

ORIENT- NM

<u>Organi</u>sation of the <u>European</u> Research Communi<u>ty</u> on <u>N</u>uclear <u>M</u>aterials

A Coordination and Support Action in Preparation of a Co-Funded European Partnership on Nuclear Materials



This project has received funding from the Euratom research and training programme 2019/2020 under grant agreement No. 899997

Start date of project Duration Reporting period 01/10/2020 30 months

2 - 01/04/2022 - 31/03/2023

Work Package 4 – Interaction with other bodies, initiatives and stake-holders, including infrastructures

Deliverable D4.11: Draft report on synergies with nonnuclear energy technologies

Author(s) r affiliation	name and	(1) Lorenzo MalerbaCIEMAT(2) Angelika BohnstedtKIT			
Date of issue	e	16/03/2022			
Date of final	approval	29/03/2022			
Disseminatio	Dissemination Level				
PU	Public		Х		
CO	Confidenti FC	al, only for partners of the ORIENT-NM Action and the			

Version Date Description





Disclaimer

This project has received funding from the Euratom research and training programme 2019/2020 under grant agreement No. 899997.

The information contained in this document has been prepared solely for the purpose of providing information about the ORIENT-NM project. The document reflects only the ORIENT-NM consortium's view and the European Commission is not responsible for any use that may be made of the information it contains.

While this publication has been prepared with care, the authors and their employers provide no warranty with regards to the content and shall not be liable for any direct, incidental or consequential damages that may result from the use of the information or the data contained therein. Reproduction is authorised providing the material is unabridged and the source is acknowledged.

Table of contents

Disclaimer
Table of contents
List of abbreviations5
Summary6
Introduction7
The EM4I initiative9
The main outcomes of the EM4I workshops10
Materials Discovery & Development: 10
From Lab to Engineering: materials manufacturing and industrial upscaling:10
Approaches for the implementation of Digital Twins:
Sustainability Assessment of materials and technologies for a clean energy transition:
Energy Materials for Harsh Operating Conditions12
The main outcome of the final EM4I workshop: the future of energy materials 13
Concluding remarks and caveats 17
Appendix I: programme and minutes of the workshop on energy materials for harsh operating conditions
Appendix II: programme and extended summary of the final workshop on the future of energy materials





List of abbreviations

Summary

The goal of this deliverable is to identify possible synergies in terms of research between materials for nuclear applications and materials of application in other low-carbon, non-nuclear energy technologies, with mutual benefit. For this purpose, three EERA JPs (AMPEA, DfE and NM) have launched the EM4I initiative (Energy Materials for Innovation): a series of five technical workshops that were held online in 2021/22, each dedicated to materials science topics that were perceived as cross-cutting through different applications, with the involvement of other EERA JPs, as well.

This series of workshops was followed by a final meeting that provided an overview on the previously touched topics, blended with policy and implementation issues. This meeting was organised with the participation of the community of the Advanced Materials Initiative 2030 (<u>https://www.ami2030.eu/</u>), particularly of EMIRI, the Energy Materials Industrial Research Initiative (<u>https://emiri.eu/</u>). It took place on 13-14 March, 2023, also online.

The main outcomes of the workshops are here reported and analysed, with special emphasis on the workshop on energy materials for harsh operating conditions, which was deemed to be the most relevant for nuclear materials, and on the final workshop.

Conclusions are eventually drawn on the commonalities between nuclear and nonnuclear energy materials research. In addition, lessons learnt of value for the partnership on nuclear materials and possible open ways of collaboration with the non-nuclear community are highlighted, together with some reflections on the caveats connected with the modern materials science approaches that are being currently pushed forwards, especially thinking of nuclear energy applications.





Introduction

The goal of this deliverable is to identify possible synergies in terms of research between materials for nuclear applications and materials of application in other low-carbon, nonnuclear energy technologies, with mutual benefit. This goal has twofold implications. On the one hand, it serves the purpose of understanding to which extent research done on materials in the nuclear field may be of use for other applications, thereby providing additional motivation to support it, even for countries that have no specific interest in nuclear energy. On the other, it provides grounds to imagine that research on nuclear materials may also be part of a wider European programme dedicated to energy materials at large, in which some materials research activities may be beneficial both for nuclear and non-nuclear energy technologies. Strictly speaking, the latter makes sense only provided that suitable instruments for the funding of transversal research programmes between Euratom and the EU functioning treaty exist, which is not the case at the moment, as far as the ORIENT-NM community is aware. However, it is expected that beneficial interactions and (formal or informal) collaborations may be set up by identifying the non-nuclear communities that work on materials issues adjacent or overlapping with corresponding nuclear materials activities.

EERA, the European Energy Research Alliance, is the ideal framework to look for synergies between nuclear and other, non-nuclear, low-carbon energy technologies. Through its joint programmes (JPs), EERA includes experts in all these technologies, from solar to hydropower, from wind to geothermal, from bioenergy to ocean energy. In addition, one EERA JP is specifically dedicated to Advanced Materials Processes for Energy Applications (AMPEA). The transversal JP (tJP) on Digitalization for Energy (DfE) is also of relevance, because the most recent materials science approaches rely heavily on modern digital techniques, such as high performance computing, artificial intelligence (AI), big data and data analytics, blockchain, sensoring, digital twins, 3D visualisation, robotics, and so on. Promoting materials science research as such is important for both the nuclear and non-nuclear community because, in the Horizon Europe (HEU) work-programme, this discipline has been somehow "forgotten", either hidden behind more general circularity aspects, or related to specific energy applications, batteries in particular. Cross-cutting and methodological aspects have been largely forgotten. In contrast, in the framework of Mission Innovation specific attention has been devoted to materials for energy as such, specifically to the concept of materials acceleration platforms (http://mission-innovation.net/our-work/innovationchallenges/clean-energy-materials/; http://mission-innovation.net/platform/materials-forenergy-m4e/). However, Mission Innovation has no connection with Horizon Europe and concerns only a small subset of the EU member states.

In this endeavour, JP AMPEA and tJP DfE have been the obvious interlocutors for the JP on nuclear materials (JPNM) to set up a dialogue on these topics, also because of their inherent transversal nature. These three JPs agreed therefore in spring 2021 on the opportunity of organizing a series of technical workshops, each dedicated to materials science topics that were perceived as cross-cutting through different

applications, with the involvement of other JPs, as well. This initiative was baptized "Energy Materials for Innovation", EM4I.

The series of five online workshops, organised between July 2021 and April 2022, was highly successful, with the participation of, on average, about 50-60 attendants.

Interestingly, while EM4I was progressing, the involved EERA community came across the <u>Advanced Materials 2030 Manifesto</u>, which, signed by 7 authoritative persons, representing 7 institutions that range from research to industry, also answers the same need, i.e., to promote advanced materials science and applications as important in themselves on the EU research funding arena.

Importantly, materials in this Manifesto cover an extremely wide spectrum of applications, not only energy: nine "materials markets" are identified (healthcare, construction, energy, transport, home & personal care, packaging, agriculture, textiles, electronics). However, the philosophy remains the same; i.e., the approaches are cross-cutting through all material classes and applications. Here are some **excerpts of the Manifesto** that, as will be seen, are largely consistent with the outcome of the EM4I initiative and also with the vision and strategic agenda of ORIENT-NM (see deliverables D2.5 Vision Paper and D2.6 SRA, http://www.eera-jpnm.eu/orient-nm/):

- "Europe must maximise the sustainability features of new advanced materials and their visibility using advanced digital technologies."
- "High performance computing, big data and AI revolutionise the digital modelling, simulation and screening of materials properties, materials development and production processes."
- "Sustainable advanced materials are a key driver for innovation, creating new opportunities on multiple dimensions and sectors."
- "We call for a systemic approach to develop the next generation solution-oriented advanced materials which will offer faster, scalable and efficient responses to the challenges and thus turn them into opportunities for Europe's society, economy and environment."
- "We recognize that "Blue sky research" and applied research both play an integral part in this approach."
- "Critical to R&I is discovery-led research, as ultimately it feeds directly or indirectly into end-user applications and industry. In short, there is no applied research without fundamental research in the long-run."
- "It is critical for Europe to create a world-wide unique ecosystem that connects discovery-led low TRL research with application-orientation and links it synergistically with industry, including small and medium sized enterprises."
- "All 27 Member States should contribute to the efforts towards levelling up advanced materials development."

