

[7] https://cordis.europa.eu/project/id/760907

ONTO COMMONS
ONTOLOGY-DRIVEN DATA DOCUMENTATION FOR INDUSTRY COMMONS

VIMMP
VIRTUAL MATERIALS MARKETPLACE

www.vimmp.eu

www.ontocommons.eu

Thank you for your attention!

Questions?

Contacts: silvia.chiacchiera@stfc.ac.uk
martin.horsch@stfc.ac.uk
gerhard@goldbeck-consulting.com
welchy.leite.cavalcanti@ifam.fraunhofer.de
rafael.mundim@osthus.com

UKRI Science and Technology Facilities Council

GOLDBECK CONSULTING

OSTHUS

Fraunhofer IFAM

VIMMP "Virtual Materials MarketPlace" has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement no. 760907.

OntoCommons "Ontology-driven data documentation for Industry Commons" has received funding from the European Union's Horizon Programme call H2020 -NMBP-TO-IND-2020-singlestage, Grant Agreement number 862136