M. T. Horsch, S. Chiacchiera, M. A. Seaton, I. T. Todorov, **UK Research and Innovation**, B. Schembera, **High Performance Computing Center Stuttgart**, P. Klein, **Fraunhofer ITWM**, N. A. Konchakova, **Helmholtz-Zentrum Geesthacht**

# Pragmatic interoperability and translation of industrial engineering problems into modelling and simulation solutions

VIMMP
VIRTUAL MATERIALS MARKETPLACE

13th October 2020

**DAMDID 2020**

Science and Technology Facilities Council

EMMC

FORCE

VIMMP VIRTUAL MATERIALS MARKETPLACE

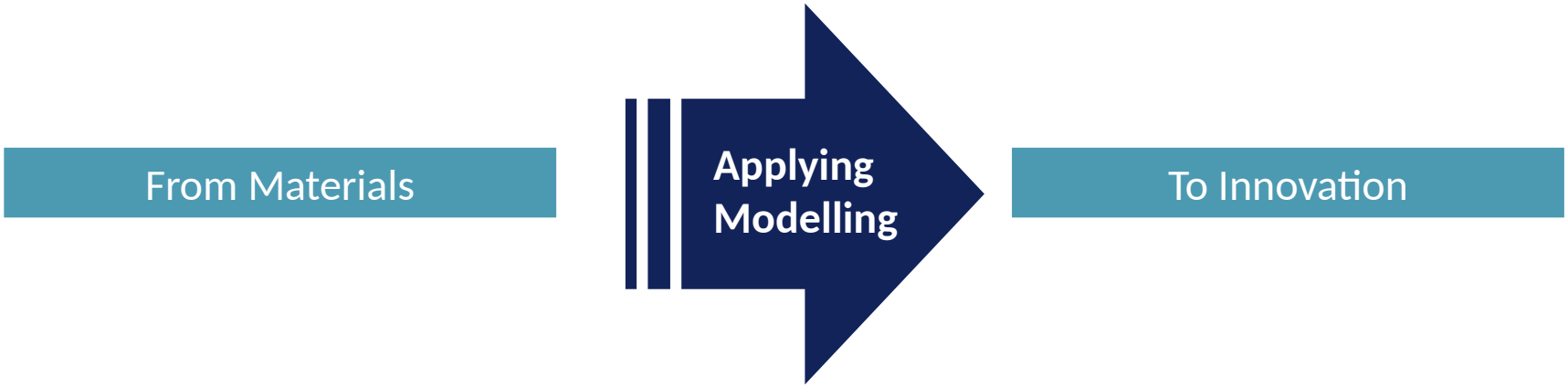
# Virtual Materials Marketplace (VIMMP)

VIMMP
VIRTUAL MATERIALS MARKETPLACE

http://vimmp.eu/

- Horizon 2020 project
  - Innovation action, grant agreement no. 760907
  - H2020 (NMBP-25-2017)
  - 4 years project – started on 01.01.2018

To support accelerating innovation in manufacturing industries by using materials modelling solutions.



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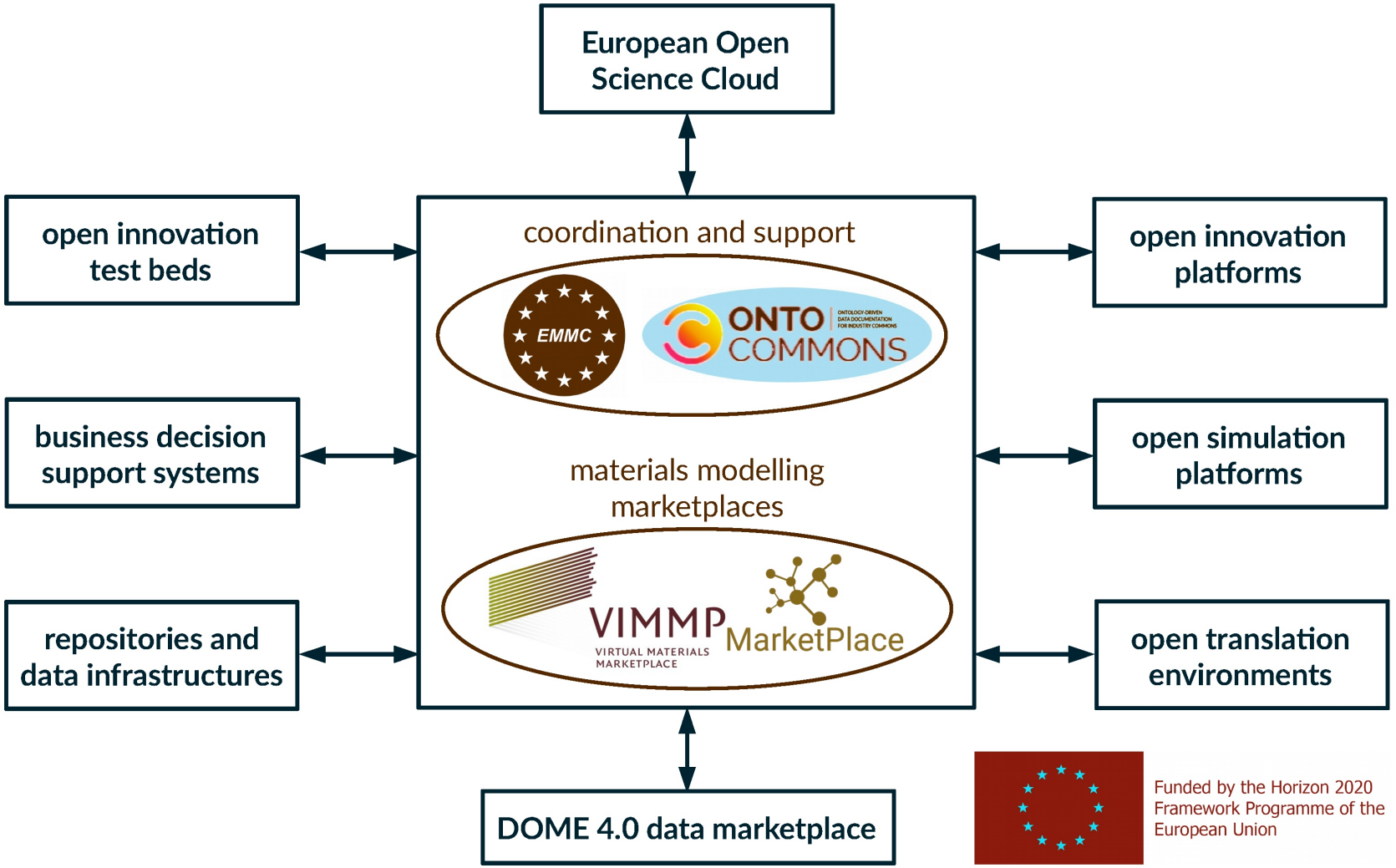
# European digital platforms in materials modelling




Funded by the Horizon 2020 Framework Programme of the European Union

# European Materials Modelling Council

https://emmc.eu/

**European Materials Modelling Council (EMMC ASBL)**

The non-profit association EMMC ASBL was created in 2019 to ensure the continuity, growth, and sustainability of community activities for modellers, materials data scientists, software owners, materials modelling translators, and manufacturers in Europe. The EMMC regards the **integration of materials modelling and digitalization** as critical for an advancement of industrial process and product design.

**EMMC Focus Area on Digitalization**

In computational engineering, digitalization encompasses aspects of representing, managing, accessing, and utilizing digital information about products, components, materials, their behaviour, and their processing.

