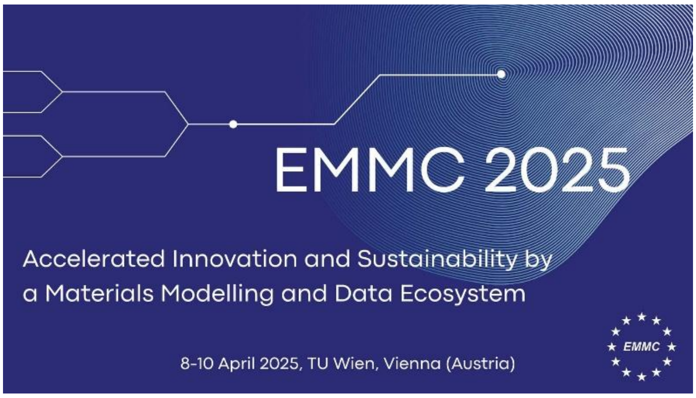
5th EMMC International Workshop 2025

APR 8-10, 2025 | TU Wien | Vienna (AT)



The EMMC 2025 International Workshop discussed advances and future directions in how both accelerated innovation and sustainability are supported by a Knowledge Ecosystem based on materials modelling and data integration.

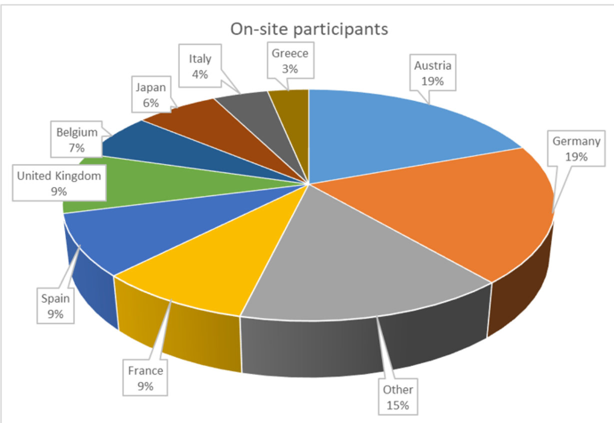
The workshop discussed following points from different perspectives including

- Advancements in modelling and integration with characterisation
- Digitalisation and Interoperability including Materials Commons
- Software development, deployment and maintenance
- Adoption in industrial ecosystems
- Sustainability
- Policy

The EMMC International Workshop is a leading, cross-cutting event where stakeholders from different materials & digital fields in industry and academia get together to discuss topics of strategic importance and elaborate on gaps and potential actions to move the field forward. Previous EMMC International Workshops had more than a third of participants coming from industry, benefitting from the opportunity to get a high level overview of key trends.

EMMC 2025 was again located in central Vienna, in the main building of TU Wien. It featured high-level plenaries from leading experts in industry and academia, discussion sessions stimulated by invited "Impulse" talks, and contributed posters with short presentations in each session.

Statistics



Other* from

- Cyprus
- Czech Republic
- Denmark
- Luxembourg
- Netherlands
- Poland
- South Korea
- Sweden
- Switzerland
- USA

* Less than 3 participants

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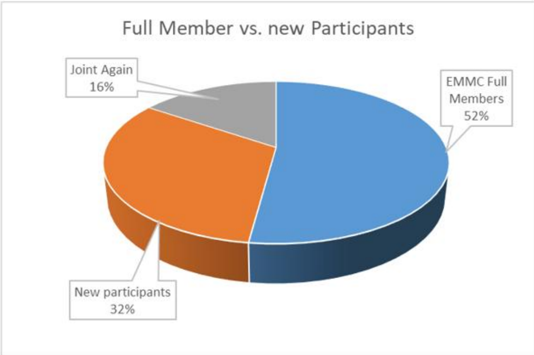