The series of EM4I workshops was therefore followed by a higher level strategy meeting, in which the various cross-cutting materials science research approaches were





overviewed, blended with aspects that concern policies and implementation, as well. This final meeting was organised on 13-14 March, 2023, with the participation of the community linked to the above Manifesto, called the Advanced Materials Initiative 2030 (https://www.ami2030.eu/). Because of the prominence given in EERA to energy applications, it was especially EMIRI, the Energy Materials Industrial Research Initiative (https://emiri.eu/), to be involved in this final meeting.

In this report, details about the EM4I initiative and the outcomes of the workshops are given. Important outcomes stemmed in particular from the final workshop. Conclusions are eventually drawn on the commonalities between nuclear and non-nuclear energy materials research. In addition, lessons learnt of value for the partnership on nuclear materials and possible open ways of collaboration with the non-nuclear community are highlighted, together with some reflections on the caveats connected with the modern materials science approaches that are being currently pushed forwards, especially thinking of nuclear energy applications, which are put forward in the conclusive remarks.

The EM4I initiative

The objectives of the EM4I initiative were set to be:

- To identify materials research topics that are shared by several energy technologies (cross-cutting issues).
- To provide a snapshot of the landscape concerning research activities and needs in Europe concerning Energy Materials, including and especially beyond the priorities identified so far in HEU.
- To highlight towards key stakeholders the importance of fundamental materials science in the future energy research roadmap for achieving the Clean Energy Transition (CET) and bring Materials Science at the forefront of EU research priorities.
- To contribute to EERA's objective to become an advisor to European Commission (EC) and Member States (MS).

This was done in two steps:

- The two former objectives were mainly pursued through a series of focused online technical workshops on topics that are expected to be cross-cutting, over the year 2021-2022:
 - Materials Discovery & Development July 1st, 2021
 - From Lab to Engineering: materials manufacturing and industrial upscaling -October 4-5-6, 2021
 - Approaches for the implementation of Digital Twins December 21st, 2021
 - Sustainability Assessment of materials and technologies for a clean energy transition - February 25th, 2022
 - Energy Materials for Harsh Operating Conditions: April 7-8, 2022

• The two latter objectives were mainly connected with the final meeting: The Future of Energy Materials, organized on 13-14 March, 2023, by EERA, with the participation of AMI2030.

The main outcomes of the EM4I workshops

The main outcomes of the series of five workshops can be so summarized:

Materials Discovery & Development:

- The need for fast & efficient energy materials development is quickly transforming the way we practice materials research.
- Accelerated materials & technology development require a systemic, cross-cutting approach taking into account the whole value chain, from basic research to scale-up production, market acceptance, cost performance and durability.
- High throughput materials design (discovery & screening) has seen a great success owing to the development of numerical tools (e.g., artificial intelligence/machine learning – AI/ML).
- Large sets of experimental data on material properties (including microstructure, insitu/operando) must be made available.
- High-throughput approaches (e.g., combinatorial characterization, miniaturized samples) are effective.
- Continuous feedback loop between real-data and simulations is the key.
- Once the TRL 5/6 is achieved, the issues hindering the materials exploitation are no longer technical, but mainly socio-economic.

From Lab to Engineering: materials manufacturing and industrial upscaling:

- The workshop addressed the strategy from science to product and analysed case studies
- The following technology areas were covered: batteries, nanotubes, thermoelectric materials, fossil-free steel production, electromechanical components....
- Keys for success in "Lab to engineering products":
 - Scientists should have entrepreneurial mind-set beyond science: making money or improve society;
 - Multidisciplinary teams are needed: science, business + others, e.g., communication;
 - Partnerships should include the whole range of relevant ingredients: public and private R&D actors - academia, laboratories, industry, finance
 - Matching technology: the final market and its implications should be taken into account from the beginning of materials development ("design and control", or "safe-and-sustainable by design" paradigms):
 - Technology challenges: product/application/innovation, upscaling
 - Market challenges: customer, economy, need





- Market vs Technology: uncertainty must be addressed
- Challenge: Reduce time from lab to commercial product from 20 to 2 years
 o Apply above "Keys for success";
 - Use digital tools (AI etc.) and reduce testing needs;
 - Regulation & politics can help or block
 - Don't overdo science, bring to market at reasonable TRL based on marketfeedback

Approaches for the implementation of Digital Twins:

- Digital platforms successfully simulate the operation of non-destructive examination, even in harsh conditions, joining physics-based and data-driven modelling with nondestructive testing and AI capabilities.
- Augmentation of data for a correct training of neural networks offers a valuable line of research and development.
- Decision-making capabilities can be integrated in monitoring schemes, as well, providing valid assessments about predictive maintenance, precision, repeatability, and efficiency.
- New possibilities are offered by joining non-destructive testing and sensor intelligence.
- Data-driven workflows integrating physics-based simulations and AI can simulate materials phenomena in a holistic way.
- Digital twins are being developed as a service provider in the industry, in which the ontologies that are defined are key for a valid reproduction of the real asset and the avoidance of malfunctions.
- Digital twins also rely on an accurate provision of input data from sensors and a proper sensor data quality control.
- The combination of physics-based and data-based digital twins are obtaining excellent results nowadays.

Sustainability Assessment of materials and technologies for a clean energy transition:

The aim of this workshop was to evaluate Sustainability Assessment methods and tools for the reduction of economic, environmental and social impacts of the clean energy transition, focusing on critical materials. Four topics were addressed, followed by a Round Table: (i) Tools for Sustainability Assessment and case studies; (ii) Sustainable Manufacturing; (iii) Critical Raw Materials (CRM); (iv) Nanomaterials, safe-and-sustainable-by design.

Outcomes

- Importance of **interdisciplinary competence** for reliable use of sustainability assessment tools; there is a **lack** of industrial qualification and industrial operators for sustainability assessment; cooperation between academy and industry needs to be pushed.
- Several tools **are available** with different capabilities and level of difficulties, but there is not yet an exchangeable standard format that could increase collaboration among different players.
- There is a **need** for flexible/intelligent tools for (early-stage) evaluation of sustainability issues, including circularity.
- Life-Cycle and Safety Assessment (LCSA) interpretation is questionable: we still **need to understand** how it can contribute to the **decision-making approach**.
- Need for **reliable data** (general usefulness) **and customised data** (national, regional for specific scopes).
- Sustainable innovation needs to integrate safety (Risk Assessment, RA) and sustainability (LCSA) into a unified concept;
- New approach for sustainability assessment of materials, processes and products is the way for going beyond uncertainties and lack of transparency;
- Value Chain approach for sustainability of CRM. Need to involve all the stakeholders of value chains. Increase circular use of CRM by End of Life and full LCSA methodologies.

Energy Materials for Harsh Operating Conditions

This workshop was especially important in connection with nuclear materials, which are part of the wider family of materials operating under extreme conditions. For this reason, the programme and the minutes of this workshop are given in Appendix I.

- Eminent need: safely increase lifetime of components and efficiency of systems. This implies: need to have capabilities to test and qualify materials; need to have capabilities to suitably manufacture materials in a scalable way, with flexibility in terms of composition for the target application (critical materials); need to have capabilities to accelerate materials discovery and development including all variables; need to have capabilities to continuously monitor materials performance and anticipate degradation and subsequent failure; need for models at all stages, from production to use; need to have sufficient and qualified data.
- Corrosion (partly erosion and wear too) are clearly the most common problem in terms of harsh conditions through several applications and energy technologies: nuclear, geothermal, bioenergy, thermal solar, energy storage under various forms
- Environments are very different, but, eventually, the solutions are similar: passivation and coatings. FeCrAl is clearly a cross-cutting material (though not for electrolysers). Other common materials are: high Cr stainless steels and Ni-base alloys (partly also austenitic steels, but less). Protective coatings are almost ubiquitous, of various types but mainly Al- or Co-oxides. Coatings are also used for other aims than corrosion protection (e.g. thermally driven adsorption machines).