# Knowledge representation in materials modelling

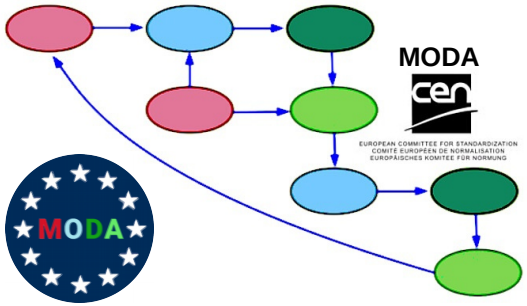
**Community-governed development of metadata standards**

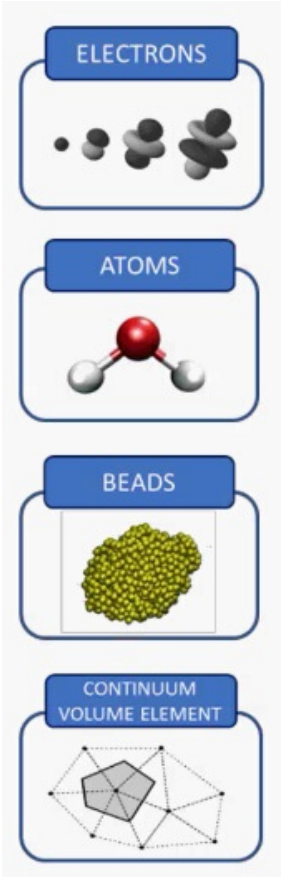
**RoMM VI** **MODA** **CWA 17284**

**Review of Materials Modelling (compendium)**

**MODA (“Model Data”)**

**CEN workshop agreement**




*electronic*

*atomistic*

*mesoscopic*

*continuum*

# Knowledge representation in materials modelling

**Community-governed development of metadata standards**

**RoMM VI** **MODA** **CWA 17284** **Ontologies**

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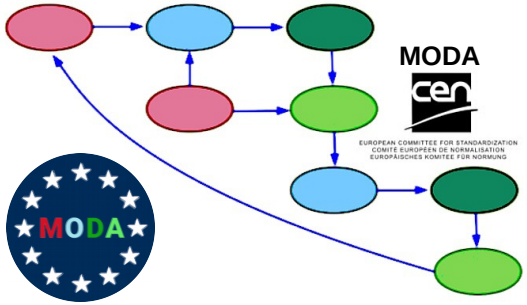
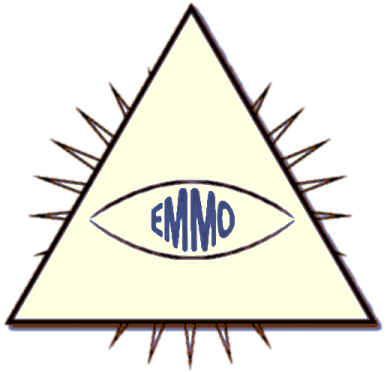
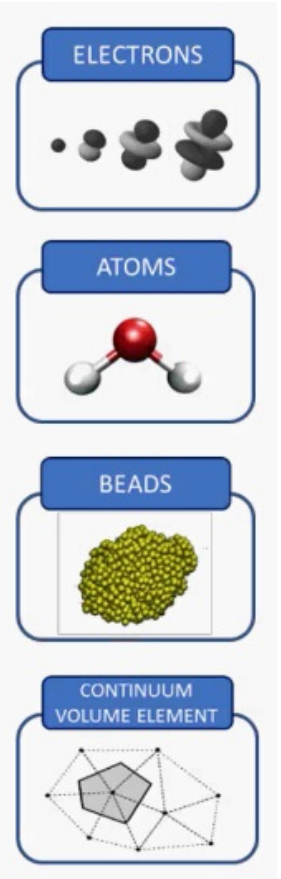
**Domain ontologies**

**EMMO top-level ontology**








*electronic*

*atomistic*

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# Provenance description of simulation results: MODA

| 1 | Aspect of the User Case/System to be Simulated | |
|---|---|---|
| 1.1 | Aspect of the User Case to be Simulated | *Describe the aspects of the user case textually.*<br><br>*No modelling information should appear in this box. This case could also be simulated by other models in a benchmarking operation!*<br>*The information in this chapter can be end-user information, measured data, library data etc. It will appear in the pink circle of your workflow picture.*<br>*Simulated input which would have been calculated by another model should not be included (but in chapter 2.4)*<br><br>*Also the result of pre-processing necessary to translate the user case specifications to values for the physics variables of the entities van be documented here.* |
| 1.2 | Material | *Describe the chemical composition, ...and the values used for properties and from which database these are taken. If pre-processing was needed please specify the methodology.* |
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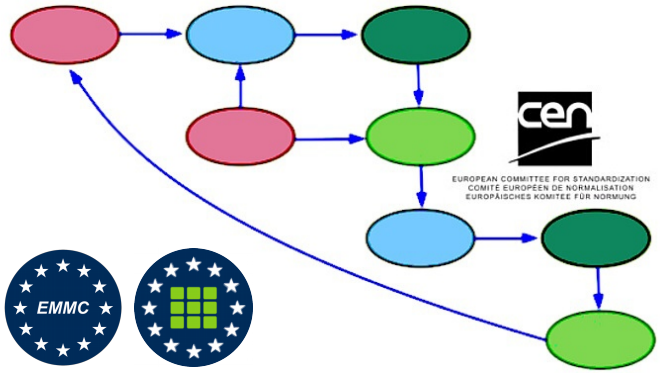
| 1.6 | Publication on this data | *Publication documenting the simulation with this single model (if available and if not already included in the overall publication).* |

