The European Materials Modelling Council

MODA and CHADA: Terminology and standardized documentation for materials modelling and characterisation

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Targeted impact of WP 2020 LEIT-NMBP

THE THREE 'Os'

Open Innovation — OITB projects
Open Science
Open to the World

Open to the World: 40 M€
Flagships in nanosafety, global health care and biotechnology for the environment.

Open Science: 105 M€
Activities in materials characterisation and modelling

FOCUS AREAS NMBP contribution

Digitising Industry	Circular Economy	Low Carbon
+1.5%	+2.2%	+15%
713M€ (250M€ in 2020)	378 M€ (143.5M€ in 2020)	284 M€ (105M€ in 2020)

BIG TICKET →

Industry Commons 2 topics – 8M€

sharing industrial research data

linked to the

- Open Access (structured and unstructured data)
- Science Cloud

Slide source: courtesy of Anne de Baas

•WP2020 Industrial Commons

➢ Objectives

- Standardise the documentation of data through taxonomies and ontologies
- Making data accessible and enabling its re-use across different domains
- Enable domains to connect, link and exchange information
- Create a common information system that would allow data sharing and enable new or improved materials, products, processes and services

•Make the data FAIR

- **(Findable, Accessible, Interoperable and Re-usable)**

- Slide source: courtesy of Anne de Baas

European Commission

Overview

1. Introduction
2. Terminology and classification for materials modelling
3. Materials Modelling Data (MODA)
4. CEN Workshop Agreement

The Vision: Targeted Material Development

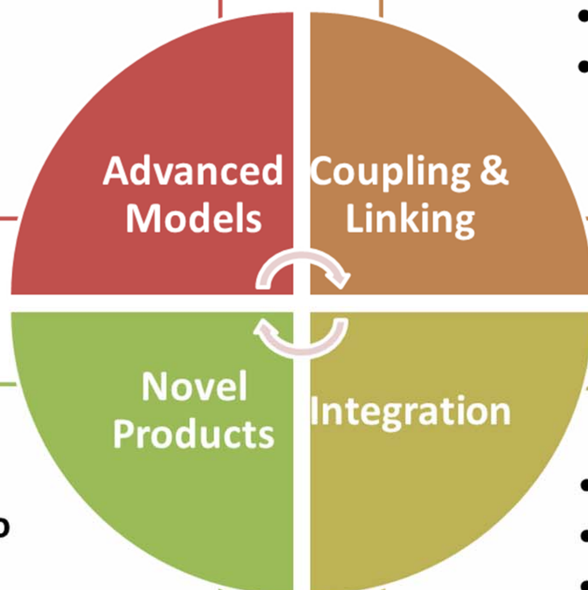
- Paradigm shift in the way materials are developed

http://emmc.info

https://mgi.nist.gov/

- Accurate Predictions
- Various Levels of Hierarchical Material Structures
- Error Estimates

- Multiscale
- Multiphysics
- Varying Degrees of Freedom



- Lower Costs, Lower Risks, Reduced Time to Market
- Sustainability, Energy…

- Material Informatics
- Experiments
- Databases
- Models

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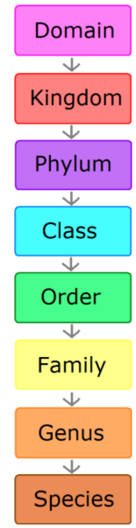
Goals

1. A common vocabulary



2. Classification for materials modelling

3. Metadata enriched materials modelling information

4. Ontologies for interoperability

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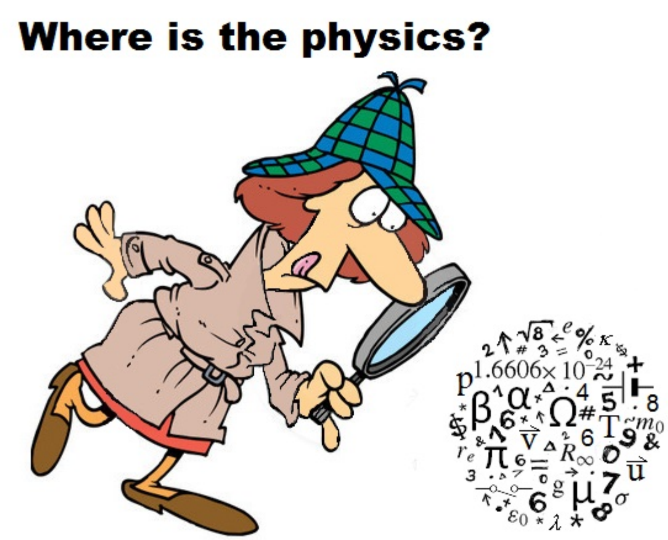
Typical materials model descriptions ...

- By **phenomena (application)**:
  - "I have a mikro-kinetics model."
- By **scale** of the phenomena:
  - "I have a mesoscale model."
- By name of the **software (code)**
  - "I use the Uppsala model"
- By **solver**:
  - "I have a FE model"

But…….