- Corrosion resistance needs however to be accompanied by other properties, e.g., typically good mechanical properties.
- High temperature is another limiting factor, but what is high temperature changes significantly from application to application: from 100°C to 1000°C can be considered high temperature depending on the technological environment. Temperature limits, among others, the possibility of continuous structural materials health, because sensors fail at high temperature. However, that main effect of not being able to increase temperature because of limited resistance of materials, often to corrosion, is that this imposes a limit to high energy efficiency.
- The Materials Acceleration Platform (MAP) that is dedicated to discovering corrosionresistant materials, which is being developed in the framework of the German-Canadian cooperation, will certainly have work to do. It would be desirable that wider participation and more extended collaboration could be focused on this goal, perhaps to include the discovery of materials with good mechanical properties at high temperature.

The main outcome of the final EM4I workshop: the future of energy materials

The programme and the extended summary of this workshop are given in Appendix II. Here the essence is extracted, together with specific thoughts and analyses of use for the CEP on NM.

This final workshop, combined with the previous ones, very clearly highlighted that, with total independence of the technology (or market) of final application, **modern materials science is based on a unique paradigm**, which can be expressed in terms of two objectives (whether fully achievable or not remains of course to be seen, but these are the guiding principles):

Materials should be designed from the start in view not only of their final application, but also maximizing their sustainability in terms of: (1) replacement of critical raw materials with less critical ones in their chemical composition; (2) full consideration of their possibility of second use after their first life.

The processes of materials discovery and development need to become significantly faster and more sustainable than now; manufacturing processes also need to become more sustainable and better controlled; in fact the whole material/component lifecycle, from fabrication to recycling or re-use through of course operation needs to be monitored to ensure functionality and made more sustainable.

The tools that enable these goals to be achieved are:

1. <u>High throughput</u> fabrication and characterization (mainly via fast <u>non-destructive</u> <u>examination and testing techniques</u>), as well as calculation (mainly of <u>ab initio</u> type),

to gather a large amount of data on the properties of several materials under several conditions. This should possibly be fully automated through robotics.

- <u>Data-driven modelling</u> based on the use of artificial intelligence/machine learning to analyse data, classify them in multi-dimensional phase spaces, find correlations between properties and use these correlations to provide a feedback and iteratively identify the best candidate materials for the final application. Also <u>advanced physical</u> <u>models</u> based on computer simulation, thus with the use of <u>high performance</u> <u>computing</u>, can be a crucial tool, especially if blended with data-driven models.
- 3. <u>Advanced manufacturing</u>, in particular additive manufacturing or other advanced methods that a priori enable full or at least significant control on materials composition and architecture, with minimal waste.
- Lifecycle sustainability assessment tools that provide criteria to identify the best research paths from the point of view of overall sustainability, taking into account all aspects, from raw materials to the manufacturing process and the decommissioning phase.
- 5. <u>Digital twins</u>, i.e. digital copies of materials and components, of their production and transportation phase, their behaviour in operation and thus evolution, and even their second life. Digital twins may make use of all kinds of models, empirical, semi-empirical, physical, and of course data-driven. To fully act as virtual replicas of the material/component they refer to, their predictions are continuously verified and adapted through sensors that make use of <u>non-destructive examination techniques</u> connected to the real material/component.

The tools 1 and 2 (and potentially also tools 3 and 4) can be combined, conceptually and physically, in <u>materials acceleration platforms</u>, i.e. self-driving autonomous materials laboratories featuring closed loop synthesis and characterization using robots, see Figure 1.

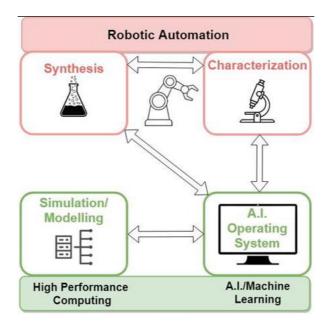






Figure 1. Schematic representation of how a MAP works (courtesy of M. Kozdras, <u>http://mission-innovation.net/platform/materials-for-energy-m4e/</u>, Mission Innovation, Materials for Energy)

The full exploitation of data-driven approaches requires that data are not only collected, but especially connected through fast networks that adopt, in order to appropriately search and classify new data, suitable <u>semantic technologies</u>. These are controlled vocabularies that enable the machine to identify what a human expression corresponds to and thus to look in the right place for relevant data and also to logically connect additional data, so as to extend the network. Techniques based on semantic technologies make it possible to think of virtual discovery centres that are physically delocalized, but functionally connected through appropriate data-exchanging networks.

The above objectives and enabling tools certainly apply to all energy materials, of which nuclear materials are a subset, but in fact they apply to materials for any application. The above "universal" objectives and methodologies make that any case study, which can be electrochemical storage or materials operating under harsh conditions, such as in nuclear applications, can be a good playground to develop and apply the above techniques, for the benefit of, a priori, any other material and technology, provided that cross-sectoral applicability is kept in mind. Thus the ground for collaboration between nuclear and non-nuclear energy applications as to materials definitely exists. If barriers to this exist, these are mainly the consequence of the "silo organisation" that, at political level, prevents actual collaboration (i.e. joint projects, or inter-project connection) between nuclear and non-nuclear materials topics.

Additional useful suggestions of use for the CEP on nuclear materials (as well as for many others) can be extracted from the workshop presentations:

- MAPs should be considered eminently as a research tool, which do not necessarily
 make use of the best manufacturing path for the material that is discovered, nor
 provides a full qualification or directly looks at commercialization aspects. However,
 through fast exploration of the configuration space, MAPs enable effective solutions
 to be found more quickly. Intellectual property management is a potential problem,
 but it is possible to think of an exploitation of the tool the result of which is proprietary,
 even if the platform itself is not.
- The indications on sustainability of given research paths obtained at low TRL using lifecycle assessment tools are affected by large uncertainties that come from the lack of information on the full technological details of the life cycle. The results can be different also depending on whether the focus is on the material, on the component or on the full device. It is sadly still difficult to make these tools actually useful for decision-making. Their use in connection with a MAP would put them under "further

stress", so it is not clear at the moment that sustainability variables can actually be included in the configuration space exploration.

- One of the programmes of the European Innovation Councils seeks for acceleration
 of innovation by considering inter-project interactions, i.e., by promoting clustering of
 projects, identifying emerging challenges and networking with other programmes.
 The EIC probably cannot provide support for nuclear materials, however it might
 advise through involvement in the innovation group of the CEP on nuclear materials.
 In addition, the practices of project clustering and networking can and should be
 applied also within the research lines of the partnership.
- The AMI2030 strategic agenda clearly indicated that advanced materials design, development and production is only the first step. Then comes the part of transformation (fabrication) and integration into components, products and systems, followed by operation and finally the end-of-life and the possible second life of the material/component. All along these steps, advanced digital technologies, as well as advanced manufacturing, processing and characterization technologies, are key, but equally important are also standardization, and accompanying regulatory and policy frameworks (Figure 2). At any rate, in an optic of industrial upscaling, while it is important to accelerate materials development, materials need to have "revolutionary performance, but evolutionary nature", in order not to require significant changes in the industrial production chain, thereby ensuring supply chain.

		RGIES TRANSPI	HOME A PERSONAL CA	PACKAGING		
The main segments materials circular va	of the advanced		E		AGRICULTURE	
	Advanced Materials design, development & production	10 m	characterization instrumentation,	<u>к</u> (;;		TEXTILES 9
	Advanced Materials transformation and integration into components, products & systems	Digital technologies for Materials (AIML, data mgt anoiogies, modeiling,)	≪ਰ ਦੁੱ	Regulatory and Policy s (Circularity, LCAs, SSbD		ELECTRONICS
	Use Phase	tologies f	processsing (tools, equipme	Standards, Regulatory Frameworks (Circularity,		
	End-of-Life	gital techr ML, data my	Production, F technologies automation,)	andards, ameworks		
2 Cross-sectional ena	ablers	NO.	ter Pr	B.H.		
3 The Materials Innov	ation Markets					

Figure 2. Schematic of the AMI2030 SRA (from F. Stassin, "Advanced Materials 2030 Initiative", presented at: <u>The Future of Energy Materials</u>, 13-14 March 2023).