## MODA workflow description




MODA section 1 — use case

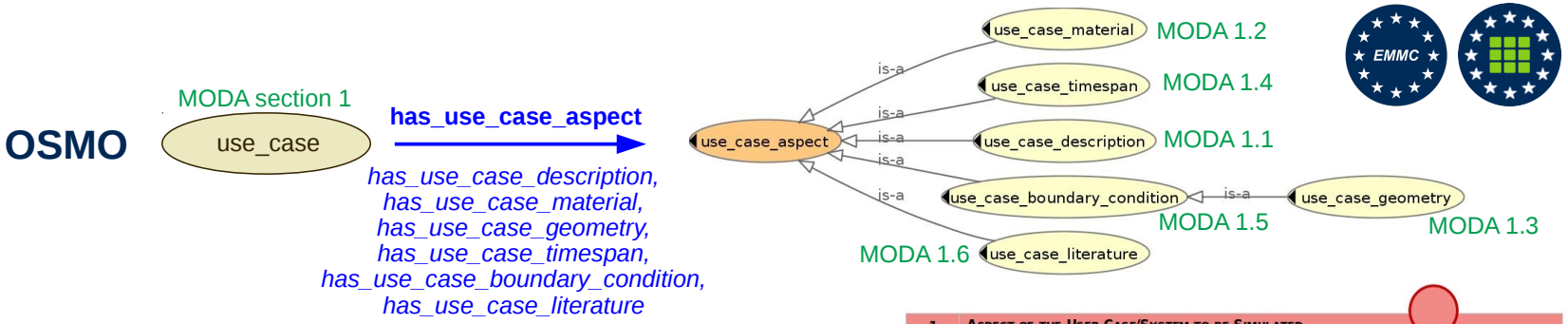
MODA section 2 — model

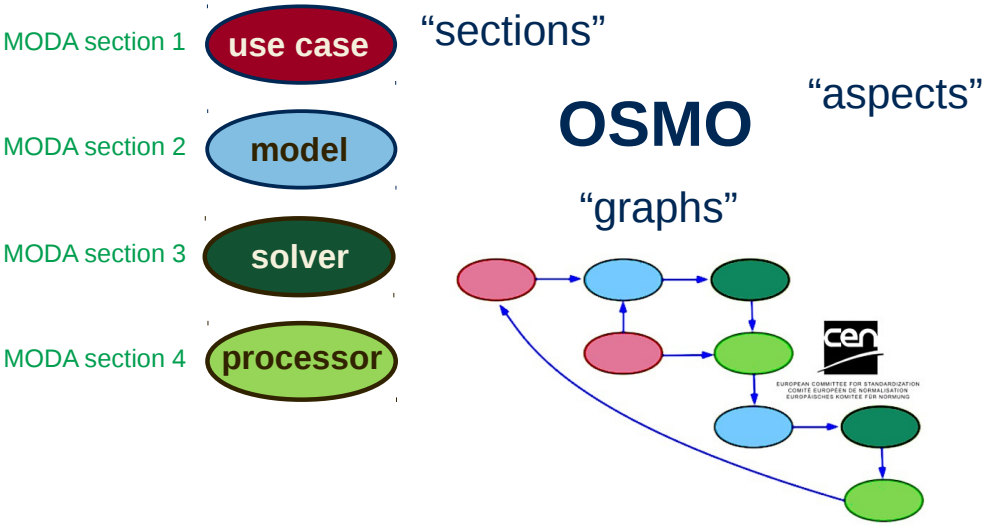
MODA section 3 — solver

MODA section 4 — processor

MODA

# Provenance description of simulation results: OSMO

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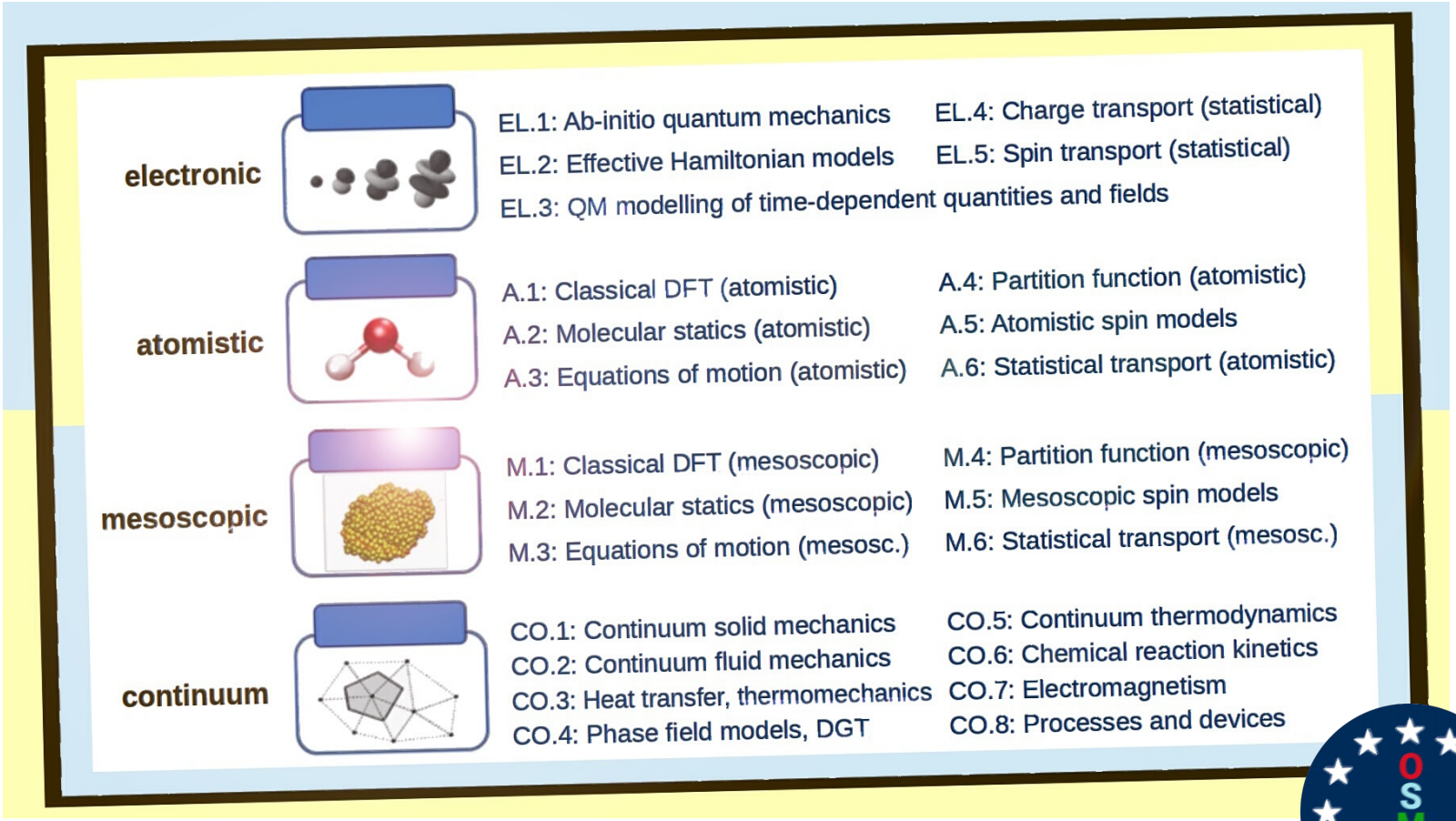
**Ontology for Simulation, Modelling, and Optimization**
J. Chem. Eng. Data 65(3), 1313–1329, 2020

# Provenance description of simulation results: OSMO

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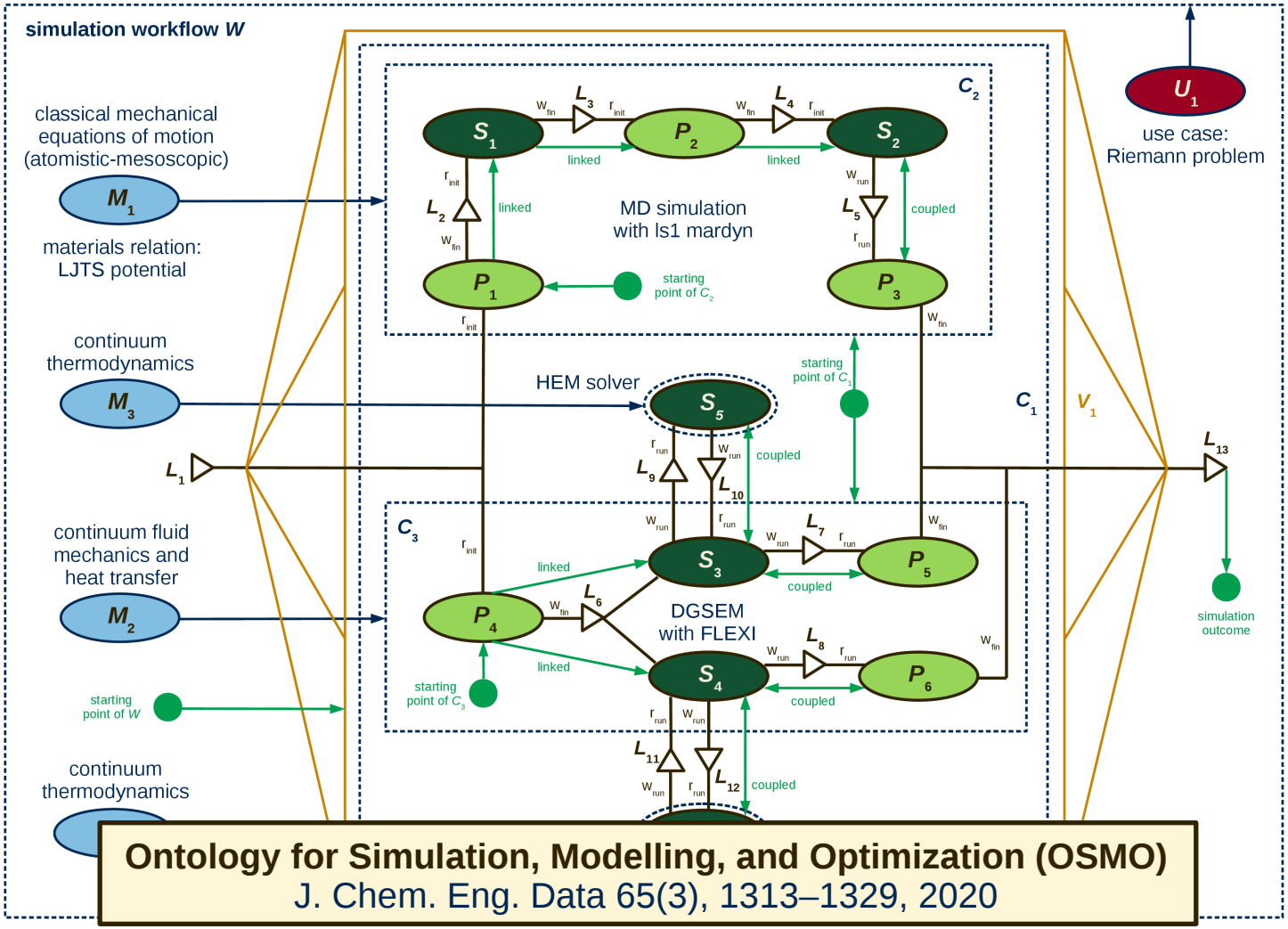



**Ontology for Simulation, Modelling, and Optimization (OSMO)**
J. Chem. Eng. Data 65(3), 1313–1329, 2020

OSMO-based **provenance description** as an extension of the MODA workflow meta-data standard:

For all elements of the graph notation, there are corresponding concepts and relations from the ontology OSMO.