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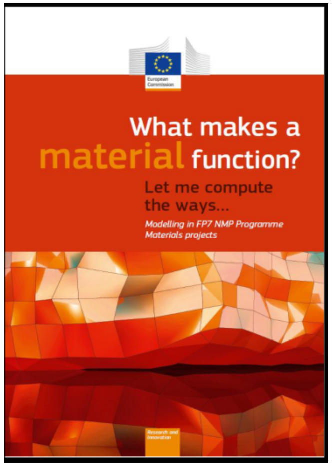
Review of Materials Modelling (RoMM)

- Catalogue EU projects involving materials modelling
- Foster **dialogue** and mutual **understanding** between industrial end-users, software developers and theoreticians.
- Establish a **terminology** for materials modelling concepts harmonising the language of subfields.
- Definition of **concepts**, **classification**
- Basic **metadata** for describing modelling



a compendium of >100 projects and classification/terminology of materials modelling

http://ec.europa.eu/research/industrial_technologies/modelling-materials_en.html

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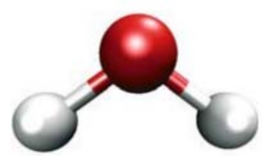
Classification concept: Entities

Modeller chooses to describe the material at a certain level of **granularity** and does this in terms of the behaviour of a set of **entities**.

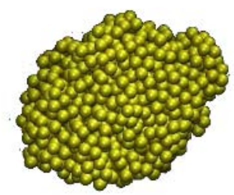
MODEL ENTITY → Self-contained, physically distinct, internally frozen, physical 'thing'

ELECTRONS

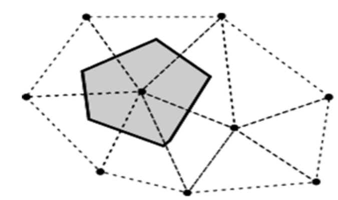
ATOMS



BEADS



CONTINUUM VOLUME



Bead: Discrete entity consisting of more than one atom (e.g. groups of atoms, nanoparticles, grains).

Continuum Volume: Volume in which the material is averaged.

Models are described by ENTITY
not according to the **size** of the application or system
nor according to the **length scale** of the phenomena to be simulated
nor according to the **solver type**

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Classification concept: Physics Equation

PHYSICS-BASED MODEL

PHYSICS EQUATION

PE

Equation based on a **physical/chemical theory** which describes the spatial and temporal evolution of a chosen physics quantities of the entity

PHYSICS QUANTITIES

MATERIALS RELATIONS

MR

Information on the material needed to **close the PE** and to make the system of Governing Equations **solvable**

EXAMPLES

CLASSICAL MOLECULAR DYNAMICS

PE

Newton's equation of motion

$$\frac{dV}{dr} = -m\frac{d^2r}{dt^2}$$

MR

Lennard-Jones potential

$$V_{LJ} = 4\varepsilon\left[\left(\frac{\sigma}{r}\right)^{12} - \left(\frac{\sigma}{r}\right)^{6}\right]$$

FLUID DYNAMICS

PE Navier Stokes equation

$$\frac{\partial}{\partial t}(\rho\mathbf{u}) + \nabla\cdot(\rho\mathbf{u}\otimes\mathbf{u}) = -\nabla\cdot p\mathbf{I} + \nabla\cdot\boldsymbol{\tau} + \rho\mathbf{g}$$

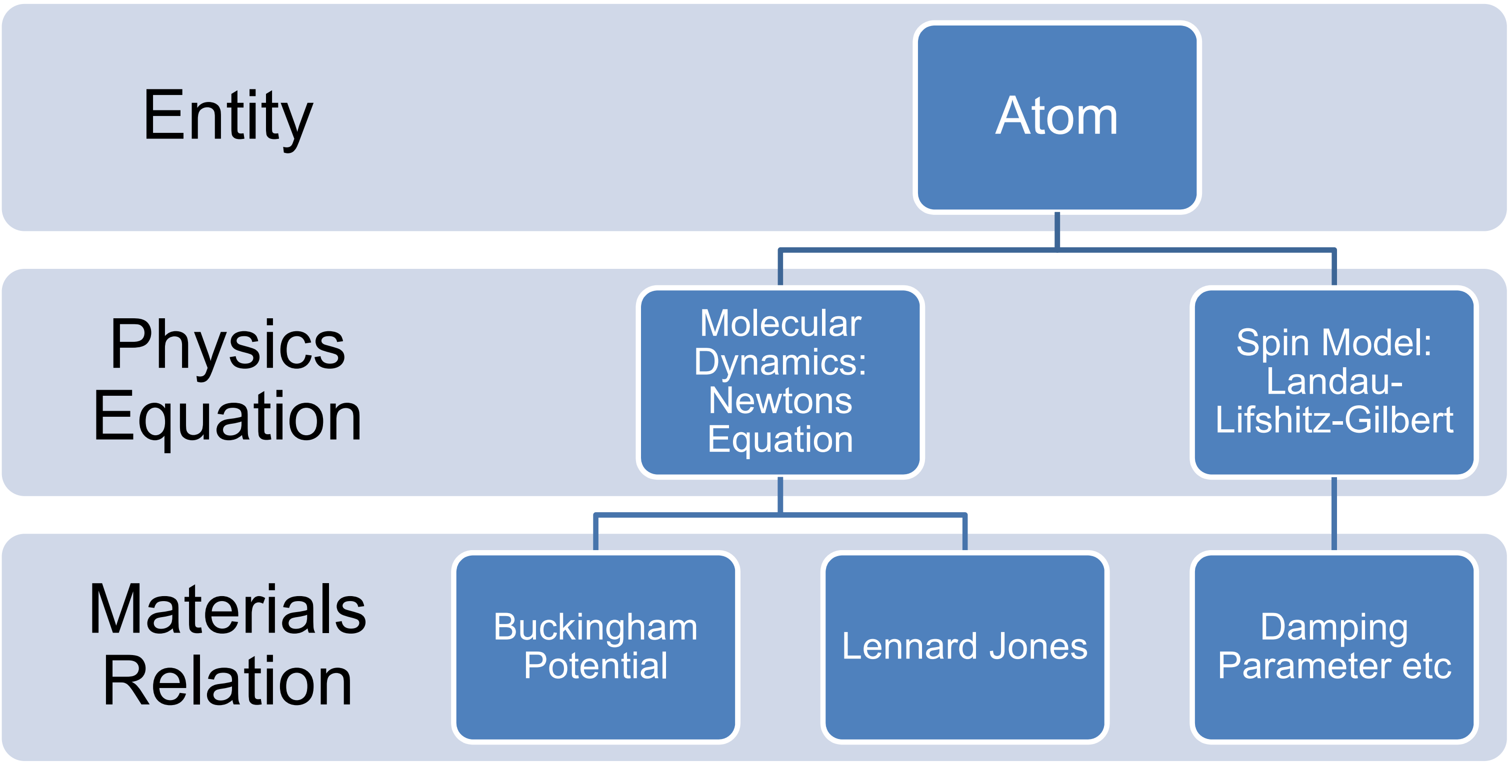
MR Stress tensor for incompressible flows