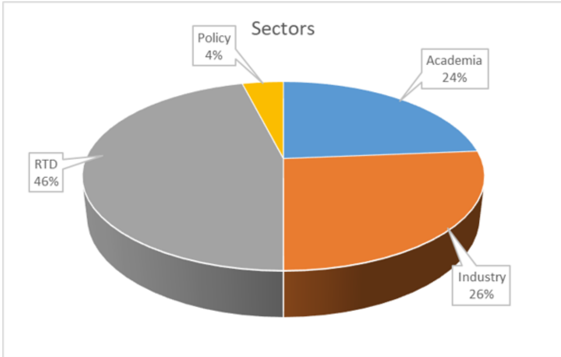

Summary

The EMMC 2025 workshop covered multiple sessions on advancing materials modelling, sustainability, and digital innovation

- **Session 1:** Explored AI's role in materials modelling, emphasizing the need for physics-based data to support AI and ML. Discussions highlighted the importance of balancing physics-based and data-driven modelling while ensuring collaboration among experts.
- **Session 2:** Focused on sustainable materials in industries like motorsports and aerospace. The integration of materials characterisation, modelling, and data ecosystems is driving innovation. Digital twins and cobotic cells were discussed as key tools.
- **Session 3:** Addressed data sharing and interoperability across platforms such as the Materials DX Platform (Japan), DIADEM (France), and European initiatives. FAIR data principles and ontology-driven digitalisation were emphasized.
- **Interlude:** Austria and the EU's efforts in supporting materials R&D were explored, including the concept of a Materials Commons—a federated digital infrastructure for research and innovation.
- **Session 4:** Examined AI's impact on software design, digital infrastructure, and materials modelling workflows. Machine-learned potentials (MLPs) were highlighted alongside the role of quantum computing in electronic modelling.
- **Session 5:** Discussed industrial adoption of materials modelling, highlighting FAIR data, AI integration, and hybrid modelling approaches. The IAM-I partnership was introduced as a driver for innovation.
- **Session 6:** Covered sustainability-driven innovation, including Safe and Sustainable by Design (SSbD) materials, digital twins, and advanced coatings. Industry collaboration in sustainable material development was emphasized.

The workshop underscored the need for interdisciplinary collaboration, FAIR data practices, and AI integration in materials modelling and industrial ecosystems.

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SESSION 1: Next Generation Materials Modelling

The session started with the pertinent question of "**Can AI revolutionise materials discovery**?". It soon became clear that AI is not a materials modeller with knowledge but rather very dependent on data; data that is provided by materials modelling and characterisation, for example via the Materials Project[1] and the Open Quantum Materials Database.[2] Machine Learning (ML) and Artificial Intelligence (AI) require a sound appreciation of Independent and Identically Distributed (IID) variables, which refers to data where each sample is independent of the others and comes from the same underlying distribution. Conversely, one must consider Out-of-Distribution (OOD), which describes data where the test data is drawn from a different distribution than the training data. The idea is to generalise IID, for example to generate universal forcefield parameters. However, if materials scientists strive to discover novel materials, i.e., predicting the future by explaining the past, the generalisation of OOD needs to be tackled to generate new data. Data generated from science-based models will, for the foreseeable future, play an important role to generate data to train ML and AI, and to verify and validate them.

With all the advances, are we finally reaching the ability to design new materials on a computer? For decades each major new advance in modelling, be in DFT, linear scaling, or machine learning, made the promise. It remains doubtful whether purely computational advances, be it AI or quantum computing will finally predict a viable, novel material. In contrast, a "Materials Modelling 2.0" should return to utilising modelling to gain insight and understanding, am approach that has led to breakthrough materials. Materials Modelling 2.0 should synergise with characterisation, human materials modelling translators, ML, AI, etc. and aid with what is needed to advance materials and address specific challenges.

For typical modelling projects that involve a complex challenge which requires fine-tuning of numerous parameters and/or disparate length scales are too disparate. Modellers are confronted with the question whether **physics-based vs data-driven modelling** The modellers will still have to think about a multiscale workflow to describe the physics of their system correctly; however, computational efforts must be considered and if they are too time consuming or not feasible at all, it is time to think about data-driven modelling. Hence, data-driven modelling is still based on input from physics-based models or characterisation data and firmly rooted in physics.

Likewise, current EU projects[3] require a close collaboration between characterisation and modelling experts and offer a unique sandbox to get to know each other. Communication, as always, is key, and a common language must be found to convey each other's results.