# Community-governed top-level interoperability layer

**Relations covered by the European Materials and Modelling Ontology[1] (EMMO)**

1) **Taxonomy**: Conceptual hierarchy (subclass relation)

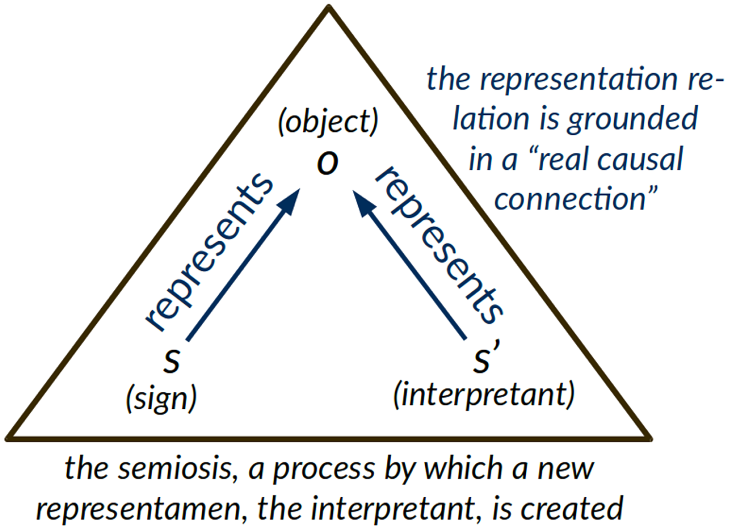
2) **Semiotics**: Representation of physical entities by signs

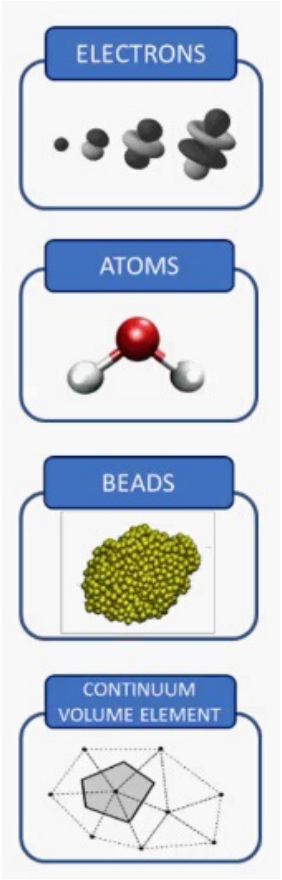
3) **Mereotopology**: Spatiotemporal parthood and connectivity

**semiosis**

C. S. Peirce

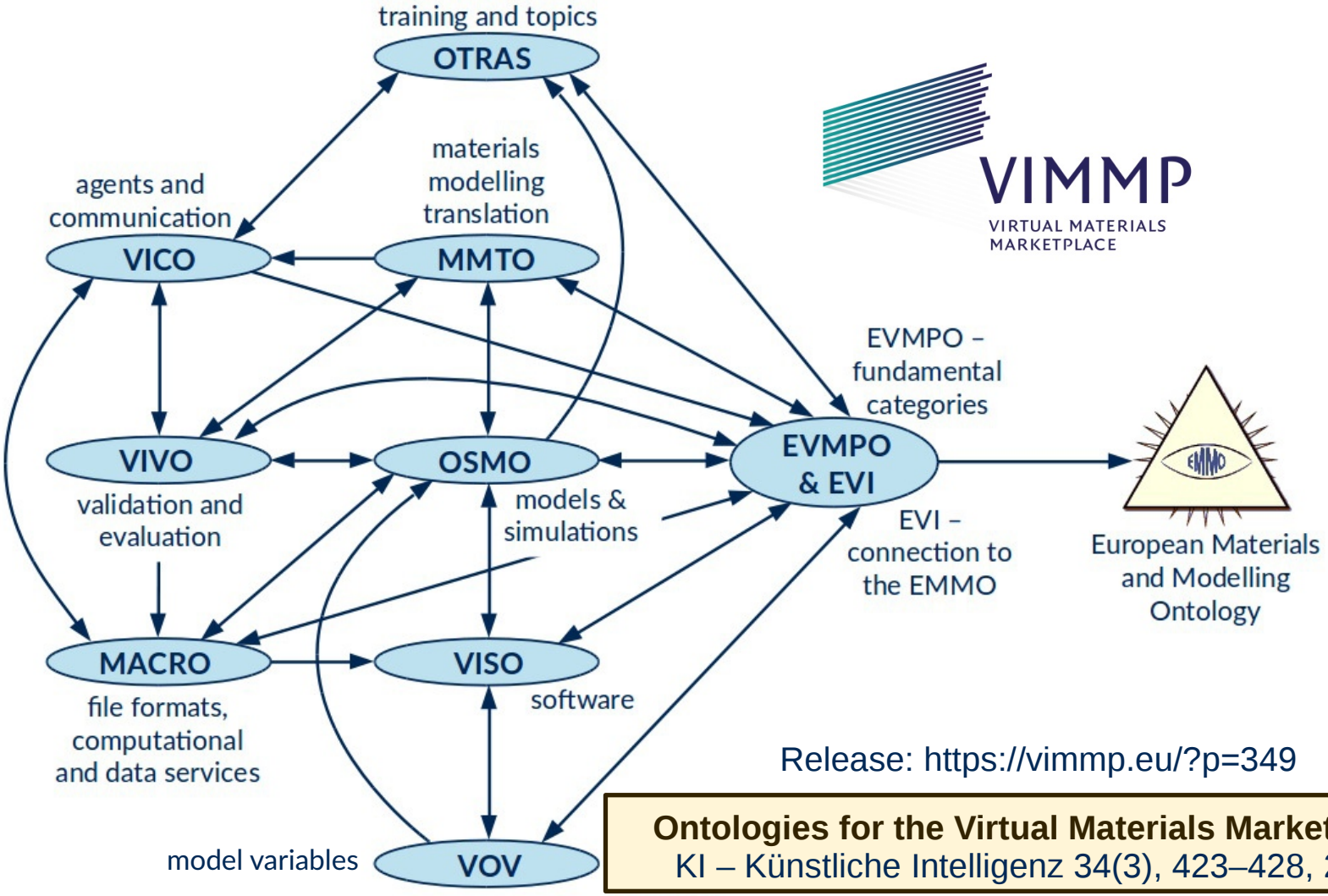
**Peircean semiotics**




[1]E. Ghedini, J. Friis, A. Hashibon, G. J. Schmitz, G. Goldbeck, *et al.*, **2020**; http://emmc.info/emmo-info/.