$$\nabla\cdot\boldsymbol{\tau} = 2\mu\nabla\cdot\boldsymbol{\varepsilon} = \mu\nabla\cdot\left(\nabla\mathbf{u} + \nabla\mathbf{u}^{\mathrm{T}}\right) = \mu\nabla^2\mathbf{u}$$

Hierarchy of classification

1. Entity type (4): **generic, fundamental physics**
2. Physics Equation (about 24); **fundamental physics**
3. Materials Relation (1000s): **domain specific**

EXAMPLE



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Modelling-Data (MODA): Standardised documentation

MODA for <*user-case*>
***Simulated* in project <acronym>**

OVERVIEW of the SIMULATION			
1	USER CASE		*General description of the User Case.* *Please give the properties and behaviour of the particular material, manufacturing process and/or in-service-behaviour to be simulated. No information on the modelling should appear here. The idea is that this user-case can also be simulated by others with other models and that the results can then be compared.*
2	CHAIN OF MODELS	MODEL 1	*Please identify the first model. Note these are assumed to be physics-based models unless it is specified differently.* *Most modelling projects consist of a chain of models, (workflow). Here only the Physics Equations should be given and only names appearing in the content list of the Review of Materials Modelling VI should be entered. This review is available on http://ec.europa.eu/research/industrial_technologies/e-library.cfm). All models should be identified as electronic, atomistic, mesoscopic or continuum.*
		MODEL 2	*Please identify the second model.*
		DATA-BASED MODEL	*If data-based models are used, please specify.*
3	PUBLICATION PEER-REVIEWING THE DATA		*Please give the publication which documents the data of this ONE simulation.* *This article should ensure the quality of this data set (and not only the quality of the models).*
4	ACCESS CONDITIONS		*Please list whether the model and/or data are free, commercial or open source. Please list the owner and the name of the software or database (include a web link if available).*
5	WORKFLOW AND ITS RATIONALE		*Please give a textual rationale of why you as a modeller have chosen these models and this workflow, knowing other modellers would simulate the same end-user case differently.* *This should include the reason why a particular aspect of the user case is to be simulated with a particular model.*

Simulation

- User Case
- Model Physics
- Computational representation
- Post Processing

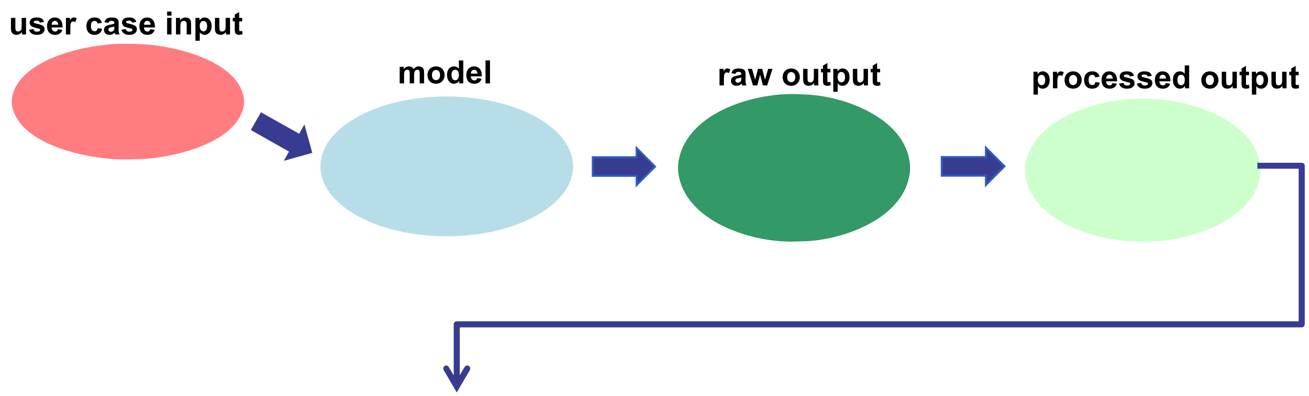
Finding a common language and formal approach how to log my simulation project