Another pertinent question explored in the workshop was what currently drives the relation between software provider SMEs[4] and their customers. In the 1990ies early adopters wanted to know if materials modelling can help them at all, while nowadays they might consider if it can replace their experiments fully. SMEs will consult their customers about areas of research where indeed this is possible and why. This sensible approach accompanied with validation and verification did create many that have confidence in modelling and are ready to embark on the next generation materials modelling.

[1] https://next-gen.materialsproject.org/about
[2] https://oqmd.org/
[3] https://emmc.eu/emmc-related-initiatives/
[4] https://emmc.eu/members/

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SESSION 2: Driving Innovation and Sustainability in Advanced Materials

This session explored the combined role of materials characterisation, modelling, and data ecosystems in fostering innovation and sustainability within the materials industry. Both industry leaders and research projects demonstrated how advanced characterisation methods and computational modelling are essential for developing sustainable materials and enhancing the resilience of European industry in line with the European Clean/Green Deal's goals.

For example, implementing **advanced and sustainable composite materials in motorsport** is not an easy task. Besides these novel materials performing as good and save as the conventional materials, their whole lifecycle is expected to be perfect and in alignment with regulations. Reinforced bio-based resins seem of great interest, as they perform as well as standard resins. Also recycled composites are of interest; not only do they help to reduce the carbon footprint, they further require the need for specialist recycling facilities, and thus generate new ways of employment. Motorsport needs to be safe, hence testing of materials is pertinent; for example, the bonding strength between a composite and the aluminium frame of the chassis is of importance. Computer aided engineering is used to virtually design a car and materials characterisation provides experimental data. The latter are captured in a so called cobotic cell.[5] Ultimately, all the data are used to generate a digital twin of a particular component and testing new materials digitally will reduce testing and saves several 100k of Euros. It is expected, that the development of sustainable materials will go together with the development of combined materials characterisation, modelling, and data ecosystems, and thus, will drive the digitalisation process.

Characterisation and modelling are finding their place in developing **next-generation power devices** and shedding light on degradation processes that may occur in these materials. Complex processes demand an adaptation of characterisation techniques and the use of synchrotrons (see also below). The characterisation experiments serve as pointers to what may happen in the material, and reveal the physics needed for selecting the most suitable materials model for elucidation of the underlying degradation processes. It becomes clear, that interoperability between characterisation and modelling data is key and both MODA and CHADA[6] are valuable tools to describe workflows, i.e., the data acquisition process.

Synchrotrons are an important infrastructure when it comes to materials characterisation and are important to the characterisation of semiconductors, for example. Industry will demand more advanced methods for in-operando measurements, democratisation, service provision and available beam time.

Also, the **aerospace industry** is harnessing AI to further the development of new composite materials. The challenge here is to estimate from coupon testing the properties of an actual component, and a combination of materials modelling, characterisation and AI are expected to address this challenge. While developing workflows, finite element methods have been improved to better model how composites behave under fatigue. Especially for the aerospace industry, data management is important, as engineers would like to be able to go back and see, where data originate from.

Amongst all the advanced characterisation and modelling, we must not forget about **data ecosystems** and the importance of data sharing and knowledge transfer; the Horizon Europe projects

[5] A cobotic cell is a specialised workstation that integrates one or more collaborative robots (cobots) with other equipment and systems to perform automated tasks within a defined workspace.
[6] https://emmc.eu/moda-chada/ - Moda Chada

MatCHMaker[7], AddMorePower,[8] AID4GREENEST,[9] CoBRAIN,[10] KNOWSKITE-X[11] and D-STANDART[12] came together in Vienna before and during the EMMC 2025 workshop to provide their approaches to, and issues with each of the stages of the data lifecycle. The projects, besides developing knowledge platforms and tools, will in due course provide a separate report[13] and elaborate on how to bring standardised data lifecycles into the world of materials modelling and characterisation.