- The problem of critical raw materials is very serious, because it will potentially create, if suitable measures are not taken or cannot be fully implemented, levels of dependency on one single country that are even higher than in the current case of fossil fuels. In addition, recycling can only solve part of the problem, and perhaps only a small part. Nuclear energy does not seem to be high in the ranking of technologies that are threatened by the supply of CRM, however it is an aspect that should be taken into account (it certainly affects fusion), which liaise with non-nuclear materials research.
- EMIRI developed technology sheets, on each of which experts identified and ranked the main technology challenges and defined quantitative targets to be reached overtime in each case. This, which complements and extends the idea of materials ID cards prepared in ORIENT-NM, is also an approach that could be attempted with all the various nuclear technologies.

Concluding remarks and caveats

The EM4I initiative has been successful in its objective to identify commonalities concerning materials research throughout energy technologies. The crucial conclusion, as amply described above, is that modern research approaches for the discovery, development, manufacturing and monitoring of materials are cross-cutting not only through several energy applications and technologies, but also well beyond energy applications. Thus nuclear materials research necessarily also shares several issues with all other applications, being especially close to the issues related with materials for harsh operating conditions. The common enablers of the paradigm shift in materials science are **modern digital techniques**: *in primis* artificial intelligence/machine learning, but also high performance computing, big data analytics, robotics, 3D printing High throughput techniques are also important in the framework of acceleration in materials research, in order to increase the number of data that can be collected per unit time: accelerated fabrication, characterization, and calculations. Finally, an important aspect is that innovation as such is promoted and accelerated through a multidisciplinary approach that includes not only science, but also business and communication, taking into account from the beginning the market trends and the customers' needs.

Taking all of the above into account, it turns out that <u>the research lines identified in the</u> <u>SRA of ORIENT-NM¹ are really on the same wavelength as those that are currently</u> <u>pursued for other, non-nuclear applications</u>. They are therefore very suitable to establish a seamless link with materials for non-nuclear energy technologies.

There are, however, some caveats that need to be taken into account in the specific case of nuclear energy.

1. Fast-track to qualification

¹ Namely Materials and Components' Qualification, Advanced Modelling and Characterisation, Materials and Component Health Monitoring, Advanced Fabrication Processes and Innovative Nuclear Materials, Data Management.

MAP-type approaches are in practice sophisticated and fast screening methods that propose especially promising possibilities for a given application. Later these possibilities need to be further tested and qualified in a more standard way, to verify their actual suitability for the expected purposes. If the expected purposes require exposure to harsh environment for long times, as is the case for nuclear materials, a truly useful MAP should include the capability of assessing long term materials performance from rapid measurements, carried out on the as-received material, or on materials exposed to conditions that are not representatives of those that are actually expected. Currently, this capability is more often than not unavailable and represents a major challenge.

In addition, in order for the selected material to be eventually usable for the fabrication of specific components, it has to be introduced in design codes, following the relevant instructions and recommendations. In the nuclear field, and perhaps also in other fields where extreme conditions are involved, the qualification of materials has a strong connection with safety. Thus, the testing and gualification plan for nuclear materials needs to comply with the requests, expectations and in essence the standards of the safety authorities. This is often the bottleneck where innovative materials for nuclear applications get stuck and this is the reason why the nuclear industry tends to be very conservative. Thus, accelerated nuclear materials' discovery is of little help without any gualification fast track. For full qualification, suitable facilities to expose the material to conditions of relevance are needed, and these include, in the specific case of nuclear materials, reactors for exposure to neutron irradiation. Acceleration in this case can only be achieved, at least in part, by defining safety-complying, standardized qualification paths and by pooling laboratories to ensure the coordinated and efficient use of facilities that should, altogether, cover exposure to all the conditions of interest: this is what has been called nuclear test-beds in the ORIENT-NM SRA. This part of the materials acceleration paradigm is, as it seems, not equally emphasised in the case of applications different from nuclear, even though it can be surmised that it does concern also other fields of application.

2. Graded approach to the acceleration of materials for nuclear

MAP-type approaches and ontologies for data-driven modelling are, in fact, strongly specialised tools. It is in general difficult to imagine that developments applied for specific classes of materials and technologies of applications can be extended to other materials and applications in a simple way. At the same time, it makes sense that a given MAP should be used for the widest range of applications possible. Given the above-described relative importance of materials qualification fast-tracks with respect to materials discovery acceleration in the case of nuclear applications, <u>the most affordable MAP option for the CEP on NM consists here in liaising with a project dedicated to harsh conditions in a non-nuclear framework, adding an extension to include, e.g., radiation <u>effects</u> (most likely using ions instead of neutrons for screening purposes). This is a winwin situation because, on the one side, the selected MAP-type approach is exploited beyond its original purposes and, on the other, re-inventing the wheel only for nuclear applications is avoided. A liaison with the corrosion-oriented MAP developed in Germany is, in this context, an excellent option, if it does not imply breaking any silo logic.</u>

3. Materials acceleration and supply chain

MAPs are inherently a research product. Even though additive manufacturing is a suitable technique for samples to be automatically produced in a MAP, the optimisation of advanced manufacturing as part of, e.g., industrial upscaling, does not necessarily enter the MAP design. As said in the previous section, it is also not obvious that the





optimisation of the overall life cycle sustainability can be addressed at MAP's level. On the other hand, MAPs are conceptually designed to be taking into account the problem of critical raw materials. They may also be tuned to obey the principle that materials need to be "revolutionary in performance, but evolutionary in type", in order to make industrial production easier. Thus, the optimisation of advanced manufacturing for industrial upscaling or repair purposes and aspects related with the supply chain, although conceptually decoupled from MAPs, can be put in the same pot, but only to some extent.

4. Big versus small data and data-driven versus physical modelling

Data-driven modelling based on artificial intelligence/machine learning implicitly calls for a series of conditions that data should comply with. Namely, data need to be of sufficiently high quality, fully consistent with each other, and, especially, abundant. In the nuclear field, however, especially because of the difficulty of getting data under irradiation, it is not so frequent that data are abundant. Moreover, without established practices for the microstructural characterisation, many valuable data that connect also with physical models are not necessarily consistent with each other, if they are coming from different laboratories (this certainly also outside the nuclear field). Under these conditions, the application of conventional data-driven techniques may become questionable. Data-driven techniques need to be made reliable also with a limited number of data. "Few-shot learning" is a field that clearly needs to be further developed for nuclear materials applications. These approaches rely on the appropriate use of few high, and many low, fidelity data, and in general call for the coupling of physical and data-driven models. Thus, blending data-driven and physical models, which is in fact a good idea for all applications, to avoid the "black-box" danger that is implicit in purely data-driven methods, is especially important in the case of nuclear materials.

Appendix I: programme and minutes of the workshop on energy materials for harsh operating conditions

The workshop dedicated to energy materials for harsh operating conditions was especially relevant for nuclear materials. It is therefore here reported in full detail. In red: statements that can be of interest for the CEP-NM. <u>Underlined:</u> <u>summarizing statements</u>.