Online tool to document and register projects on EMMC.info

MODA portal

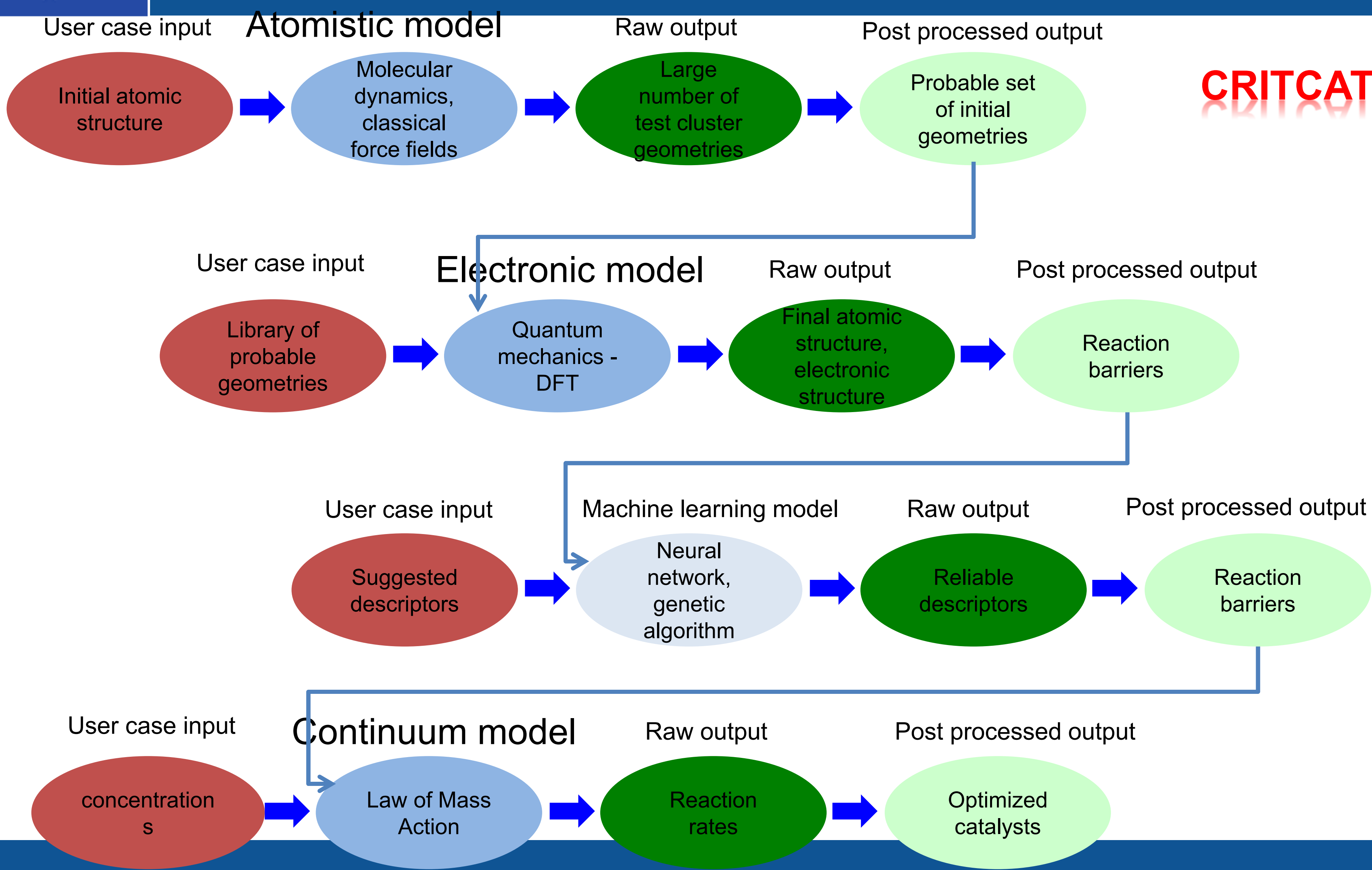
MODA: Graphical representation

Simplest case: simulation with **one** model



RoMM VI

Models used for microkinetics



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CEN Workshop Agreement (CWA): materials modelling - terminology, classification and metadata

- Formal agreement on a terminology and classification of materials models; organises the description of materials modelling applications in order to achieve more efficient communication; lower the barrier to utilising materials modelling.