SESSION 3: Interoperability and data sharing across boundaries

In Japan, we find with the **Materials DX Platform**[14] of the National Institute for Materials Science (NIMS) an initiative to leverage large datasets to spur new innovations in the development of materials. Besides literature data, also daily generated data from high quality laboratories are of interest. NIMS has developed a data structuring and collection system to ensure standardised data ingestion. The only thing that is public is the data structure; the data itself can be open or closed, in compliance with an organisation's policy. Users of the platform can train their ML/AI models even with confidential data. The platform enables that collected data become widely utilised.

France offers with **DIADEM**[15] a programme that accelerates materials discovery and together with the European synchrotron, ESRF, works on a project for high-throughput, smart and automated material characterisation. Within the DIADEM ecosystem, DIAMOND[16] provides a platform dedicated to materials modelling software and the processing of results using AI; additionally, data are available from both experiments and simulations. The ecosystem is enriched by NUMPEX[17], a software stack for exascale computing, needed to perform resource intensive calculations often inherent to materials modelling.

As can be deducted from both platforms, large datasets in a standardised form are needed, and **autonomous labs** can aid with producing them. Robots can work 24/7 and continuously explore and probe materials. As many data sources are continuously producing, the data handling will have to be automatised as well. Such scenarios invite the creation of a digital twin, as the corresponding physical twin can dynamically deliver life data.

The last part of this session covered **ontology-driven digitalisation** of laboratory research in materials science. The aim here is to make data available to other persons or computers, which can only be done sensibly if these data are FAIR. One also needs to control their vocabulary and collect terms and uniquely define them. Then concepts shall be organised hierarchically to formally represent domain knowledge. This requires knowledge engineers and domain experts working closely together. It is wise to choose an Electronic Lab Notebook (ELN) that can assist with the data ingestion and by using semantics already at that stage, FAIR data practises are put in place. The **use of ontologies** is advanced

[7] https://cordis.europa.eu/project/id/101091687
[8] https://cordis.europa.eu/project/id/101091621
[9] https://cordis.europa.eu/project/id/101091912
[10] https://cordis.europa.eu/project/id/101092211
[11] https://cordis.europa.eu/project/id/101091534
[12] https://cordis.europa.eu/project/id/101091409
[13] To be distributed via EMMC's dissemination channels.
[14] https://www.nims.go.jp/rnfs/en/materials-data-platform/
[15] https://www.pepr-diadem.fr/en/
[16] https://diamond-diadem.github.io/en/
[17] https://numpex.org/

by both the German Initiatives Platform MaterialDigital (PMD)[18] and NFDI-MatWerk,[19] respectively. This comprises the PMD Core Ontology (PMDco),[20] which is a comprehensive framework for representing knowledge that encompasses fundamental concepts from the domains of materials science and engineering (MSE), and the MatWerk ontology,[21] which represents research data and related activities of the MSE community. Both ontologies are developed collaboratively and members of the MSE community are welcome to contribute. EMMC's very own ontology, the Elementary Multiperspective Material Ontology (**EMMO**),[22] underwent its 1.0.0 release. EMMO supports a knowledge framework consistent with scientific principles and methodologies. EMMO 1.0.0 achieves complete multiscale representational capabilities relating all entities from elementary particles to continuum and includes physical models such as Schrödinger and classical electrodynamics. The development team meets on a weekly basis and offers dedicated slots to everyone who would like some help with developing their own EMMO-based ontology.

INTERLUDE: A European State's and the EU's perspective on Materials Commons and Advanced Materials for Industrial Leadership

Two talks provided insight on how both Austria and the EU work towards the Materials Commons and advancing materials, respectively. The Republic of Austria offers primarily national funding and supports calls in the fields of energy, environment, mobility, and technology-oriented areas such as space. Further, digital and key-enabling technologies and circular economy are covered. The expectations for deploying digital technologies are more resource efficiency, automation, and flexibility of the manufacturing process. Austria harbours a range of research and technology organisations (RTOs), industry and universities who are already or looking into using digital technologies for advancing materials such as ML and AI. The Austrians cooperate or are involved with several European organisations such as AMI2030,[23] EuMaT,[24] EMIRI,[25] SusChem,[26] Manufuture,[27] and IAM-I (Innovative Advanced Materials Initiative). [28] They are also very supportive of a Materials Commons as they are of the opinion that international collaborations and knowledge sharing are key for advancing materials. The key elements a Materials Commons should have, are a federated data ecosystem with trusted management and access control, access to workflows, software and tools, a marketplace, and an integration of Safe and Sustainable by Design (SSbD), Life Cycle Analysis (LCA) and digital product passports.