Agenda:

7th April						
Worksho	Workshop Introduction					
13:00	L. Malerba, CIEMAT					
13:15	Adel El Gammal, EERA	N Contraction of the second seco				
Session	1: Chairs - L. Malerba, E	3. Tanguy				
13:30	F. Feyel, Safran Tech, France	Mastering high performance aerostructures by the help of models				
14:00	M. Kowal, NCBJ, Poland	Non-destructive testing of components used in a scientific reactor. Review of methods.				
14:30	G. Ribay, CEA, NDT and SHM of materials under harsh conditions used in Energy France Applications					
15:00	M. Frignani, Ansaldo Nucleare, Italy	Materials requirements and qualification strategy for the European lead-cooled fast reactor prototype: analysis of the challenges				
15:30	Break					
Session	2: Chairs - O. Suminska	-Ebersoldt, P. Pohjanne				
16:00	M. Kozdras, Canmet, Canada	Accelerated development of corrosion resistant materials				
16:30	G. Skulason Kaldal, ISOR, Iceland	Materials engineering for geothermal applications				
17:00	B. Acosta, JRC, The Netherlands	Hydrogen enhanced fatigue of compressed hydrogen storage vessels				
17:30	J. Mykkola, VTT, Finland	Protective Coatings for SOEC interconnects	REPLACED BY P. Pohjanne			
18:00	End first day					

8th Ap	8th April					
Sessio	Session 3: Chairs - S. Vasta, M. Roeb					
9:00	T. Jonsson, Chalmers, Sweden	Power-production from biomass - material development and corrosion prediction in harsh environments				
9:30	F. Sutter, DLR, Germany	Materials for harsh conditions in CSP				
10:00	G. Karagiannakis, Certh, Greece	Materials in harsh conditions for high temperature solar thermochemistry	Replaced by Christos Agrafiotis, DLR			
10:30	A. Freni, CNR-ICCOM, Italy	Durability of solid desiccant materials for HVAC systems				
11:00	L. Bonaccorsi, U. Reggio Calabria, Italy	Materials for thermal energy storage in harsh operating conditions				
11:30	Break					
Panel discussion: Moderator - H. Ihssen						

12:00 Panelists:

P. Jacques, EMIRI, Belgium





	F. Schuster, CEA, France G. Karagiannakis, Certh, Greece M. Kozdras, Canmet, Canada				
Conclu	sion				
13:00	L. Malerba, CIEMAT, Spain	Wrap-up			
13:15	H. Ihssen, Helmholtz, Germany	Announcement next (and last) technical workshop			
13:30	Workshop ends				

Minutes:

Frédéric Feyel - Mastering high performance aerostructures by the help of models

Safran is a company dedicated to make aviation more sustainable. World leader in jet engines and helicopter turbine engines.

Aviation contributes today to 2-3 % CO2 emissions, ATAG in 2008 set the goal to reduce this to half in 2050, i.e., to decrease by 90% CO2 emissions compared to 2015, because meanwhile air traffic is expected to increase. This will be done by reducing fuel consumption (40-50%), optimizing air traffic (10%) and moving to low-to-zero carbon fuels (30-40%). One turboengine generation needs to be skipped to anticipate what should have been developed in 2030-35: pressure increased to 40 atm to lower velocity, temperatures up to 1500°C, beyond the melting point of several alloys. To decrease CO2 inlet T41 and outlet T30 temperature need to further increase, while decreasing maintenance costs: resistance to severe mechanical loading (creep, HC fatigue), temperature (up to melting), corrosion (gases, salinity, ...), erosion (sand, ash ...) are needed: efficient blades cooling and high performance materials. More and more complicated cooling circuitry (multicavitiy multi-trombone-like). Materials: Ni super alloys, single crystals (half hand big) with Ru replacing Re: the removal of GB improves creep resistance. Thermal barriers protect the single crystal from external attack and oxidation: minimal protection layer thickness with compatibility and adhesion, 3 parts optimized together to get highest mechanical performance.

Definition: To observer B an object A* is a model of an object A to the extent that B can use A* to answer questions that interest him about A (Marvin Minsy 1965). A model can thus be anything: a representation, a set of equations, a set of data, ... Modelling and simulation are usde through the whole product lifecycle: design, manufacturing, exploitation: legacy simulation (so far called computational physics) + data assimilation (machine learning & artificial intelligence, or deep learning): physical based, component design and manufacturing; alloy-by-design procedure; from chemical composition through experiments metamodels are created with ML and AI to screen quickly across compositions (in progress), or to go from composition to constitution (Calphad) to microstructure (not done yet) and properties. Improve design by simulation: analyse costs and risks, simulation based design cycles: exploit models at any scale, multifidelity approach combined with multiscale approach, take advantage of state of the art computing and software ecosystem. Simulation is used everywhere, for example for manufacturing (wax filling for mould eg, casting process, solidification: grain nucleation and growth, ...). Models are all continuum models, from single or polycrystal scale upwards. Validation? Thermomechanical sollicitation of specimens. AI is supposed to foresee result of tests for thousands of compositions when only a limited amount of testing is performed.

Marcin Kowal - NDT of components used in a research reactor (Maria) - review of methods

The Maria testing reactor is the only nuclear reactor in operation in Poland. It has a power of 30 MW; it was commissioned in 1974 and is licensed until 2025, the request for extension of operation being in progress.

It was designed for radioisotope production, materials research, semiconductor doping and training. The associated materials research lab is accredited.

NDT laboratory deals with: visual testing, penetrant testing, magnetic particle testing, eddy current testing, ultrasonic testing ...

Visual testing: cheapest and easiest, but requires experience and sees only surfaces.

<u>Penetrant testing</u>: allows detection and size assessment of discontinuities, including complex geometries; only surface discontinuities, though: it is not suitable for porous materials and needs cleaning and regular surface (a stain on the surface after application and cleaning reveals a crack).

<u>Unmanned/online) inspection</u>: extreme conditions generally hamper direct inspections, so remote inspection is needed in these cases and components should then be properly designed to allow this.

Eddy currents: an alternate current coil induces currents on the surface of the component, by current changes defects and discontinuities are detected, it is, e.g., usable for tubular elements, but it only works for conductive materials and

magnetism introduces complexity. Highly qualified operators are needed, only surface and subsurface defects are visible; but the process can be automated.

<u>Radiographic testing</u>: volumetric method which is effective for most materials; test results are permanently recorded and concern surface and subsurface: devices are portable. However, radiation can be hazardous, delamination is not detected, the equipment has high cost and it takes a long time to have results. Highly skilled operators are needed.

<u>Ultrasonic testing</u>: propagation of ultrasound waves, the method is based on wave reflection and can detect internal defects and discontinuities, and measure thickness and sizes. It can be automated. Devices are generally portable. Like radiography, it cannot detect discontinuities that are parallel to direction of the wave beam: it requires coupling agent and calibration blocks. A scanning vehicle is used on Maria the reactor shell.

Guillemette Ribay – NDT and SHM of materials under harsh conditions used in Energy Applications

Development of new sensors/methods and software for multi-technique applications: ultrasound testing, guided waves, structural health monitoring, eddy currents, radiography, computed tomography, infrared thermography ... Simulation is used to understand the physical phenomena and for the optimization of non-destructive techniques: sensitivity analysis to predict performance; diagnosis using AI.

Monitoring of materials using ultrasound testing: it detects reduction in thickness, microcracks, macrocracks, before it is too late (penetrant testing is considered environmentally unfriendly and visual examination cannot see buried defects).

NDT versus structural health monitoring (SHM): the latter finds physical quantities that are sensitive to material degradation and uses sensors that are able to monitor them. Proper analysis of signals is needed, but it is possible to think of automatic diagnosis to avoid expert eye need. NDT is done during shutdown for fast inspection. SHM is based on sensors that are permanently attached and monitor the system when in use (with the risk of possible noise); wireless data transfer used if possible.

<u>First example:</u> <u>solutions for NDT in SFR during shutdown</u>: Liquid sodium is opaque, there is therefore a need for localization of unwanted objects inside the vessel and ultrasounds are sensitive to materials properties and geometry, but sensors must withstand chemical aggression, irradiation (low, like in pressurised water reactors), at 200°C during shutdown. Classic piezoelectric sensors are not sufficient: insulated piezoelectric sensors or alternative solutions like electromagnetic acoustic transducers. For localization, telemetry is used in liquid sodium with ultrasound compression waves: waves are emitted and reflected by an object, by knowing the speed of the ultrasound waves the distance can be calculated, but one sensor is not enough: multi-element sensors need to be arranged in an array, with appropriate excitation times.

Electromagnetic sensors with coils (eddy currents) and magnets, without contact with transducers are under development to be compatible with liquid sodium, which should be able to steer the ultrasound beam for fast inspection. The challenge: many parameters, good ultrasound transmission needed and good sensitivity of reception; combination of simulation and experiments, with multi-element electronic devices. A new electromagnetic sensor is being tested in liquid sodium at 200°C to be permanently attached, but only where the temperature is not too high.

<u>Second example</u>: Corrosion in pipes. It is crucial to avoid thickness reduction and prevent leakage. Ultrasound guided waves are used, SHM instead of simple NDT: two rings of transmitters and receivers. Reference images are built with artificially created thickness reductions. Optical fibres are used for very high temperature.