- **Terminology used to describe materials modelling**
- **Classification of materials models**
- **Standardised documentation of Simulations (MODA)**

CWA 17284 “Materials modelling - terminology, classification and metadata” is now published.

https://www.cen.eu/news/workshops/Pages/WS-2017-012.aspx

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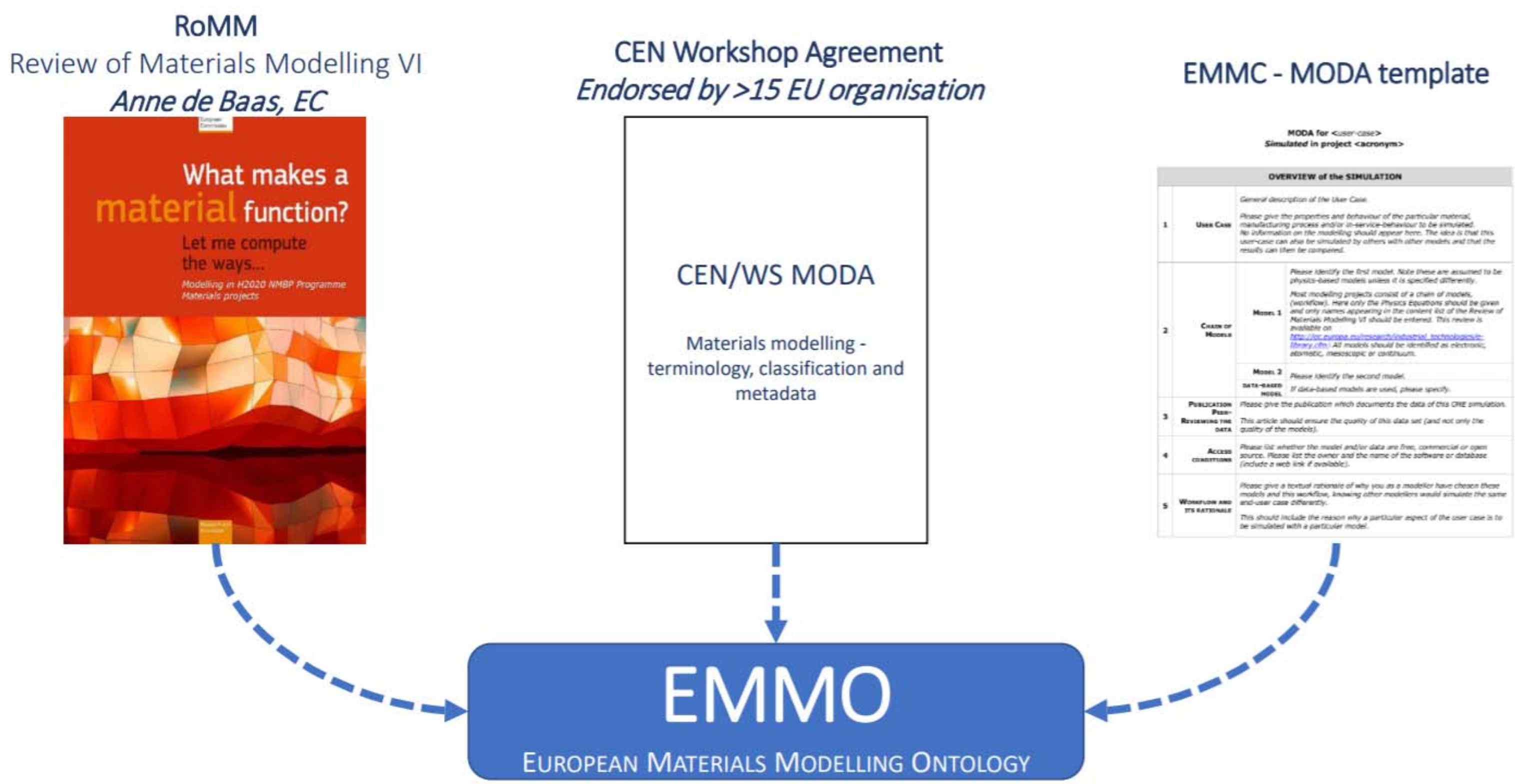
European Materials Modelling Ontology (EMMO)



FOCUS ON CHARACTERISATION - EMCC

The EMCC paradigm, shown below, describes the Open Innovation Environment for the optimisation of materials, materials behaviour and/or nano-device manufacturing processes, and for the validation of materials models based on experimental characterisation.