# System of marketplace-level domain ontologies

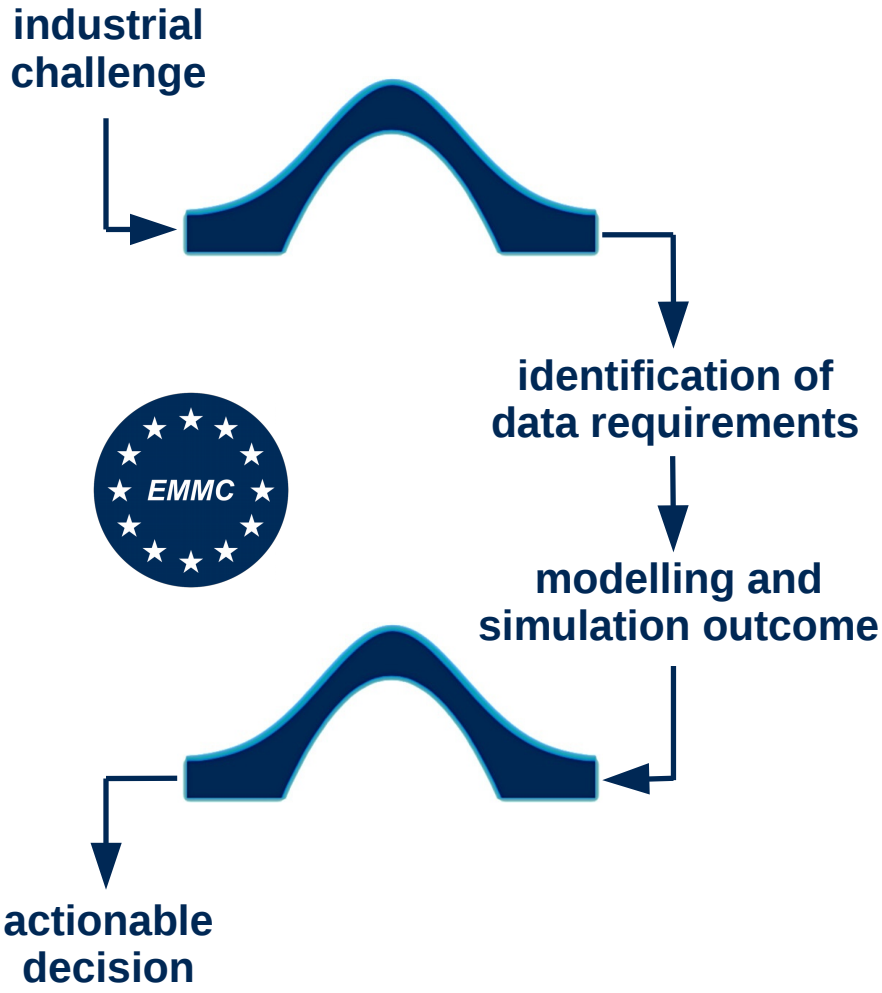



Release: https://vimmp.eu/?p=349

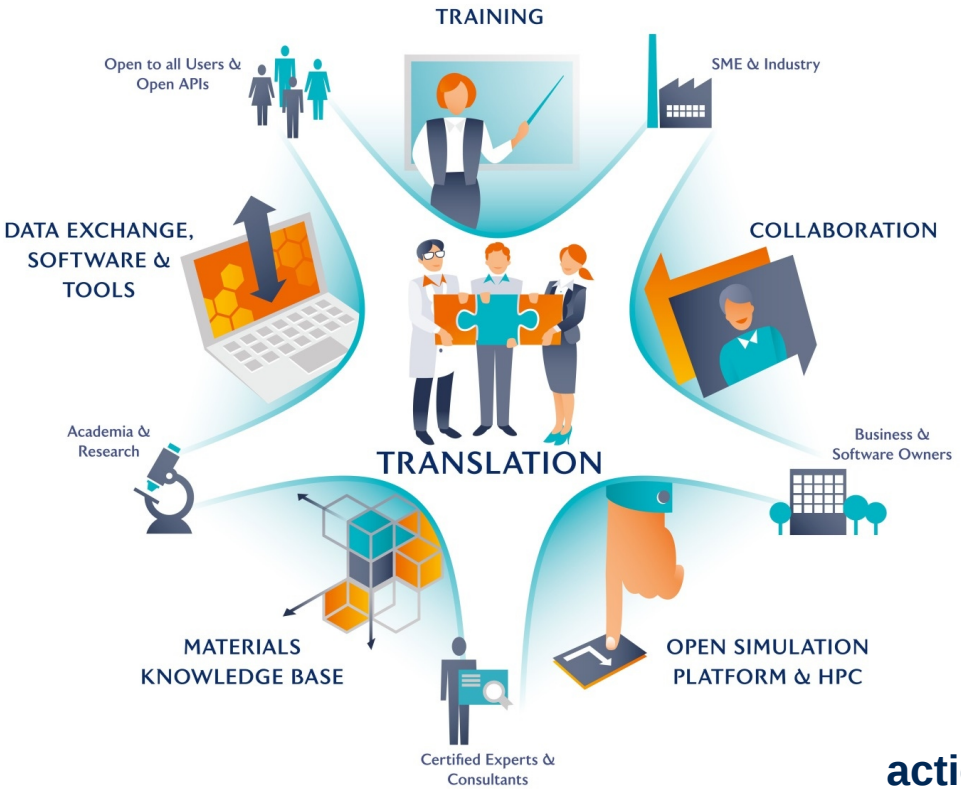
**Ontologies for the Virtual Materials Marketplace**
KI – Künstliche Intelligenz 34(3), 423–428, 2020

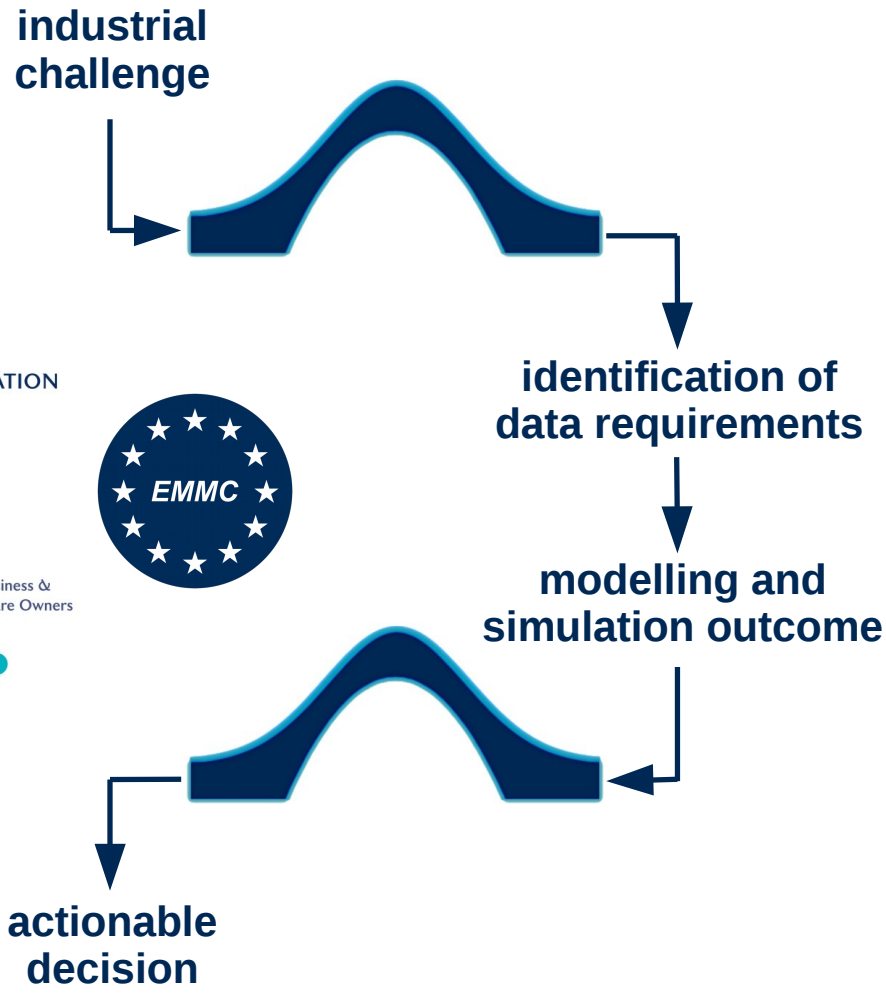
# Translation in materials modelling

**Task:** Facilitate the translation of industrial R&D challenges into solutions using scalable and quantitatively reliable materials modelling and simulation.