Ocean breeze: large amount of data from wind farm, NDT of welds: km of measurements, months of manual analysis was done in less than one day by automatizing

Questions:

- Is it possible to have sensors always in a nuclear reactor? Electromagnetic sensors are not for high temperature, optical fibres should be able to withstand up to 1000°C, but are still far away.
- Under different operating conditions temperature will influence wave propagation, are there ways to take this into account? Yes, this is not a major problem, but sensors need to withstand high temperature.
- Will continuous monitoring be acceptable from the licensing point of view? Is monitoring sufficient or it is just a
 way to point to additional investigations? If SHM provides proper image no further investigation is needed, but it
 depends on the performance reached by the technique.

Michele Frignani - Materials requirements and qualification strategy for the European lead-cooled fast reactor prototype: analysis of the challenges

LFR is a GenIV reactor included in the EU roadmap, one of the most promising designs in terms of sustainability and safety, also as SMR: for this reason there is increasing attention from the industry.

Opportunities: high boiling point of liquid lead avoids criticalities in accidental situations, enhances natural circulation thus providing passive safety, etc. But liquid lead is highly corrosive (so issue of materials) and requires chemistry control. A disadvantage of liquid lead is its high melting point, which requires continuous heating and cooling at the same time to avoid freezing.





ALFRED is the name of the EU LFR prototype: very simple design with high safety features, the design is ready, but with caveats in terms of compatibility of liquid lead with materials, which impacts industrial deployment.

Compatibility of steels with liquid lead and lead-bismuth eutectic: low alloy steels are of no use because their operating temperature must remain <370°C); F/M are affected by embrittlement at 475°C, welding difficulties, and susceptibility to radiation and liquid metal embrittlement; the current solution are austenitic stainless steels, although they have low thermal conductivity and are susceptible to stress corrosion cracking and have limited irradiation resistance. However, there is experience on their use: they are not the best, but reasonably good.

The highest temperature is reached close to the fuel pins in the core region, the outlet temperature is not as high, but is what defines efficiency: these hottest temperatures need to be taken into account. Another issue is the control of oxygen control: if O concentration is above a certain value lead oxides are produced which may plug pipes, with potential danger of no circulation; but below another value the steel dissolves; it is thus necessary to remain within a band to form stable oxide layers. The window of operation depends on temperature: temperature and oxygen concentration windows are thus mutually fixed.

The highest temperature is limited to 450°C with current materials (500°C is the maximum accepted temperature). These limiting temperatures need to be increased because from the point of view of the properties of liquid lead we could go as high as 1000 or even beyond without any danger: new materials or protective measures are thus needed to fully exploit the competitiveness of this technology.

<u>Staged approach is used to progressively qualify new materials</u>: build a prototype of reactor that works within permitted limits of temperature and use it to test better materials in operation. Westinghouse is looking at making this technology s competitive as possible by going to as high temperature as possible. Test rigs are being developed in the UK to test materials in lead and lead thermo-hydraulics. The main reason to perform irradiations in the case of the LFR is to check the absence of synergy between corrosion and irradiation.

Mark Kozdras - Accelerated development of corrosion resistant materials – a closed loop approach.

An autonomous lab is being built to tackle the problem of corrosion: ideas and concepts to attempt accelerated materials discovery for corrosion resistance (corrosion materials acceleration platform, MAP) are presented here.

An example of accelerated experimentation of this type is being built in Erlangen, Nürnberg. It is built in stages to produce samples and do high throughput characterization with Al/robotic system to enhance dramatically the result obtained, with very small quantities of materials for samples.

Sample preparation: must be highly reproducible and repeatable, with novel materials and a variety of sample geometries.

Sample handling: simple geometries, flexible gripping tools, discs and rods (plate, extruded, 3D printed), easy manipulation.

Surface operations: machining, grinding, polishing, etching, degreasing, coating, plating.

Sample analysis: proxy parameters and development of suitable proxy tests for automated cyclic evaluation of descriptors: open circuit potential, linear polarization resistance, passivity, critical pitting potential, pit propagation tests, rotating disc electrode, tomography (atomic force microscopy, laser profilometry), corrosion produced analysis via spectroscopy, gas and liquid analysis blue chromatography, inductively coupled plasma ...

Machine learning based: bias free parameter optimization, selection of best performed, improvement of data analysis during test campaigns (requires searching phase space effectively).

Advanced analysis is then performed on candidate samples that are promising, eg: SEM, TEM, EDX, detailed electrochemical analysis ...

Long term exposure: scanning kelvin probe, in-situ scanning electrochemical microscopy, synchrotron or neutrons.

Material development: biggest challenges for integration into a MAP are the metallurgical processes involved, using alternative fabrication methods (e.g.plasma-based ...).

Simulation and modelling: assisting an acceleratign materials development, further information on mechanical and thermal properties.

Electrocatalysis MAP for fuel cells: platform being built for electrodeposited materials by M. Eikerling in Jülich. The corrosion one is only starting

Q: How much does it cost in terms of money and time to build a MAP? Time and cost depend on which equipment is already available. Planning takes a long time. Workforce is needed: hardware and software, multidisciplinary teams ... The different parts are generally not so costly, because costly equipment is difficult to automate.

Gunnar Skulason - Materials engineering for geothermal applications

Iceland GeoSurvey is a no-profit organization that provides specialized services to the Icelandic power industry, government and international companies.

Geothermal drilling: make a hole to access deep resources (temperature and permeability), or extract energy in the form of hot water or steam.

Geothermal drilling established standards in 1970s learning from oil industry.

Temperature increase from drilling to production results in high compressive forces that generate plastic deformations in casing, typically high temperature is 200-250°C, but in some cases 450°C are reached; the current aim is 550°C. Corrosive fluids with huge contents of H₂S and CO₂ or chlorides: uniform corrosion, pitting, crevice, SCC, HIC, SSC and high temperature (>200°C), which cause strength reduction and thermal expansion. More extreme conditions are found in the hottest wheels at 450°C.

Normally API materials are used: low yielding materials, resistant to H₂S attack, essentially carbon steels, sometimes with 9 or 14%Cr. Main problems are hydrogen attack, temperature gradients and subsequent thermal expansion: flexible couplings are used to compensate and reduce SCC.

Economic materials are needed, while technology is key to enable drilling or geothermals power production. Wells should last at least 30 years and preferably longer. Current design is ok below 150°C, but there is a need to move above 200°C, where thermal expansion and fluids are an issue.

Q: How easy is for you to change material? (For licensing/safety)?

It is relatively easy to change material, the community is sufficiently equipped to do operando testing. Probably the main limiting factor is cost. Drilling is not a big problem, but casing is because there is no cooling system.

Beatriz Acosta - Hydrogen enhanced fatigue of compressed hydrogen storage vessels

Different tanks exist for hydrogen storage: type 1 tank (standard gas cylinder, with stainless steel casing holding compressed gas); type 2 tank (more durable, cylinder shell made of aluminium or stainless steel and with partial wrapping); type 3 tank (metallic liner and composite wrapping); type 4 tank (fully wrapped, liner made of plastic, cheaper and lighter; may have glass fibre wrapping to protect against external effects). Nominal working pressure up to 70 MPa, T -40-85°C.

JRC is equipped for testing of high pressure hydrogen storage tanks, although it simulates wrong operative conditions at the hydrogen refuelling station.

Hydrogen embrittlement is obviously the main problem for metallic tanks. Tests are made on actual vessels with artificially created defects, with cycling temperature and pressure to simulate filling and emptying, counting the number of cycles after which a leakage is produced: much lower number of cycles with hydrogen than with, e.g., water: hydrogen enhances crack growth.

Conclusion: tanks 3 and 4 are the best. The difference is related to creep effects.

Q: Are these tanks the most likely means to store and transport hydrogen?

Q: Is there any moment in the hydrogen cycle (from production to use) where extreme conditions (perhaps more extreme than in the case of storage) are produced for containing materials? What are the features of these conditions?