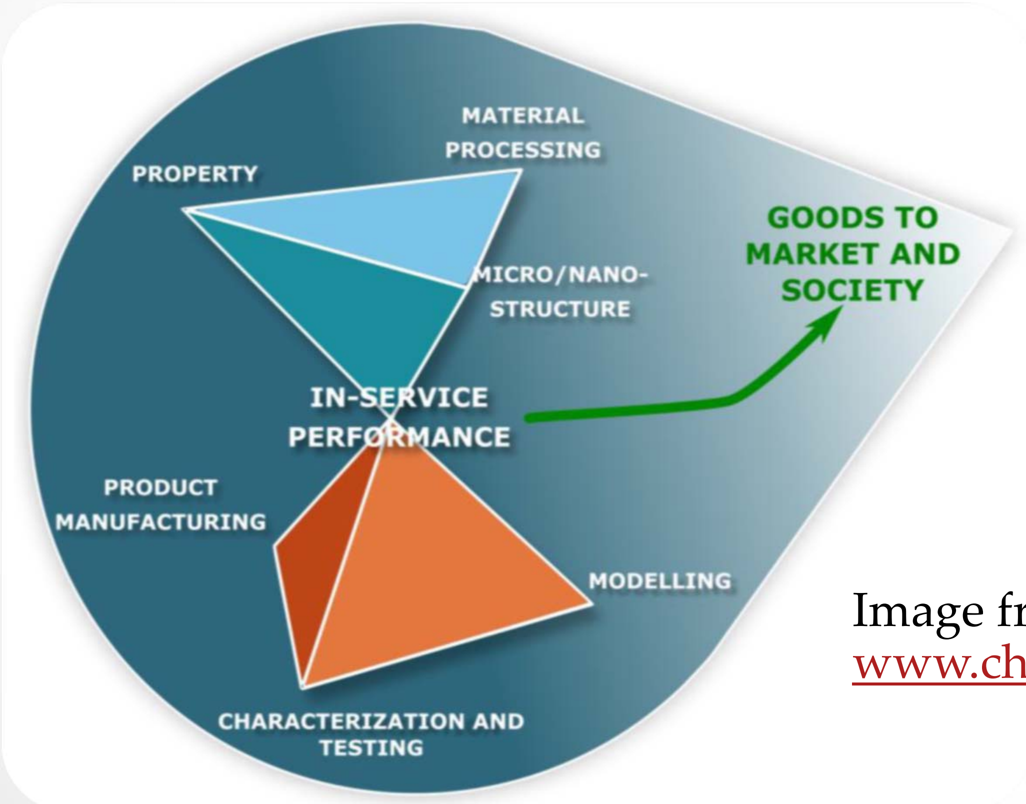


Image from EMCC 2017 roadmap, www.characterisation.eu

CHARACTERISATION DATA – WHAT DO WE NEED?

OYSTER

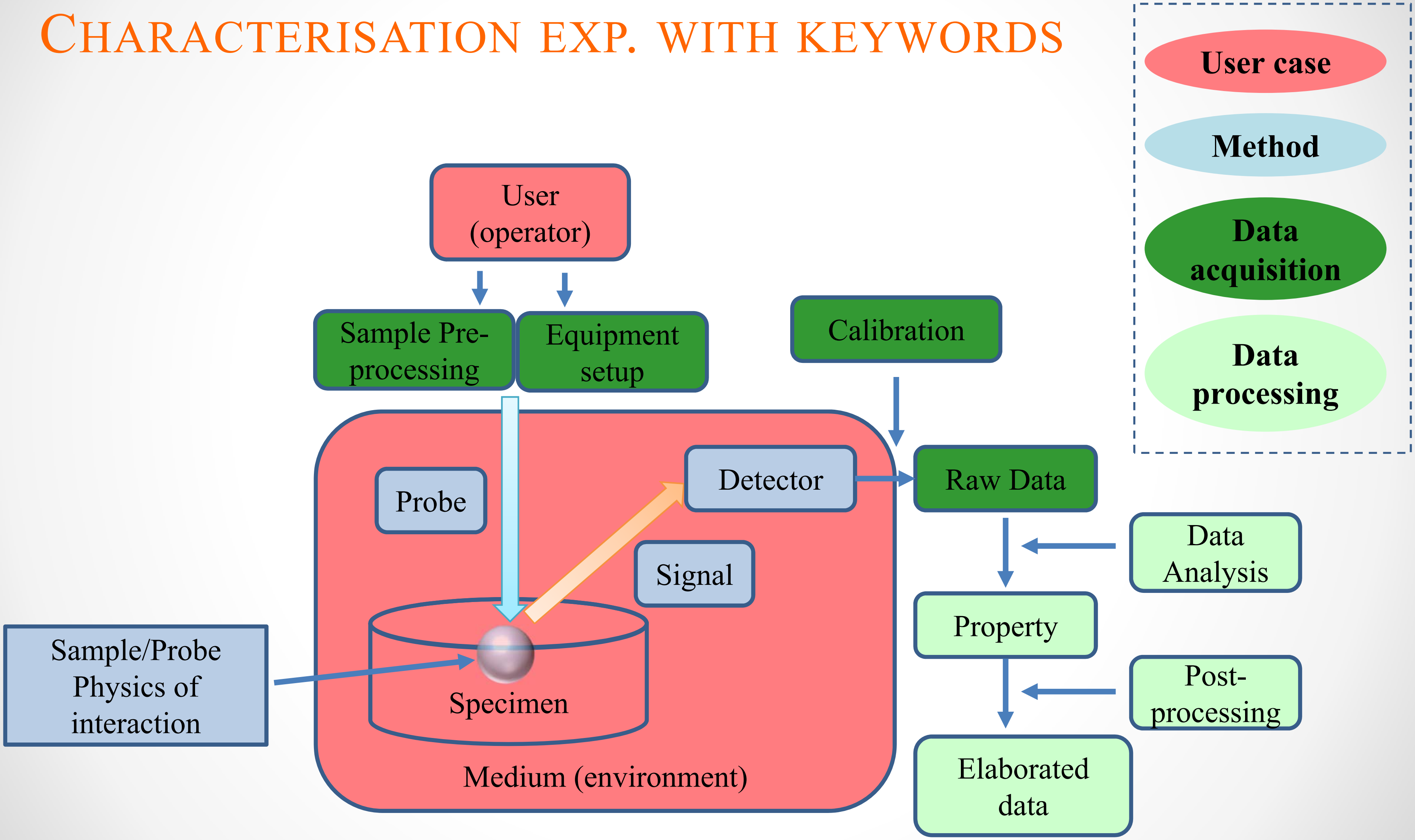
- Data from materials characterisation can be very different, depending on the adopted characterisation method;
- Nonetheless, the availability of **FAIR DATA** on materials properties (behaviour) is probably one of the most precious need for industries and SMEs;
- The **real challenge** here is to seek for a STANDARD DATA STRUCTURE for a range of experimental methods that can be very different;
- The **expected impact** can be extremely wide, e.g. reduction of resources and time needed for product development, with clear associated environmental and societal benefits.