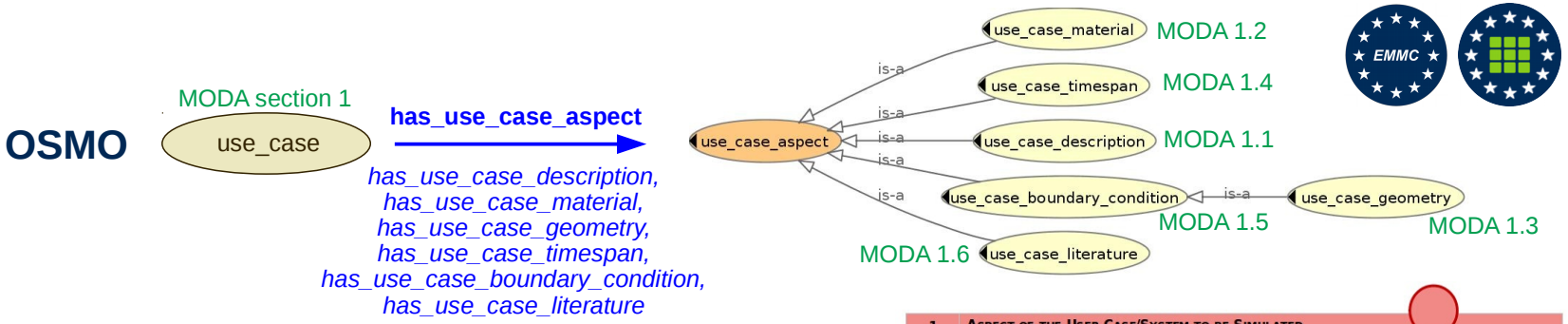


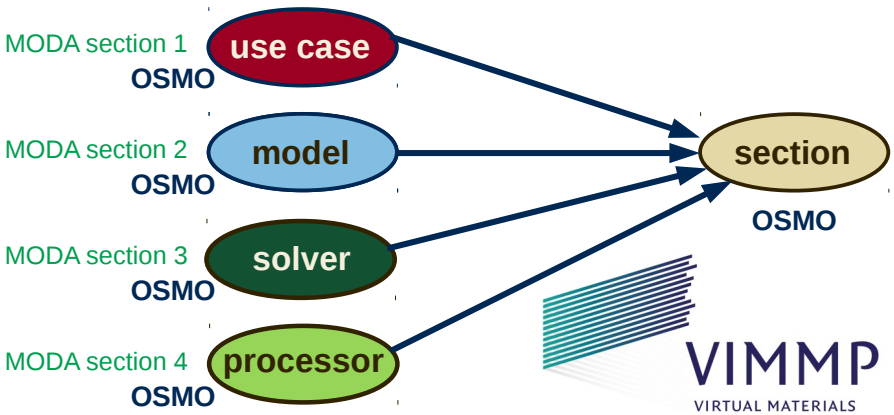
# Translation in materials modelling

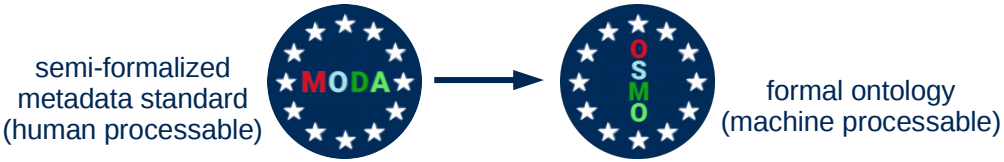


# Ontologization of EMMC metadata standards

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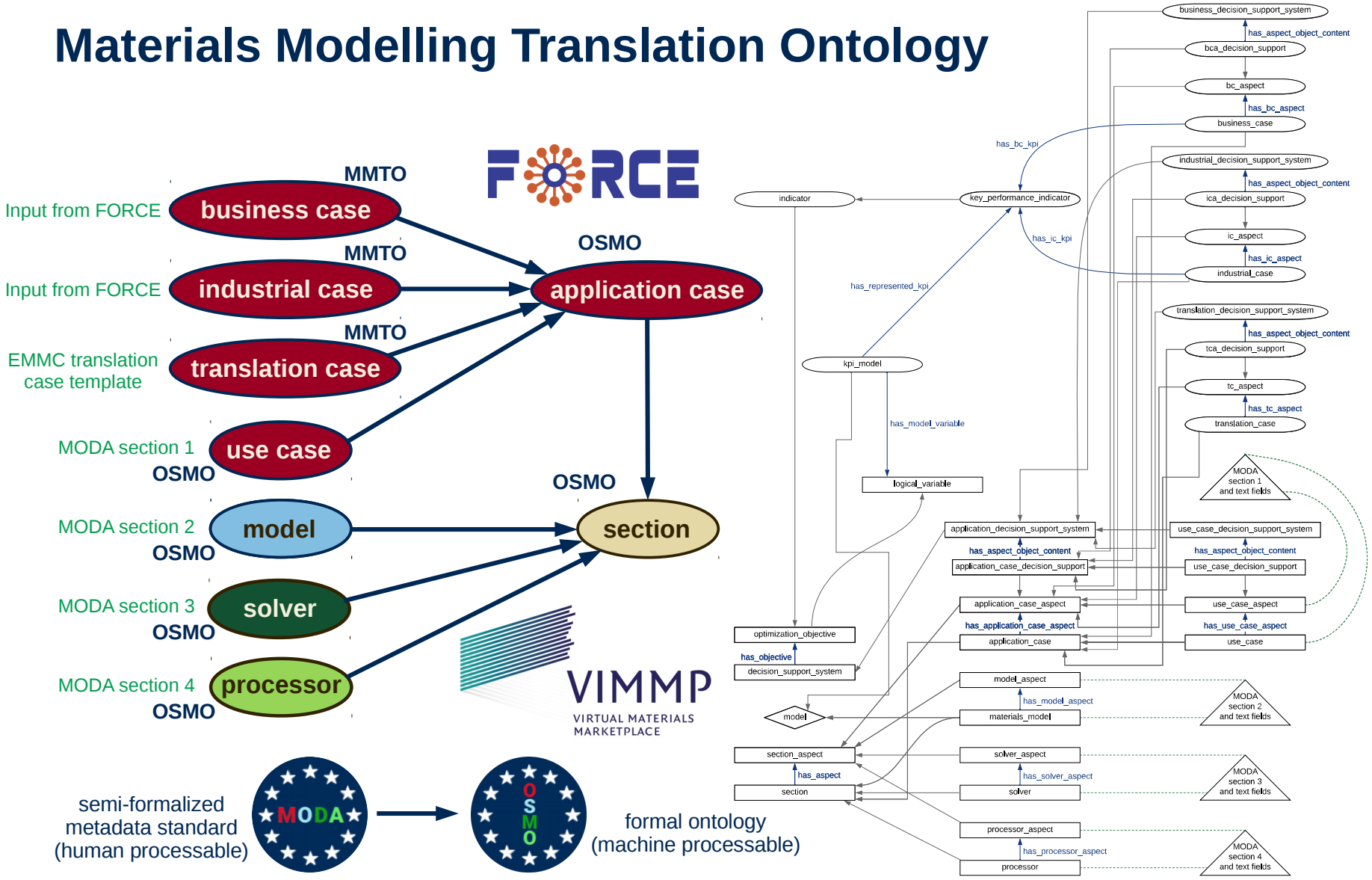

