European Materials Modelling Council

European Materials Characterisation Council

Report on Advanced materials modelling and characterisation: strategies for integration and interoperability

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1. Background

This satellite meeting of the EuroNanoForum2021[1] was organised by the European Materials Modelling Council (EMMC ASBL)[2] and the European Materials Characterisation Council (EMCC).[3]

European industrial manufacturing requires the developments of novel, and integrated, characterisation methodologies and computational modelling, especially for establishing the process-microstructure-property correlations in advanced materials in a reproducible and efficient way, allowing design of new and sustainable materials and processes, and rapid upscaling. The ultimate goal is to increase the efficiency and effectiveness of materials and product development by reducing costs and time for product design and time-to-market which will enable the transition to a decarbonised economy

Such developments must be based on knowledge transfer facilitated by data documentation standards and the exploitation of open repositories for data exchange that would be accepted as trusted, efficient and reliable for European industrial manufacturing.

To address this challenge, EMMC and EMCC as well as related projects have been engaged in actions to define a classification and formal documentation of materials modelling and characterisation, the MODA (CWA 17284, 2018) (de Baas, 2014) and CHADA (Sebastiani, Charitidis, & Koumoulos, 2019), respectively. Furthermore, EMMC has been spearheading the development of an ontology (EMMO)[4] that serves the applied sciences and in particular materials science including modelling and characterisation.

In this workshop, some current activities regarding interoperability and integration were presented. In particular, EMMO, MODA and CHADA were discussed to highlight their usability and utility as a basis for moderated discussions related to the following topics:

- Interoperability between materials characterisation and modelling.
- Supporting complex, integrated characterisation and modelling workflows.
- Data traceability for materials throughout multiple lifecycles

[1] https://euronanoforum2021.eu/
[2] https://emmc.eu/
[3] http://characterisation.eu/
[4] E. Ghedini, G. Goldbeck, J. Friis, A. Hashibon and G. J. Schmitz. The European Materials & Modelling ontology (EMMO). Available on https://github.com/emmo-repo/EMMO

2. Summary of Talks and Discussion Session

2.1. Welcome and Introduction of participants

Esther Hurtós welcomed the audience and introduced Materials Modelling and Characterisation as crucial for European industrial manufacturing. The European H2020[5] funding effort has been enabling development in both fields and the new Horizon Europe[6] programme is encouraging closer interoperability between Materials Modelling and Characterisation data. Thus, the community involved will have to identify and address challenges that may hamper such integration. Overarching schemes such as Open Innovation[7] (Pillar 3 in Horizon Europe) and Open Innovation Testbeds[8] will function as incubators for a symbiosis of Materials Modelling and Characterisation. The experts taking part in this event are experienced participants in European projects and avid networkers. Their presentations will aim to engage more stakeholders to enable interoperability between Materials Modelling and Characterisation.

2.2. Overview of EMMC and its activities on interoperability

Nadja Adamovic gave an overview of the European Materials Modelling Council (EMMC) that started with a stakeholder consultation in 2014 to become a non-profit organisation in 2019 after a successful EU CSA[9] project. Membership is continually increasing and currently includes 594 Associate members, 43 Full Individual members and 32 Organisational members.

The EMMC enables stakeholders to form and join focus areas and use a bottom-up approach to develop methods, policies, strategies, and best practises. It caters for its stakeholders with events, workshops, surveys and encourages discussion which is key to enabling changes and realising the benefits of Materials Modelling. The EMMC captures more than 140 outputs in reports, whitepapers[10] and case studies and its community provide input to Horizon programmes. To this date, the EMMC hosted about 50 events with 20-200 participants. It avidly collects input from the community to update strategic documents and roadmaps. EMMC offers six Focus Areas for its members to become active in:

1. Model Development: Everything that has to do with the capabilities and qualities of the materials models and the modelling workflows: development, validation and application.