WHERE TO START FROM: HARMONIZATION

- Our proposal for a strategy is to pursue the concept of an **Open Characterization Platform** based on a **semantic footing** and open standards.
- This is basically one step removed from an actual common platform implementation, but provides the **interoperability standards** for it.
- On this basis, **different platform implementation can exist**, but would be highly interoperable if the same standard is used (starting from **CHADA** and **ontology**);

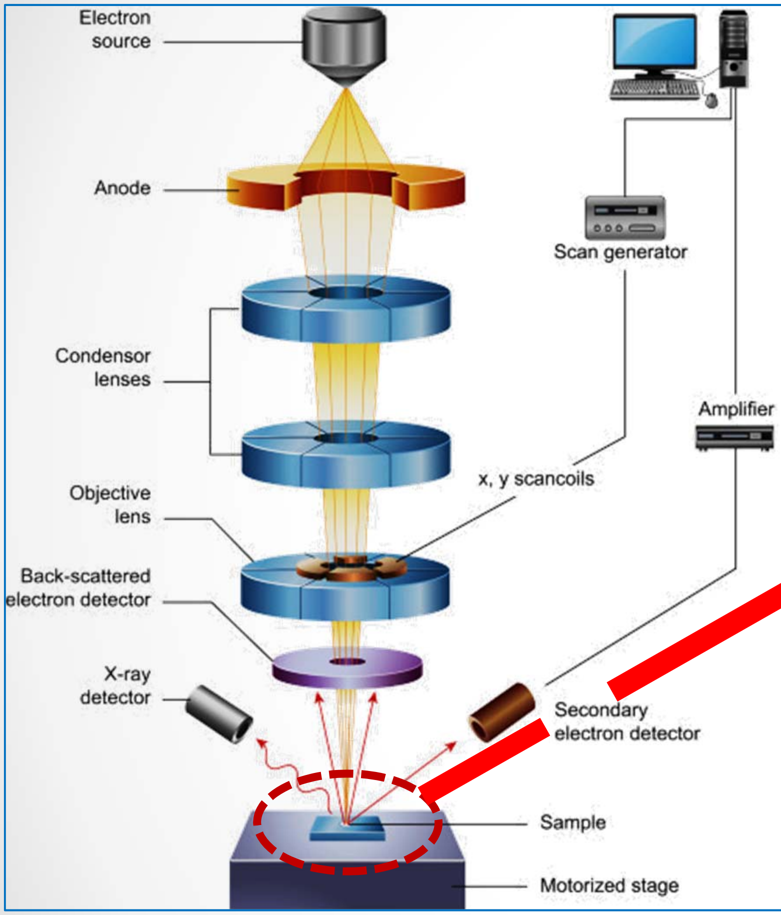
The main step to start this is the development and wide adoption of CHADA

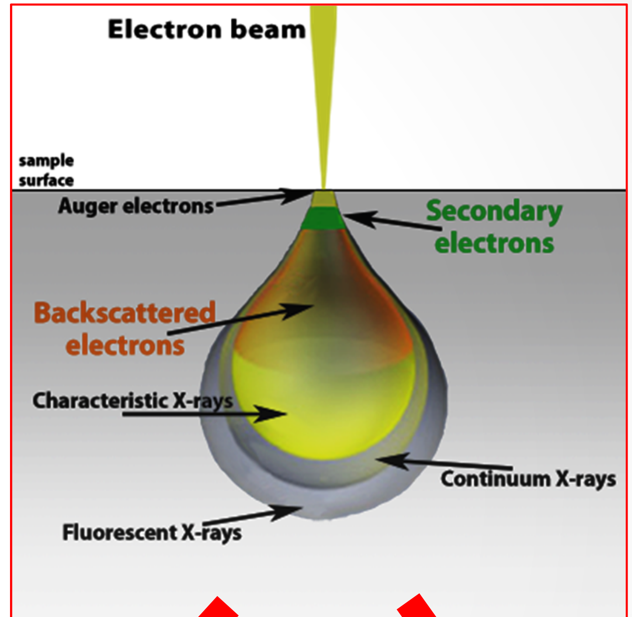
VISUAL REPRESENTATION OF A GENERAL CHARACTERISATION EXP. WITH KEYWORDS



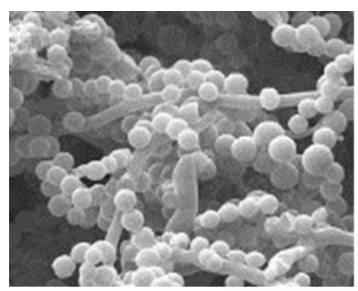
https://www.preprints.org/manuscript/201903.0205/v3

EXAMPLE: Scanning Electron Microscopy (SEM)