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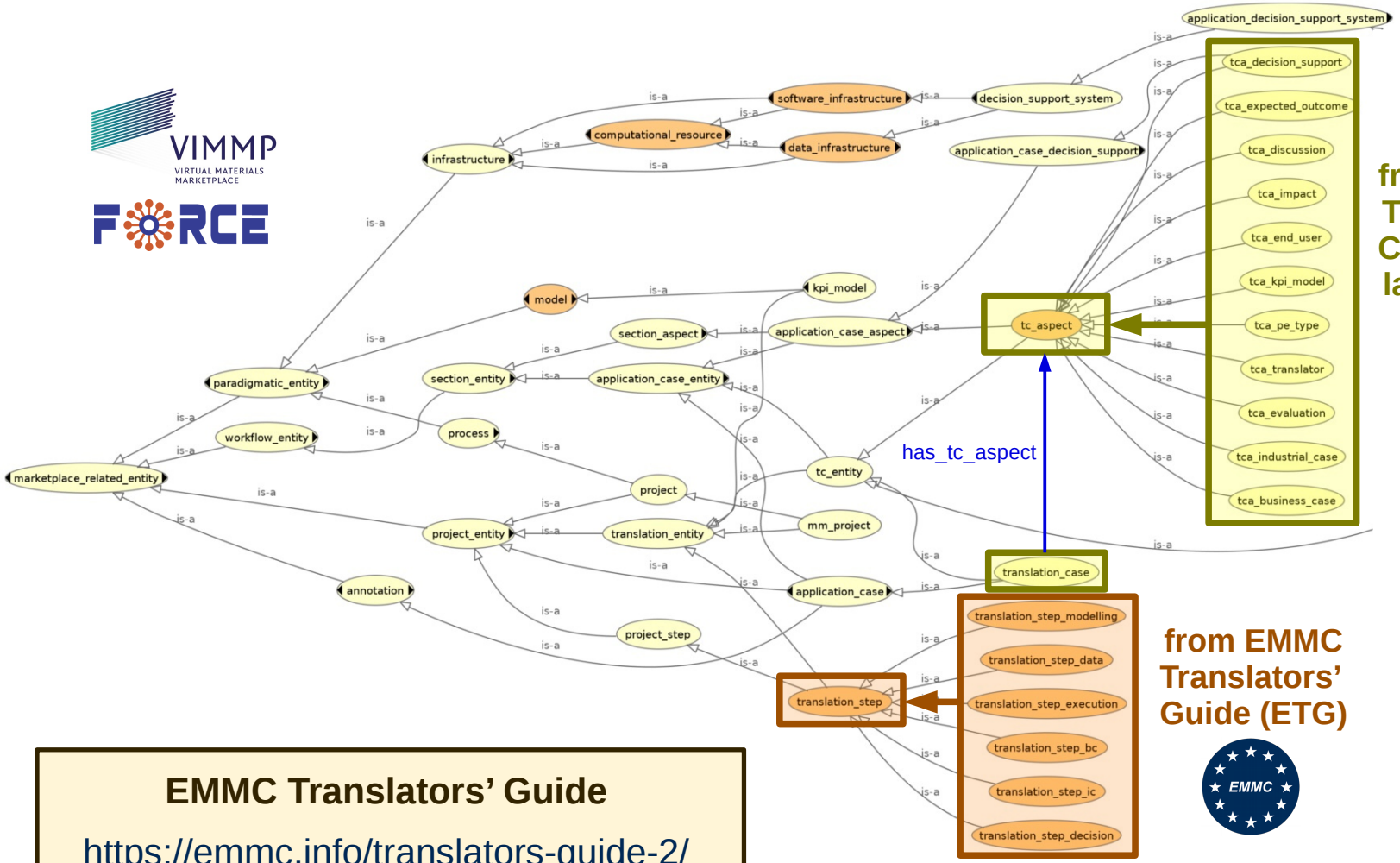


from EMMC Translation Case Template (ETCT)

from EMMC Translators' Guide (ETG)

**EMMC Translators' Guide**

https://emmc.info/translators-guide-2/

# VIMMP ontology-based translation router

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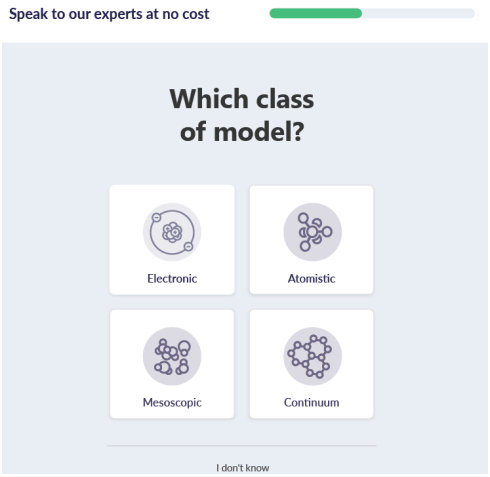
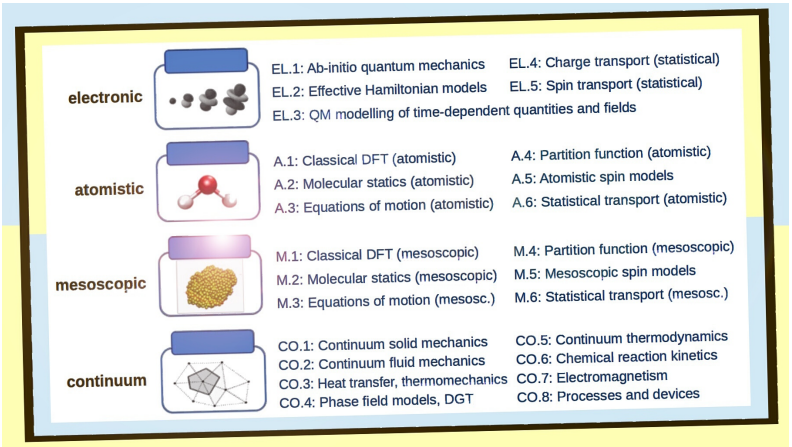
Basic prerequisites for materials modelling.
**mm_topic_computational** (codes **3XXX**):
Computational and numerical aspects of materials modelling.
**mm_topic_data** (codes **4XXX**):
Data science and technology aspects.
**mm_topic_materials** (codes **5XXX**):
Topics related to fluid and solid materials.
**mm_topic_social** (codes **6XXX**):
Social, economic, and community aspects.
**mm_topic_theoretical** (codes **7XXX**):
Theory (non-computational aspects).
**mm_topic_interdisciplinary** (codes **8XXX**)
**mm_topic_side** (codes **9XXX**):
Topics from other disciplines.

- 3100, 7100 electronic
  - 3120, 7120 physical equation EL.1
  - 3130, 7130 physical equation EL.2
  - *etc.*
- 3200, 7200 atomistic and mesoscopic
  - 3220, 7220 equations A.1 and M.1
    - 3222, 7222 physical equation A.1
    - 3225, 7225 physical equation M.1
  - 3230, 7230 equations A.2 and M.2
    - *etc.*
  - *etc.*
- 3300, 7300 continuum
  - 3320, 7320 physical equation CO.1
  - 3330, 7330 physical equation CO.2
  - *etc.*



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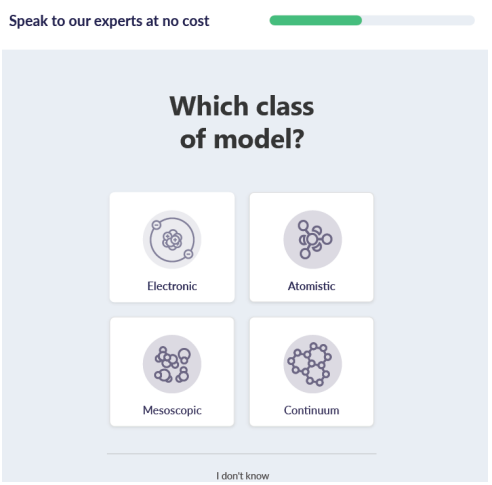
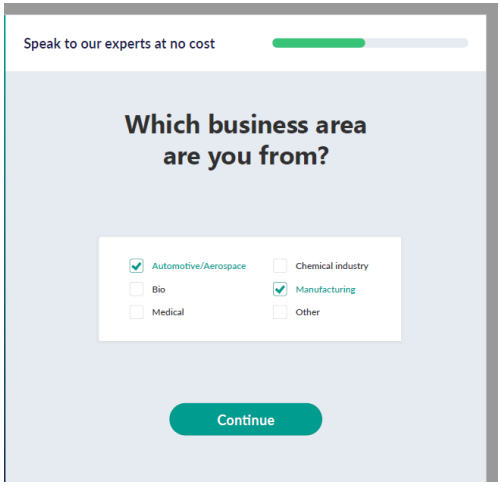
**mm_topic_side** (codes **9XXX**):
Topics from other disciplines.

under 61XX: industrial

- 6120 chemical
- 6130 petrochemical
- 6140 transport
  - 6142 aerospace
  - 6144 automotive
  - 6148 railway
- 6150 biotechnology
- 6155 food
- 6160 medicine
- 6165 paper
- 6170 electrical
- 6175 machinery
- 6180 metal (basic and fabricated)
- 6190 special topics