[5] Horizon 2020 is an EU Research and Innovation programme, that was running from 2014 to 2020.
[6] https://ec.europa.eu/info/horizon-europe_en
[7] https://ec.europa.eu/info/sites/default/files/research_and_innovation/strategy_on_research_and_innovation/presentations/horizon_europe_en_investing_to_shape_our_future.pdf
[8] https://ec.europa.eu/research/participants/data/ref/h2020/other/guides_for_applicants/h2020-im-ac-innotestbeds-18-20_en.pdf
[9] https://cordis.europa.eu/project/id/723867
[10] https://zenodo.org/communities/emmc

2. Interoperability: Topics include the semantic foundation (from terminology to ontology), standardised documentation and cross-domain interoperability platforms.
3. Digitalisation: This refers to the process of making use of digitised information to formulate and to create new knowledge enabling the extraction of insight out of such digital data.
4. Software: Successful materials modelling software uses the best algorithms, it is numerically robust, carefully validated, well documented, easy to use, and continuously maintained during decades.
5. Impact in Industry: This Focus Area is concerned with all aspects that play a role in the impactful use of materials modelling in industry, including People, relevant research and business Processes, Models use and simulations, and Data Infrastructures and Analysis.
6. Policy: The RoadMap recognises the importance of making advances in materials modelling and digitalisation of materials sciences to support the competitiveness of European industry.

Interoperability is the focus area[11] most pertinent for the topic of this Satellite workshop. It aims to raise awareness, to highlight benefits and impact and to support widely agreed terminology (CWA 17284, 2018), taxonomy and ontology standards (Goldbeck, Ghedini, Hashibon, Schmitz, & Friis, 2019) (Morgado, et al., 2020) (Konchakova & Klein, 2021) (Hagelien, Preisig, Friis, Klein, & Konchakova, 2021) which are key enablers for interoperability.

To reach semantic interoperability, members of the EMMC community are developing EMMO[4], the European Materials and Modelling Ontology.

Industry wants to connect models and data for innovation and novel products which can be seen as the main benefits from enabling interoperability. The latter is only possible if materials modelling and experimental (i.e., characterisation) data are FAIR and the European materials and manufacturing industry focusses strongly on data value generation. Digitalisation, as envisaged by the European Union, requires a high data information quality which goes hand in hand with utilising ontologies. The EMMO will be an enabler for materials modelling and characterisation data documentation, and its developers invite stakeholders to join the effort. Also, EMMC focus areas are open for stakeholders to collaborate in task groups with like-minded people from industry, academia and beneficiaries from H2020 projects such as MarketPlace[12], VIMMP[13], ReaxPro[14], SimDOME[15], OntoTrans[16], OntoCommons[17], DOME 4.0[18], OpenModel[19], NanoMECommons[20] and VIPCOAT[21].

[11] https://emmc.eu/activities/emmc-focus-areas/interoperability
[12] https://cordis.europa.eu/project/id/760173, https://www.the-marketplace-project.eu/
[13] https://cordis.europa.eu/project/id/760907, https://www.vimmp.eu/
[14] https://cordis.europa.eu/project/id/814416, https://www.reaxpro.eu/
[15] https://cordis.europa.eu/project/id/814492, https://simdome.eu/
[16] https://cordis.europa.eu/project/id/862136, https://www.ontotrans.eu
[17] https://cordis.europa.eu/project/id/958371, https://www.ontocommons.eu/
[18] https://cordis.europa.eu/project/id/953163, https://dome40.eu/
[19] https://cordis.europa.eu/project/id/953167
[20] https://cordis.europa.eu/project/id/952869, https://www.nanomecommons.net/
[21] https://cordis.europa.eu/project/id/952903

2.3. Overview of EMCC and its activities on interoperability

Costas Charitidis gave an overview of the European Materials Characterisation Council (EMCC), which is a European initiative that was set up at the beginning of 2016, based on and strengthening the existing European Materials Characterisation Cluster (created at the end of 2014). Similarly to the EMMC, the EMCC is a bottom-up activity based on the involvement and support of a wide range of stakeholders. The aim of the EMCC is to support the process of developing and improving characterisation tools to enable the successful conversion of nano- and advanced materials to actual products in Europe.