In a European context, Austria has been leading the design phase of an Important Project of Common European Interest (IPCEI) on Circular Advanced Materials for the application fields mobility, energy, and electronics. The objectives of this IPCEI are:

- Circularity, recyclability, and manufacturability
- Integration of circularity across the entire value chain and innovation cycle

[18] https://www.materialdigital.de/
[19] https://nfdi-matwerk.de/
[20] https://materialdigital.github.io/core-ontology/
[21] https://nfdi-matwerk.pages.rwth-aachen.de/ta-oms/mwo/docs/index.html
[22] https://emmo-repo.github.io/
[23] https://www.ami2030.eu/
[24] https://www.eumat.eu/en
[25] https://emiri.eu/
[26] https://suschem.org/
[27] https://manufuture.org/manufacturing-potentiality-and-strategies/
[28] https://www.iam-i.eu/

- Reduction of EU dependencies
- Data continuity and development of digital tools
- SSbD and scale-up
- Performance orientation

The European Union wants for its members to invent services and products, deliver and manufacture, and market in Europe. Therefore, the EU is providing frameworks to make this happen,[29] i.e., accelerate advanced materials R&D, scale up innovations and step up production. Advanced materials are the key enabler for the Green/Clean Deal and the digital transition across sectors. Hence, the EMMC community is right at the epicentre to deliver. EMMC is a member of the IAM-I[28] and will contribute to secure and strengthen European technology sovereignty. Of great importance will be the Materials Commons, expected to become the European Digital Infrastructure for advanced materials R&I. Its objectives are:

- To pioneer a federated infrastructure for advanced materials R&D
- FAIR data sources and software tools
- Support the workflows for the design and development of advanced materials
- Inclusion of self-driving labs
- To create use cases to facilitate industrial uptake
- Longterm sustainability and adaptability to future use cases/industrial needs.

SESSION 4: AI driven software and digital infrastructures design and performance

Materials modelling for advanced materials happens often **across different scales** and requires **different tools**. For example, one would like to model a fluid, but may also be interested in the behaviour of a single droplet. The fluid is well catered for by Computational Fluid Dynamics (CFD), while the motion of a particle is best resolved with a Discrete Element Method (DEM). The modeller requires a solid understanding of the underlying physics and how these methods can be coupled to a seamless workflow. Once this is mastered one has a rather time-consuming workflows and may want to speed them up. This is where ML (and data science) is brought in and a set of reliable data is used to predict parameters rather than calculate them lengthy from scratch. Another way can be to use reduced order modelling whereby the complexity of a full-scale model can be reduced. Many people have been working on generating such multiscale workflows, produced data, etc. Thus, a solution could be to collate all that domain knowledge into platforms, such as engicloud, [30]and integrate community driven workflows. **Magnetic materials modelling** faces similar challenges. Both the chemical/physical structure (particle) and the intrinsic magnetic properties (continuum) are needed to deduct magnetic hysteresis properties. ML finds its place in calculating intrinsic magnetic properties and it feeds on both ab initio and experimental data. Reduced order modelling can be used to speed up the computation of the hysteresis properties.

Can one say now that **AI in Materials Modelling** is **A Game Changer?** For molecular dyamics calculations, interatomic potentials are needed, and they can be derived from density functional (DFT)

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[29] https://research-and-innovation.ec.europa.eu/document/download/0fcf06ea-c242-44a6-b2cb-daed39584996_en?filename=com_2024_98_1_en_act_part1.pdf
[30] https://www.engicloud.ai/

calcualtions. If ML is applied to do this process, we speak of machine-learned potentials (MLPs). However, this means also that MLPs inherit all the negative aspects which DFT has. For example, a vanadium rutile structure can be described correctly as metallic with a simple DFT calculation while the insulating monoclinic structure is falsely described as metallic, too. A more expensive DFT calculation will predict both structures correctly but if one wants to develop an MLP, 1000s of such calculations are needed. The best route is to choose a medium expensive calculation, be aware of its shortcomings, and tailor the MLPs to specific problems.