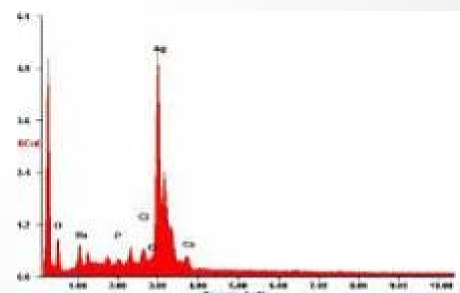




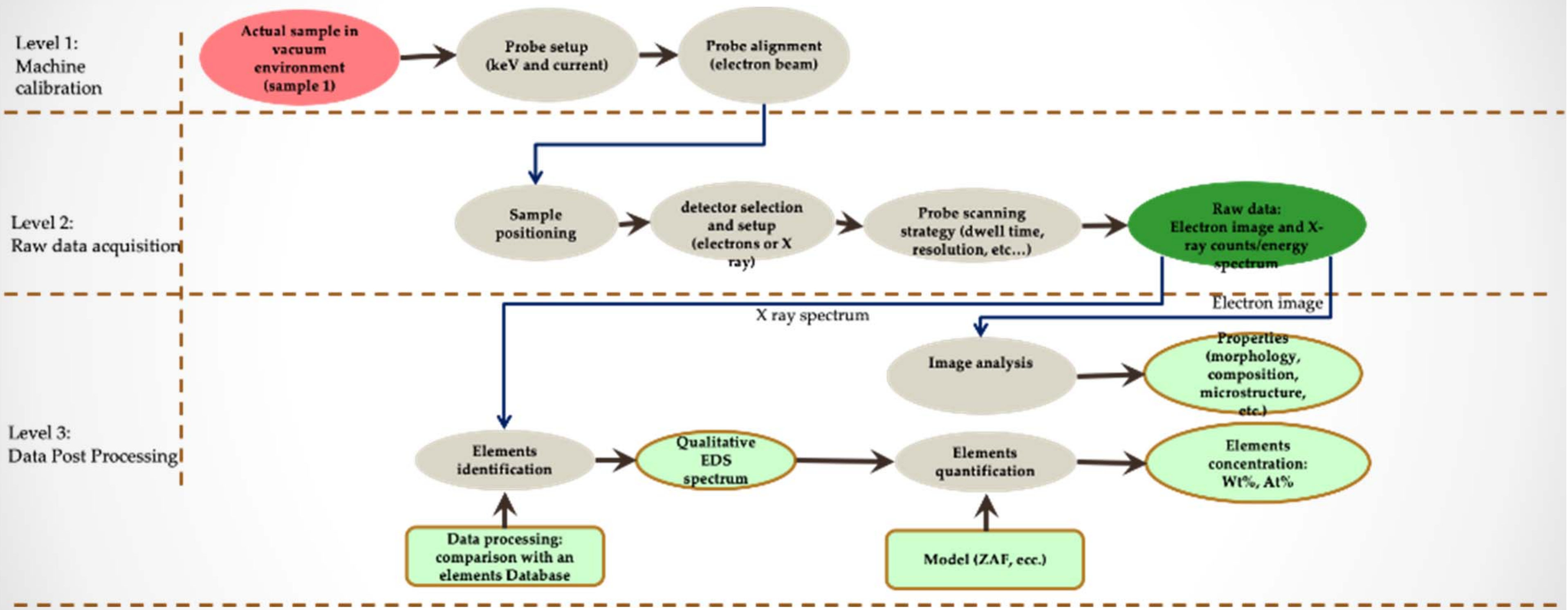
Images



Composition



Workflow materials characterisation: Scanning Electron Microscopy (SEM)



First draft for CHADA workflow

Keyword	Description
User (operator)	Human Operator
Medium (environment)	High vacuum (typically) or low vacuum (environmental SEM)
Specimen	Solid and dry materials with good electron conductibility (Metals, ceramics, biological and polimers. If electron conductibility is not enough, sample have to be metallised or carbon coated
Specimen requirements	Sample dimensions (Typically 30mm x 30mm with thickness less than 10mm). Sample have to be flat, clean and dry.
Sample/Probe Physics of interaction	Energetic electrons in the microscope strike the sample and various reactions can occur in a restricted volume with a consequent generation of secondary electrons, backscattered electrons and X ray photons (for elastic and anaelastic interactions). The probe rasters the sample pixel by pixel
Equipment setup	Probe alignment and setup, sample positioning,
Calibration	Generally only during instrument maintenance
Probe	Energized electron beam (0,1 -30 keV)
Detector	Solid state or photomultiplier to detect secondary signal emitted by the sample
Signal	Electrons and X-ray
Raw Data	Morphological or compositional images. X-ray counts/energy spectrum.

Keyword	Description
Data Analysis	Image quality evaluation (noise, focus, astigmatism, etc.) and X-ray energy data identification
Post-processing	Image analysis and X-ray energy data quantification using models
Property	Topography, morphology, particles metrology (dimensions and shape) etc.

Conclusions

- MODA and CHADA: Standardised documentation for materials simulations and materials characterisation.
- CEN Workshop Agreement Materials Modelling
  Standardised terminology and classification for materials models
- CEN Workshop Agreement Characterisation planned by OYSTER.
- EMMO: a common semantic framework for all NMBP

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