EMCC is constantly gathering the needs and requirements of its community for characterisation tools and supporting actions. It aims to provide a forum for discussion, problem solving and planning of R&I activities in Europe. It strongly supports policy development, underpinning the relevant EC priorities, with a stakeholder driven roadmap for characterisation techniques for engineering and upscaling of nano-materials and advanced materials in Europe. This activity is to support the strengthening of Europe's industrial capacity and competitiveness.

EMCC has also a strong focus on interoperability, as one of its objectives is to create a platform for (nano)characterisation, with the attempt to interact with Open Research Data. Another objective of great interest is to link (nano)metrology with in-situ monitoring and industrial needs. However, to enable this interoperability, all stakeholders involved are required to establish the formation of standard methodologies on (nano)characterisation and find a common background.

The relevant stakeholders comprise materials scientists covering all types of characterisation expertise, developers and manufactures of analytical instruments (both in academia and industry), materials manufacturers who are using such instruments, standardisation bodies and metrology institutes.

The competitiveness of the EU depends on how strongly resources are channelled within its supply chain environment and how efficiently these resources are utilised. This is strongly connected to the digitalisation of both industry as a whole and specific manufacturing technologies. Only digitised data can be accessed fast enough to generate a holistic picture on all available resources to enable this channelling. Hence, for characterisation to become part of this solution, digitisation will be key. For example, the digital twin representation of materials in the in-situ state, e.g., at critical stages during manufacturing or during production, needs to be underpinned by robust materials characterisation. Also, not all stakeholders are able to host all characterisation tools in their organisations. To enable them to still take part, the formation of an independent platform will be pertinent to effectively connect them and these tools (characterisation, simulation and online sensing) in a sustainable and standardised manner.

All of this requires an enhancement of the (meta-)data quality by supporting standardization of EU-wide characterisation. The interoperability of characterisation protocols increases functionality of information systems to exchange data and to enable sharing of information. The EMCC seeks coordination with 3rd parties such as EMMC, the European Pilot production network (EPPN)[22], the

[22] https://www.eppnetwork.com/

Nanosafety Cluster (NSC)[23], the European Technology Platform for Advanced Engineering Materials and Technologies (EuMaT)[24], the Research Data Alliance (RDA)[25], and the NANOfutures[26] initiative to enable effective interoperability and reusability of characterisation data for the end-users. This will maximise the impact of uptake and adoption of the results by the materials and manufacturing industry.

For the time being, there is an interoperability challenge: the preliminary CHADA (see Chapter 2.4.) does not include the necessary EMMO ontologies (see Chapter 2.6.) and interoperability capability allowing for harmonisation among diverse industrial sectors. Hence, the EMCC will put effort in iCHADA (Interoperable Characterisation Data structure) development via the H2020 project NanoMeCommons[20]. There is also an ongoing CEN Workshop activity that is actively looking into this, as discussed in-depth below in Chapter 2.4.

The vision for the characterisation community is an Open Innovation Environment that facilitates sharing of data and knowledge, connects characterisation infrastructures and modelling environments for driving innovation. Such an innovative platform permits the exchange of FAIR data, the coupling of instruments, and the reusability and traceability of characterisation protocols. This ambition will bring changes and require the community to do things differently. However, the EMCC will aim to support its stakeholders all the way.

2.4. CHADA and the OYSTER CEN Workshop Agreement (CWA)

Marco Sebastiani introduced the H2020 project OYSTER[27] which has its scientific and technological focus on tailoring the surface free energy (SFE) in nano-engineered materials to improve their properties. OYSTER works with novel characterisation methods and multi-physics modelling to enable the manufacturing of novel nano engineered materials. The beneficiaries want to tailor surfaces and nanomaterials and get an in-depth understanding how a surface actually looks like. This led to development of cutting-edge characterisation methods such as next generation contact mechanics such as Atomic Force Microscopy (AFM) and nanoindentation for SFE measurement and X-ray photoelectron spectroscopy (XPS) for surface chemical analysis on nanopatterned surfaces. Additionally, multi-scale (from atomistic to continuum) modelling was deployed to understand the chemistry and topological effects on wettability and SFE. Finally, the developed methods are applied to optimise novel materials and surface with tailored surface energy. To assure innovation continuation, OYSTER aims to become an Open Innovation Environment (OIE) for the matchmaking between experts, consumers, models, equipment, data, and knowledge – it will take a whole ecosystem to make their findings accessible to everyone everywhere. To enable this, a common standard (Romanos, et al., 2019) has to be found, and a first step was made by introducing the CHADA (Characterisation Data) (Sebastiani, Charitidis, & Koumoulos, 2019). There are analogies of