Temperature is never extremely high. Temperature should be as high as affordable and safe, because the higher, the smaller the volume for the same quantity. Currently, 200 bars is the maximum accepted for transport by road in metallic tanks; standards are being studied for 300 bars. The maximum pressure in general could be 500-700 bars. Liquid hydrogen seems far at the moment, there are issues of leakage, but it's a possibility for the further future. With 200 litres in a tank 3-4 times bigger than for petrol, a car can currently cover about 400 km.

Jyrki Mikkola (replaced by Pekka Pohjanne) - Protective Coatings for SOEC interconnects

Hydrogen, to be used as fuel, is generally produced in electrocatalysers. <u>20-40 GW renewable generation can be</u> <u>accommodated by 2030 by producing hydrogen with electrolysers, but these need to be of higher efficiency</u>. Solid oxide electrolysers exist for co-electrolysis of H₂O and CO₂, with high efficiency reversible operation, but they are still at low TRL and scale 1 MW max. But they are a promising technology, at a price 1500 of \in/kW , with higher efficiency, 80-90%. One challenge is represented by the interconnecting plates in SOEC, to separate fuel and oxidant, connect cells in series, and give mechanical support. They need to offer low resistivity and high conductivity, match thermal expansion coefficients, and be chemically stable in oxidizing and reducing atmosphere, at high temperature (700-800°C).

Ferritic stainless steels are normally used, with high Cr content: AISI 44, Crofer 22 APU, also coated (but not with AI: Co based coatings).

Tornbjörn Jonsson - Power-production from biomass - material development and corrosion prediction in harsh environments





Materials challenges are common in biofuel and waste from solar and wind power: biomass burning produces water and steam in heat exchangers: the higher the temperature, the higher the efficiency. This leads to corrosion issues, because of the combination between environment and temperature. Corrosion protection has to go hand in hand with good mechanical properties, but it is corrosion that limits temperature and lifetime. Typical corrosion resistant materials used in bioenergy: FeCrAI, F/M steels (called stainless steels, Cr > 9-12%), austenitic steels, low alloyed steels (Cr<9-12%), Ni-based alloys, coatings. Comparison fossil fuel and biomass (wood/agriculture): temperature is higher, but biomass contains e.g. reactive alkali, especially waste, with high pH₂O.

FeCrAl and reactive alkali improve secondary protection.

Lifetime predictive tools: fuel, temperature, material are the variables, thermodynamic calculations including kinetics (Calphad, DICTRA, DFT) are the tools to study good primary and secondary protection.

Florian Sutter - Materials for harsh conditions in CSP

CSP materials addressed: reflectors, molten salt receivers, particle fluids. CSP has the advantage that heat can be stored (using molten salt, particles ...). The CSP installed power worldwide is currently 6.2 GW (IEA recommends 6.7 GW/yr growth, thus there should be a massive increase to hit the target). PV is cheaper and presently has 80 times more installed capacity.

Technologies: parabolic through (linear Fresnel mirrors): receiver temperatures 200-500°C, 280 MWe. The most promising is the tower, with receiver temperature up to 1200°C. Issues:

- <u>Solar reflectors</u>: Soiling, erosion, corrosion, slope deviation can cause performance loss. New mirrors are being studied to decrease cost (<12€/m²), increase lifetime and reflectance, reduce dust deposition (anti-soiling, antidew, anti-ice coatings), remove lead (toxic) from the base coat.
- <u>Secondary reflectors</u> (high temperature reflectors): Increase overall efficiency; Ni base alloys as support, as coatings are not sufficiently stable.
- <u>Heat transfer from receiver</u>: Ni-base alloy or whatever material is used needs corrosion resistance to molten salt, T91 with Ni or Al coatings is being studied to reduce costs, or even coatings on low-alloy steels. The target is to increase molten salt temperature from 565 to 600 or even 650°C. Lifetime has to be increased, at least to 20 years.
- <u>Falling particle receiver</u>: Direct absoprtion of particles, no need for expensive alloys, promising solution because it enables the highest temperatures possible, up to 1000°C. Issues: particle attrition, breakage rate, erosion; emittance. Novel particles are being studied: cheaper, with high heat capacity, high density, high temperature resistance, as spherical as possible, with high absorptance and abrasion resistant (perhaps coated).

Q: What's the composition of the particles? Often bauxite, but alternative products are being searched for: Fe-oxides, recycled materials ...

Q. What are the main shortcomings with particles? Interaction of particles with alloys: wear rates, guarantee good heat transfer in exchanger ...

Q. Have liquid metals been abandoned as heat exchange fluids? No, still on-going, even a commercial company in Australia is using liquid sodium.

Christos Agrafiotis / George Karagiannakis - Materials in harsh conditions for high temperature solar thermochemistry

High temperature solar thermochemistry: not for electricity production, but for inducing chemical reactions as a means of storage of CSP. Solar thermal advantage is indeed that heat can be stored more easily than electricity, themochemical reactions are a possibility to store and then release high T process heat.

Systems are conventional, like for electricity, but materials change because it is a chemical plant which should be working 24/7, in contrast to solar energy, so storage is essential. Conditions: temperature > 600°C, chemically harsh environment ... Thus corrosion (sulphur), and, if moving particles, erosion with creation of dust. Redox reaction: thermomechanical but also thermochemical stresses in materials, due to cyclic phase changes and high operating temperatures - cobalt and aluminium oxides are considered. Alternative materials: ceramic foams.

(De)hydration: calcium --> lime, 518 °C, fluidized or moving bed reactors: problems of particle fragmentation due to extreme thermomechanical cyclic stresses, possible to use CaO.

Angelo Freni - Durability of solid desiccant materials for HVAC systems

Thermally-driven adsoprtion machines: based on reversible physisorption of vapour on porous materials, driven by the applied ΔT : adsoprtion produces heat, desorption absorbs heat. Porous materials used: zeolites, silica gel, activated carbons; absorbed vapours: ammonia, water, (m)ethanol. Water is the best. Similar to heat pump, usable for cooling, refrigeration, heat storage, air conditioning, etc. An evaporator produces cooling and by absorption heat is produced. No mechanical devices: thermally driven. Market is small because of high capital costs, still bulky machines, no industrial players, there are problems of maintenance and performance degradation. Main needs: optimize machine and absorption materials: they need to guarantee stability over several thousand cycles.

Absorbents: silica gel is unstable, so new materials are considered: salt inside porous matrix, modified zeolites with adsorbing coatings, polymeric foams/fibers, metallic organic composites ...

Lucio Bonaccorsi - Materials for thermal energy storage in harsh operating conditions

Materials for thermal energy from low temperature heat. <u>70% of the energy produced in the world is eventually wasted</u>, <u>because in the range of low temperature (<150°C)</u>: hence the importance of waste heat recovery (sensible heat, latent <u>heat</u>, thermochemical storage via endo/exothermic reactions: store energy in chemical bonding). Thermochemical storage is ideal in the range 200-500°C, but also <100°C can be recovered. Issues: materials corrosion and toxicity/safety, limited benefit/cost ratio, mainly lab scale.

Panel discussion

Karagiannakis: Materials are always at the centre, especially active materials. Common challenge for any application is the issue of materials stability under long term operation and validation for the given application under relevant conditions. Each application has its own peculiarities.

Schuster: [It is his job to seek for commonalities between nuclear and non-nuclear technologies]. For the development of emerging processes, the way materials are processed and elaborated is always key in order to obtain the target properties. Hence the importance of the process aspect in techniques like, e.g., additive manufacturing. We also need discovery acceleration tools: high throughput calculation and characterization, artificial intelligence, data management: Other important point: how to share data. Standardization is also important. Durability in terms of sustainability, which needs to be included at the beginning of all studies: see Advanced Materials 2030 Manifesto.

Kozdras: (MAPs not yet as much developed as to use additive manufacturing). [He is working on robotic platforms]. Modelling has an important role in all materials development steps, to get stability in operation through design: the turbine blades example shows how modelling is important from production to use. It is important to have platforms where all variables are included. NDT is also an important way to improve devices: not only materials, but also materials embedded in a system.