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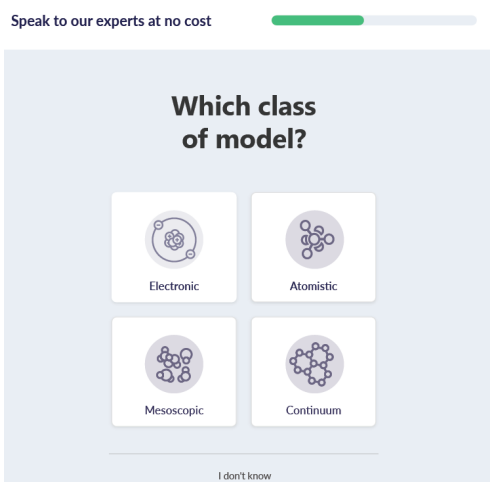
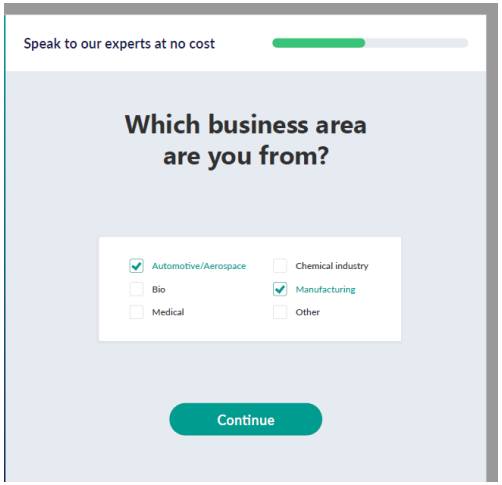
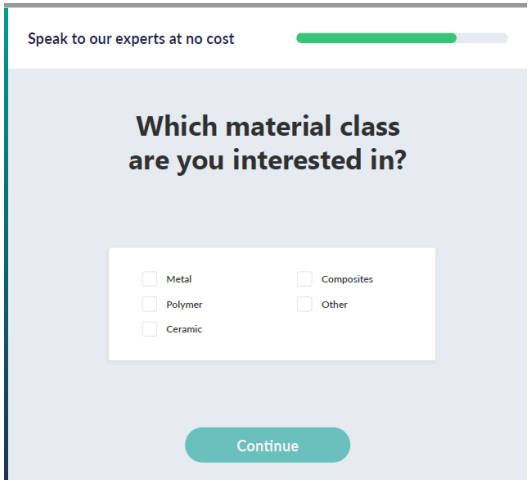
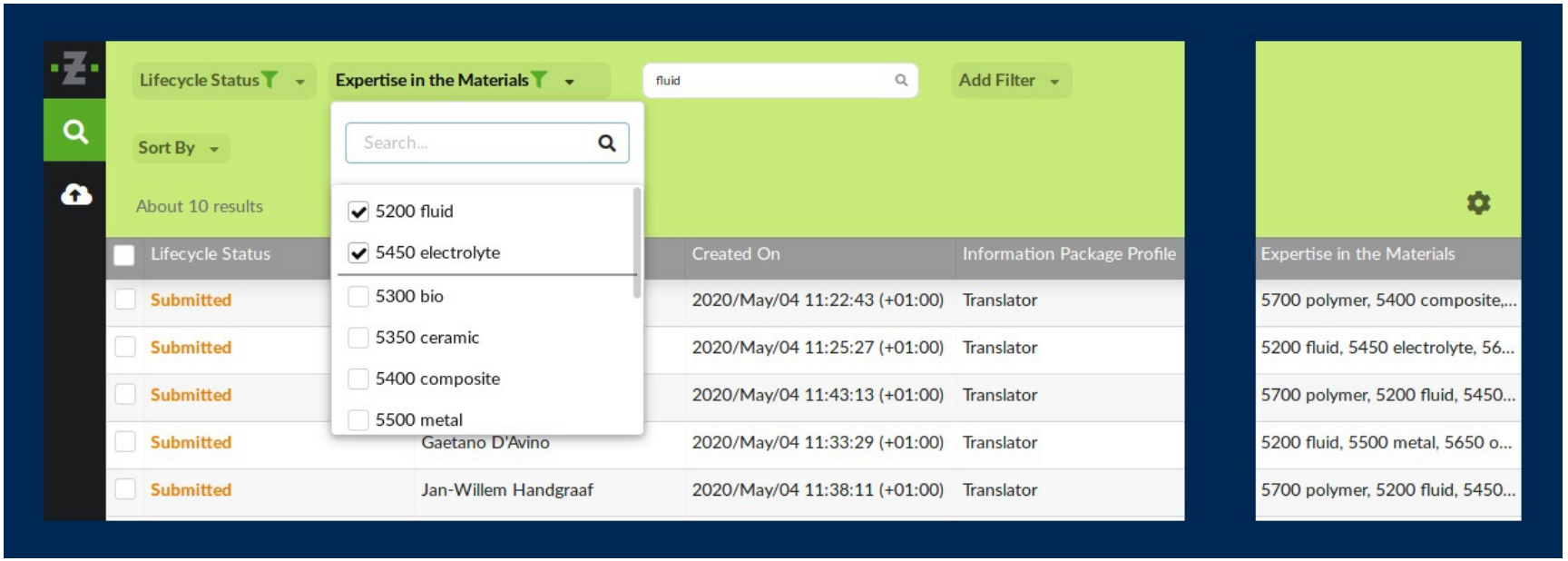
5100 general
5200 fluid
5300 bio
5350 ceramic
5400 composite
5450 electrolyte
5500 metal
5550 mineral
5600 nano
5650 organic
5700 polymer
5750 semiconductor
5800 ultracold
5850 unstable
5900 special topics

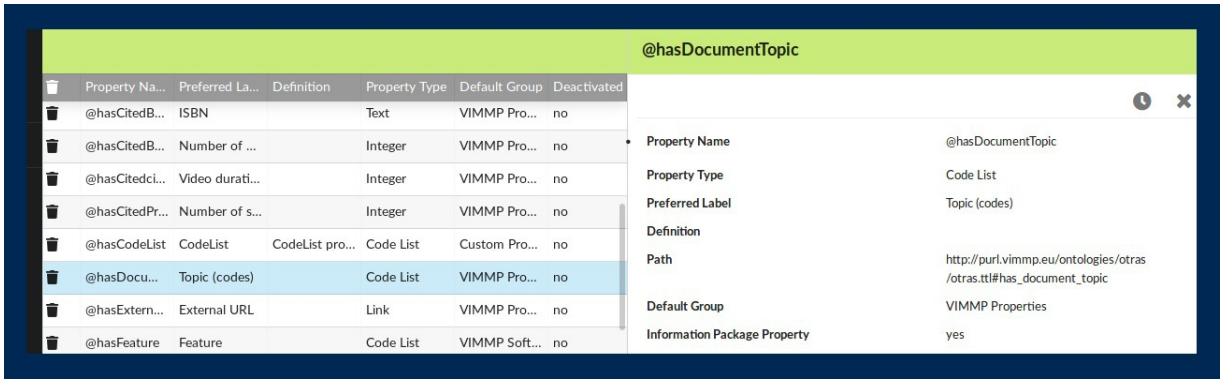


# Data management on the VIMMP back end




OSTHUS

**The present work is a collaboration of UKRI STFC Daresbury Laboratory with:**

| | | |
|---|---|---|
| **Geesthacht** | – | Natalia A. Konchakova |
| **Kaiserslautern** | – | Peter Klein |
| **Stuttgart** | – | Björn Schembera |

*This project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement no. 760907.*

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| **Kaiserslautern** | – | Peter Klein |
| **Stuttgart** | – | Björn Schembera |

**Formulations and Computational Engineering (FORCE)**

H2020 GA no. 721027

http://www.the-force-project.eu/

**EMMC Coordination and Support Action**

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http://emmc.info/

**Virtual Materials Marketplace (VIMMP)**

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http://vimmp.eu/