[23] https://www.nanosafetycluster.eu/
[24] https://www.eumat.eu/
[25] https://rd-alliance.org/
[26] http://www.nanofutures.eu/
[27] https://cordis.europa.eu/project/id/760827, http://www.oyster-project.eu/

characterisation to materials modelling: in both cases one needs an input to engage with a method to obtain some raw data and perform post processing. The first two steps for modelling are an input and a model and for characterisation a sample and a (characterisation) method. This enabled the OYSTER team to harness the already existing MODA (CWA 17284, 2018) and build the CHADA. Initial workflows and templates (Sebastiani, Charitidis, & Koumoulos, 2019) (Koumoulos, Sebastiani, Romanos, Kalogerini, & Charitidis, 2019)for CHADA have been already developed and can be obtained from the OYSTER Zenodo repository[28]. However, the sole provision of documentation is not sufficient, so the OYSTER team initiated a CEN[29] workshop[30]: CWA[31] on Materials Characterisation - Terminology, classification and metadata. This effort is assisted by UNI[32] (Ente Nazionale Italiano di Unificazione - Italian National Unification) who are the CWA secretary and provide guidance through this process. It became clear that this effort is in the interest of many stakeholders as an unusually high number of participants joined this CWA: there are more than 40 registered participants/experts, including representatives from NMBP-07-2017[33](i.e., Cornet[34] and MMAMA[35]), NMBP-08-2019[36] (i.e., NanoBat[37], NanoPat[38], NanoQI[39], and RealNano[40]) and NMBP-35-2020[41](i.e., NanoMeCommons[20]) funded projects, and relevant representatives from both the EMMC and EMCC, respectively.

The main purpose of this CWA is to propose a widely agreed and common basic architecture for characterisation data (i.e., proposing a new structure of data but not a new format), which can be used as a building block for the most complex characterisation case studies, also comprising interactions with modelling and process workflows. This will increase the interoperability between all emerging platforms and create a truly European OIE.

Future projects will look into bringing the CHADA into machine readable form and into the interoperability of MODA and CHADA workflows.

[28] https://zenodo.org/communities/oyster/
[29] CEN: Comité Européen de Normalisation - European Committee for Standardization
[30] https://www.cen.eu/News/Workshops/Pages/WS-2020-010.aspx
[31] CWA: CEN Workshop Agreement
[32] https://www.uni.com/
[33] Systems of materials characterisation for model, product and process optimisation
[34] https://cordis.europa.eu/project/id/760949, http://cornet-project.eu/
[35] https://www.mmama.eu/
[36] Real-time nano-characterisation technologies
[37] https://cordis.europa.eu/project/id/861962, https://www.nanobat.eu/
[38] https://cordis.europa.eu/project/id/862583, https://www.nanopat.eu/
[39] https://cordis.europa.eu/project/id/862055, https://nanoqi.eu/
[40] https://cordis.europa.eu/project/id/862442, http://www.realnano-project.eu/
[41] Towards harmonised characterisation protocols in NMBP