SESSION 5: Adoption in Industrial Ecosystems

In the context of developing the Horizon Europe Strategic Plan 2025-2027,[31] the Commission has proposed a co-programmed public private partnership for Advanced Materials, called IM4EU and IAM-I is the association that will operate this partnership. The guiding principles are:

- Ensure EU leadership in advanced materials innovation
- Towards a more resilient, competitive, and sustainable Europe
- R&I properties are driven by industry needs and commonalities between industrial sectors
- Support of the full innovation cycle
- Awareness of the diversity Advanced Materials

IAM-I will establish seven working groups and they cover the materials innovation markets construction, electronics, energy, transport, and health as well as Resilient & circual value chains, AI, materials digitalisation and data management. Additionally, four task forces are installed to cover (i) education and workfource, (ii) standards and norms, (iii) infrastructures, support to SMEs and upscaling, and (iv) policies, funding and strategy. Stakeholders are invited to join IAM-I and contribute to both working groups and task forces, respectively. The most recent activities can be observed on their LinkedIn page.[32]

The industrial adoption of materials modelling and characterisation is seen as big enabler to accelerating the design, development, and production of advanced, save and sustainable chemicals and materials. The session showed that industrial organisations go **beyond basic models** and have quite **strategic approaches to industrial materials modelling**. At the centre of their consideration stands their business imperative, i.e., what problems do they need to solve and what tools do they have. It is sensible to analyse the dis/advantages of experiments, mathematical models, physics-based models, and data-driven models. Especially the latter are of interest as data-driven modelling promises fast results. Industry realised one needs large data sets to fully exploit this type of modelling and that those need to be available FAIR. This is rarely the case so it will be important to promote data sharing and creating a federated FAIR company-wide data base. Hence, so far ML and IA are somewhat limited to smaller data-sets. Of interest are also hybrid models, i.e., a combination of physics-based and data-driven modelling. **Multiscale modelling** is still an important **industrial perspective** but one realises that ML finds its way into such workflows. Especially, when it comes to screening large databases for promising candidates for R&D, ML is producing faster results over traditional screening methods. Industry also keeps their eye on quantum computing which is expected to have a great impact when it comes to electronic modelling. There are certain areas where the current DFT calculations are too expensive; quantum computing may be important when it comes to investigate phenomena such as excited states, large strongly correlated systems, and quantum dynamics. A big driver for adopting

[31] https://ec.europa.eu/commission/presscorner/detail/en/ip_24_1572
[32] https://www.linkedin.com/company/iam-i/

materials modelling in industry is the **green transformation**. Organisations are keen to be transparent about their carbon footprint towards their customer and work with digital threads to follow a material from cradle to gate.

Modelling in Industry Fishbowl Conversation[33]

Not only the materials and materials manufacturing industries have to be involved but also system integrators who are using these advanced materials to ensure research, development and innovation goes in the right direction from the start. Different stakeholders need to learn how to trust each other as the development of advanced materials will need to involve stakeholders beyond an organisation. It will involve external talent such as academics and external services such as modelling, characterisation, and data engineering. Involving data and data-based modelling should be happening stepwise; one needs to know that data is available and its location, that new vital knowledge can be gained, and subsequently, one then finds a way to make this happen. The community may want to commonly shape the perfect data landscape which can be used for ML and AI tools to harvest knowledge. As many domain experts and policy makers will take part on this journey towards advanced materials, the deployment of facilitators and translators will be necessary to enable a *lingua franca* between all relevant stakeholders. Data require repositories and ideally these should be accessible to the whole community; for example, the electronic modelling community can deposit their data in the NOMAD[34] data base, but for other methods the modellers still struggle to find a common place. Data curation will be key to avoid swamping repositories with data as AI may lose its capability to find a signal in all that noise. It is noticeable that the materials community is already discussing many of these aspects concerning data. One should emphasise that FAIR does not mean open, and also it is possible share rich metadata about FAIR data, hence not exposing the actual data. This will be important for a common infrastructure which is covering academic open data as well as industrial IP data. The stakeholders working with SSbD encountered the issue of “sustainable raw materials and where to find them?”, and once they are found, who can source them? The Materials Commons will have to consider matchmaking activities which reach further ahead.