2.5. Twinned MODA-CHADA case study for electrical characterisation

Małgorzata Celuch is the president of QWED[42], a Polish high-tech SME, that serves its global customers now for 24 years with its Electromagnetic simulation and design software as well as related services. The SME has long standing experience with EU projects starting with the 6th Framework programme[43] and is currently a beneficiary with NanoBat.[37] QWED's speciality is also electrical and electromagnetic (EM) characterisation of materials to enable accurate design of new high frequency devices, development of new technologies and applications and also find fundamental knowledge about materials. Their methodology is the design of test-fixtures that provide a specific EM response to a specific material. An example given demonstrated EM field interaction with tissues ranging from beef burger to in vivo brain haemorrhage (Petrovic, Otterskog, & Risman, 2016). A typical set-up for a Split-Post Dielectric Resonator (SPDR) – operation (Celuch, Rudnicki, & Krupka, 2019) was explained. It looks, to the non-expert, very simple and one is tempted to claim "*the Dielectric constant is measured by a Vector Network Analyser (VNA)*". Indeed, there is a number, but the physics behind deserves deeper explanation. QWED's modelling is applied to fully investigate a transmission signal in the desired domain and range, i.e., a test-fixture electromagnetic response. Thus, only, if a CHADA for SPDR can be augmented by a MODA, this type of characterisation can be thoroughly described. This combination of MODA and CHADA is expected to chance to continuously improve both characterisation test-fixtures and methods and modelling solvers and material libraries. Małgorzata Celuch, together with her colleague Marzena Olszewska-Placha, is due to establish a Task Group "Linking and Coupling Computational Chemistry to Electromagnetics" under the umbrella of the EMMC Focus Area "Model Development".[44] All interested stakeholders can look forward to many more MODA-CHADA interoperability in the near future.

2.6. Modelling and characterisation interoperability facilitated by EMMO

Jesper Friis, one of the EMMO[4] developers, introduced how ontologies can be enablers for interoperability. EMMO started in 2016 and its foundation was laid within the EMMC-CSA[45] EU project and its governance is currently managed by EMMC ASBL[2]. A team of philosophers, information and communication technology experts and applied scientists worked on application cases in the project SimDOME[15]. VIMMP[13] and MarketPlace[12] saw EMMO applied to larger materials modelling communities and marketplaces infrastructures. OntoTrans[16] offers more domain ontologies and industrial application cases, while in OntoCommons[17] EMMO will join an ecosystem with other ontologies and tools to build a foundation for data documentation in materials and manufacturing industry. By 2024, EMMO will be applied to industrial data ecosystems (DOME 4.0) and open innovation platforms and workflows (OpenModel[19], VIPCOAT[21]).

[42] https://www.qwed.com.pl/
[43] https://ec.europa.eu/growth/sectors/space/research/fp6_en
[44] https://emmc.eu/activities/emmc-focus-areas/model-development
[45] https://cordis.europa.eu/project/id/723867

Knowledge graphs are useful to describe complex scientific data as they can describe unstructured data and how they are interrelated. An Ontology can be seen as a schema for a knowledge graph. The EMMO fills the role as a strong schema for knowledge graphs (Figure 1) for applied sciences.

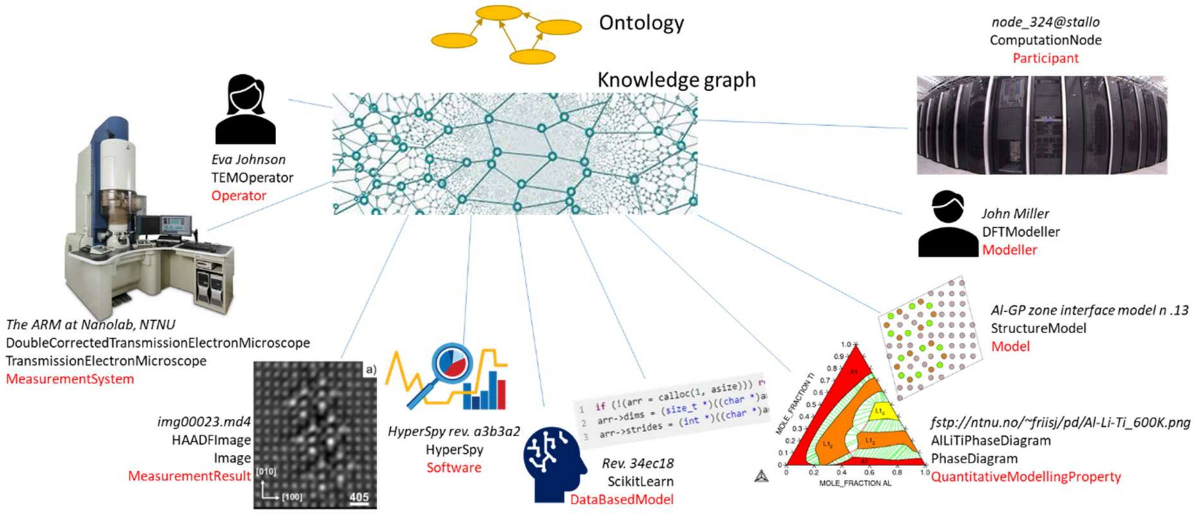

Figure 1. The ontology serves as a schema for the knowledge graph that describes and connects all the individuals that participate in a characterisation and/or modelling case. The individuals are written in italic, followed by the generalised class names in the application, domain or mid-level ontology that they belong to. The classes in red are found in EMMO.

The EMMO covers several ontological levels: top, middle, domain and application. The top level comprises "item", "Physical", and "Perspective"; the latter leads to the mid-level with "Holistic" (describes whole 4D object/process and the role of its participants), "Reductionistic" (direct parthood - material entities can be represented in EMMO by a hierarchy of parthood relations), "Physicalistic" (matter, field, material - the world as described by a physicist), and "Perceptual" (symbols, languages, metrology, mathematics - objects that can stimulate a perception).

Characterisation is the (semiotic[46]) process of measuring and determining a material's structure and properties. Quantitative properties are determined by a well-defined semiotic process, with participants:

- **Object:** real world object with a property that we want to measure → *Sample*
- **Sign:** stands for the physical that communicates the measurement (→ signal in the *MeasuringSystem* that produces the *MeasurementResult*)
- **Interpretant:** another sign that stands for the measured quantitative property → *MeasurementResult*
- **Interpreter:** the measurement instrument used to perform the measurement → *MeasuringSystem*

[46] Semiotics is the general study of signs of all kinds and in all their aspects. Semiosis is a triadic relationship between a sign, an object and an interpretant.

Modelling is the (semiotic) process of applying a model to describe or predict a phenomenon. Quantitative properties are determined by a well-defined semiotic process, with participants:

- **Object:** real world object with a property that we want to model → *Object*
- **Sign:** stands for the model that is used to produce the result → *Model*
- **Interpretant:** another sigh that stands for the modelled property → *Property*
- **Interpreter:** the person or system that runs and interprets the results of a model → *Modeller*

To capture the data for both the characterisation and the modelling process a triplestore[47] will be key. Triplestores will house ontologies, individuals representing the participants and metadata in the characterisation/modelling case, and mappings (e.g., from data sources to ontological concepts). A challenge is that the characterisation and modelling experts are seldom familiar or trained on ontologies. Instead of requiring these experts to express their datasets according to a specific ontology, a more realistic approach is to just ask them to provide a semantic description of their data structured as it is common in their field. A translator that knows the ontology can then map the semantic description to the common reference framework provided by the ontology and thereby achieve interoperability across characterisation and modelling.

This means stakeholders will have to change their way of how they work with data and concentrate on data information quality. One also has to concentrate on context; it is not only important that we have data in a standardised format, but also information on how the data has been measured/calculated.

2.7. Open discussion session "Characterisation/Modelling integration"

Bojan Boskovic and Adham Hashibon engaged with the participants and captured their thoughts and pressing issues. The idea of an interoperability between MODA and CHADA was well received, as often data from modelling serve as input for characterisation and vice versa. Especially, members of the OYSTER project could share several examples; e.g., how modelling data of a surface can enable a better interpretation of X-ray measurements. There was interest to make MODA and CHADA machine readable. The projects OYSTER and NanoMeCommons are working on EMMO implementations of CHADA, complementing work in other European projects on EMMO/MODA. It is key that both communities work together, keep aligning their efforts and develop tools that enable interoperability between both MODA and CHADA.