SESSION 6: Sustainability as innovation driver for a zero-pollution and climate-neutral future

Advanced materials ideally should be **safe and sustainable by design** so for the materials community some new characterisation and modelling methods will be added to their arsenal. One must assure that these new and advanced materials are non-toxic and do not harm humans, any other lifeforms, and the environment. Characterisation often happens in vivo and may require testing on animals, life tissue, or cells. Instead of a chemical search space, a biological search space is investigated and one wants to discover which materials are most likely non-toxic. Hereby, cells are exposed to the materials and then stained with dye (cell painting assay). Images are taken and one can then extract morphological profiles and cluster the substances according to their bioactivity properties. The materials community is quite familiar with QSAR, where one creates a training set with molecular structural properties (or descriptors) and relates them to an activity. In case of the SSbD community, this would be toxicity as obtained from the assay described above. AI can help here to relate molecular properties to the cell painting profiles, and finally, can predict from a profile whether the materials are

[33] A fishbowl conversation is a structured group discussion technique where a small inner circle of participants "in the fishbowl" discuss a topic while a larger outer circle observes and listens. See: https://en.wikipedia.org/wiki/Fishbowl_(conversation)
[34] https://nomad-lab.eu/nomad-lab/index.html

toxic or not. The **coating industry** does not only want to achieve SSbD but also use less critical raw materials, be long lasting and protect a material from corrosion. The underlying modelling workflows are multiscale and profit from data-based modelling to save computational time. As the modelling work is demanding, it should ideally happen on materials expected to be SSbD. This requires a close collaboration between domain experts who assess the hazards chemicals can pose to the workforce during the whole manufacturing process.

Finally, we are looking into the **needs of industry and innovators** when it comes to SSbD, as they should investigate the functionality of an advanced material and simultaneously if it is safe and sustainable. Some EU projects such as PINK[35] are developing innovation platforms which will enable this rather complex demand. The process of creating an advanced material goes over several stages and can undergo modification and optimisation as required. Hence, one will have to consider what was safe and sustainable to start with, still is. It is sensible to align the safety-sustainability dimension with the functionality but also the economic viability. Creating an advanced materials following SSbD is an iterative way; phases of working on the material need to go hand in hand with assessment phases, where one can check if they are still on the right path. Multi objective optimisation procedures can be helpful with this. Innovation platforms will have to run behind organisations' firewalls, as they may want to work with their own data and knowledge first, before adding 3rd parties.

SSbD Discussion Summary

It is important, that SSbD advanced materials must balance improved performance in their respective applications with economic, environmental, and social sustainability. Another layer of added complexity comes from the fact that all sustainability aspects need to not only be considered at the chemical/materials level but also at the component and overall integrated systems level. This will require the sharing of data/knowledge (collective intelligence) and requires federated FAIR data bases which are very work intensive and expensive to create. This can only be done with several partners working together and jointly financing such effort. Naturally, industry is competitive; hence, one needs to find pre-competitive synergies and cooperation opportunities. Catena X[36] is an example for a successful data-ecosystem, driven by the automotive industry.

There are many historical and current data stored in a variety of formats, often in silos. Before one consolidates this data, it will be necessary to understand what their quality and usefulness is, as that will determine the quality of knowledge one gains. Also, one must consider appropriate ML/AI solutions which uncover useful knowledge.

SSbD will require collaboration of different domain experts; for example, a materials engineer is trained to focus on the technical performance of a material in the early stage of R&D but never trained in SSdD. If the engineers however could feed their expertise into a digital twin, an SSbD expert could bring their expertise in before any costly prototypes have been produced. Hence, the usage of modern digital tools will be pertinent.

[35] https://pink-project.eu/
[36] https://catena-x.net/