The audience would like to see a terminology for meso and nano structures. Especially nanoparticles have, besides their chemical compositions, a variety of shapes and dimension they could appear in and the latter is vital to understand their properties fully. There was a recent effort (Lynch, et al., 2020) to investigate and InChI (IUPAC International Chemical Identifier) for Nano could address the need for a simplified representation of complex nanomaterials across experimental and nanoinformatics studies. However, a corresponding domain ontology does not exist yet, and the

[47] A triplestore is a database for the storage of triples, i.e., data composed of subject-predicate-object.

audience members were invited to form a task group in the EMMC, so an EMMO compliant one can be developed. A domain ontology may cause also additions to the mid-level of EMMO, thus, an interaction with the developing team will be vital.

Another interesting discussion point was concerning the reproducibility of characterisation experiments. If one uses the “same material” one would expect to obtain the “same results”. However, “material” is complicated, as there are hardly any 100% defect and inclusion free specimen around. The community is aware of this fact, but would like see reproducibly adequately defined for characterisation experiments. It will be pertinent to report more on the context of a material, i.e., what exactly do we mean by “material”, inclusions, structure, surface properties, impurities, defects, etc. This information, especially on size, shape and surface properties, is also necessary for Nanosafety as on the nano-scale (1-100 nm) the properties of materials can be different from those of a bulk material. Additionally, knowledge on evolution over time, ageing, and complexity should be included. The audience could envisage for each material/sample an InChI type string which would enable it to be compared to other materials/samples. A similarity factor could then be used to declare two materials/samples being the “same”.

Interoperability and sharing data have its advantages, however, industry holds a lot of propriety information they do not want to or cannot share. Thus, when our community talks about Open Innovation Environments, they talk about the philosophy behind not about freely available data. They want to share workflows and best interoperability practises for both characterisation and materials modelling. Many of the tools and concepts developed in recent and present EU projects can be deployed behind firewalls and in closed company ecosystems. Industry does have data management and digital infrastructure in place, with diverse levels of maturity. However, our communities’ idea of interoperability will enable industry adoption and contribute to their infrastructures becoming interoperable with novel tools. The latter need to be brought into industry for testing to proof new concepts can have benefits.

The modelling community works now more on verification and validation of methods to gain industry’s trust. Protocols and training materials are provided to enable stakeholders to test novel tools. The characterisation community works with round robin tests and reference samples to validate new characterisation tools or workflows. If both the communities want industry to move towards open innovation environments they have to commit to standards as expected from their industrial stakeholders.

3. Conclusion and Outlook

There are several topics that should be addressed by both EMMC and EMCC

- Make MODA and CHADA interoperable
- Make MODA and CHADA machine-readable
- Both MODA and CHADA should be introduced more to industrial stakeholders so they go beyond EU projects and become a standard to report on modelling and characterisation, respectively.
- Can our communities find ways to compare “materials” so one could confidently say, when two specimens are identical?
- Do our communities consider meso and nano materials in-depth?
- Interoperability and Open Innovation are not about sharing propriety data – they share concepts, ideas, better understanding of the underlying physics, ways of finding knowledge, etc.
- Make industry more confident in both our communities’ efforts by working to high standards and demonstrate the benefits of novel tools and concepts.

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APPENDIX 1: Event Agenda

Online, 4th May 2021

Time	Topic	Speaker/Moderator
14:00 – 14:25	Welcome and Introduction of participants	Esther Hurtós
14:25 – 14:35	Overview of EMMC and its activities on interoperability	Nadja Adamovic
14:35 – 14:45	Overview of EMCC and its activities on interoperability	Costas Charitidis
14:45 – 15:10	CHADA and the OYSTER CEN Workshop Agreement (CWA)	Marco Sebastiani
15:10 – 15:35	Twinned MODA-CHADA case study for electrical characterisation	Małgorzata Celuch
15:35 – 16:00	Modelling and characterisation interoperability facilitated by EMMO	Jesper Friis
16:00 – 17:00	Open discussion session “Characterisation/Modelling integration”	Bojan Boskovic and Adham Hashibon

APPENDIX 2: Event Pictures

Some EMMC and EMCC team members enjoying the EuroNanoForum 2021