Moderator: Is it good to support materials in harsh conditions the same way as batteries? (BigMap)

Jacques: Yes, it is important. EMIRI is involved in the mentioned Advanced Materials 2030 Manifesto. The ambition there is to bring back a better governance structure to coordinate cross-cutting issues on materials. The most obvious topic is how to integrate digital tools in the materials science world. Degradation under harsh conditions is one of the key challenges, requiring the understanding of physical and chemical degradation from the atomic level upward. We need accelerated testing tools to have our eyes on the materials in operation, so monitoring techniques and the infrastructures to reproduce the operation conditions. Sometimes these are very difficult to reproduce in a lab, having all the equipment is costly. The importance of digital tools that are quickly developing is becoming dominant.

Moderator: BigMap is getting 20 M€ and will get as much in its continuation. Electrocatalysers are equally complex in fact.

Karagiannakis: Yes, they are complex, but all devices are complex in fact, because the broader complex of the operation is a puzzle without single solution. A holistic approach is needed. But we also should not be relying completely on artificial intelligence because if the data and their quality are not sufficiently good, then these methods may fail. Environmental aspects are also important to take into account.

Moderator: There is no teaming up in the use of data.





Kargiannakis: There is a need for standardization and coordination. Calls should direct in the right direction. If they are fragmented, the results are also fragmented.

Moderator: How to avoid that activities stop when the project is over?

Karagiannakis: it is a matter of strategies. Member States do not work in a coordinated way.

Moderator: In batteries, the future projects will use the same ontology. But in this case a lot of resources were put there.

Schuster: The solution is to put research before application. E.g., additive manufacturing issues can be addressed at research level before intellectual property aspects arise. So projects should be just before application itself.

Kozdras: Currently 9 different MAPs exist: concrete, electrocatalysts, ... each time the MAP development starts, data and computational scientists need to be involved, to make sure the data quality is sufficient and the ontology is defined. This is application specific, though.

Jacques: It is difficult to find a solution to how having all the community focused on the single goal of standardized data (translators, connectors, ...) in a coordinated way. There is a push towards another CSA to force the community in this direction: how to further reinforce the community on the least sexy part of the AI approaches, which is the quality and gualification of the data.

Moderator: How to make data reliable? JP AMPEA or others may discuss ontologies, but is it sufficient to do so on a voluntary basis? Or is money needed? Could this be done within EERA JPs?

Kozdras: Creating ontologies takes money and there has to be widespread agreement on it, to be sure all problems are correctly taken into account in them. Do the computation, the automation and the materials science is complex. The data ontologies on top of it has to be friendly to all and able to include all the possible data and metadata.

Moderator: E.g., in mission innovation there is no money to bring people together, it relies on member states to do this and it is difficult to know a priori whether this is sufficient funding. Artificial intelligence can be used in different ways, how to merge different groups under a single umbrella?

Schuster: CEA and CNRS are involved in a big initiative, DIADEM (DIscovery Acceleration for the Development of Emerging Materials), with several M€ (8 year programme with first call for proposals in 2024). France cannot give money outside, but PhDs and students can go to different labs and this can be a way to do something jointly, also with data. This could harmonise with other initiatives in other countries, e.g. FERMAT in Germany.

Moderator: Also funding for visiting labs outside can be useful, there is a programme for storage application (CSP could be included too). What about industry's role? E.g., electrolysers and hydrogen economy at the moment is not possible if based on green hydrogen because raw materials for this technology are not available.

Jacques: Research can try to find solutions to the problem, but there are also geopolitical issues involved that are independent of research (e.g. Russia is the third producer of Ni worldwide and we need now alternative providers): it's manly about how to become more autonomous, within regions that are sufficiently stable and integrated. DG energy are defining sustainability by design and these criteria will have to be included from the beginning in the design of the materials, so we definitely need digital tools for it will be impossible for scientists to include all variables.

Kozdras: Sustainability is built around critical minerals and we need to change them, but we also need to do more in recycling technologies to recover critical elements. Replacement and recycling need to be both included.

Moderator: Final comments?

Karagiannakis: There is never a single solution concerning materials choices, but just say that it is a game of compromises trying to find the best one possible, so the holistic approach with all disciplines included is the only possible one. No easy way to do it, but some coordination from the top is definitely needed.

Kozdras: The German-Canadian materials development centre is doing this: coordination and exchange with possibility of training and exchange, multidisciplinary in essence. Needed to make sure the ontology is accepted in the future.

Jacques: EMIRI is ready to organise workshops too on topics of modern materials science and development. Key players are also the vendors supplying the information technology.





Appendix II: programme and extended summary of the final workshop on the future of energy materials

Agenda:

March 13 - 13:30 to 16:40

		Title / Topic	Speaker	
13:30	13:35	Opening welcome	Adel El Gammal - EERA, Belgium	
13:35 14:05		Introduction: EERA-EM4I series	Loronzo Molorho, Ciamat Spain	
		ORIENT-NM: towards a CEP on nuclear materials	Lorenzo Malerba - Ciemat, Spain	
		Scientific EM4I session		
14:05	14:30	MAPs r/evolution: Pathway to energy materials	Mark Kozdras - Natural Resources, Canada	
14:30	14:55	Digital Twins in the (Future) European Battery Supply Chain	Jawad Elomari - SINTEF	
14:55	15:05	Q&A session	Moderator: Sawaco Nakamae - CEA, France	
15:05	15:15	Break		
15:15	15:40	The different aspects of digitalisation in metallurgical research at ArcelorMittal Global R&D Gent	Nico De Wispelaere - OCAS/ArcelorMittal, Belgium	
15:40	16:05	Prospective Sustainability Assessment and decision support for new Energy Materials – use cases from battery research	Manuel Baumann - KIT, Germany	
16:05	16:15	Q&A session	Moderator: Lorenzo Malerba - Ciemat, Spain	
16:15	16:35	AMPEA (COST-Action)	Sawaco Nakamae - CEA, France	
16:35	16:40	Closing		
16:40	16:40	End of first day		

		Title / Topic	Speaker		
8:50	9:00	Opening welcome & 2 nd day introduction	Philippe Jacques - EMIRI, Belgium		
9:00	9:20	AMI2030: the multi-sectoral accelerator for sustainable advanced materials dedign, development and uptake	Fabrice Stassin - EMIRI, Belgium		
		Materials Research for CET			
9:20	9:40	From materials design to their scale up: the EIC hands on approach for Advanced Materials for Energy	Francesco Matteucci – EIC, EC		
9:40	10:0 0	IEMAP: the Italian platform for energy materials discovery	Massimo Celino - ENEA, Italy		
10:0 0	10:2 0	Critical Raw Materials	Stéphane Bourg - CEA, France		
10:2 0	10:3 5	Q&A	Moderator: Monica Fabrizio - CNR		
10:3 5	10:4 5	Break			
10:4 5	11:0 5	EMIRI Focus Group on Hydrogen: Advanced materials for Electrolysers, Fuel Cells and Storage & Distribution	Marcel Meeus - EMIRI, Belgium		
11:0 5	11:2 5	Harnessing semantic technologies to accelerate the discovery of next-generation battery materials	Eibar Joel Flores Cedeño - SINTEF, Norway		
11:2 5	11:4 5	EU-SOLARIS: From Solar Infrastructures and R&D Capabilities to innovative applications and solutions to meet CET challenges	Eugenia Zugasti - CENER, Spain		
11:4 5	11:5 5	Q&A	Moderator: Sawako Nakamae - CEA		
11:5 5	12:4 0	Panel Discussion	Moderator: Kalle Nilsson - JRC, Petten Panellists: M. Celino, E. Flores, M. Kozdras, L. Malerba, F. Matteucci, F. Stassin, L. Giovannelli		
12:4 0	12:4 5	Closing	Lorenzo Malerba - Ciemat, Spain		
12:4 5	12:4 5	End of Workshop			

March 14 - 8:50 to 12:30





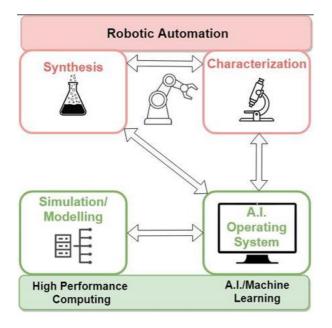
13th March

Mark Kozdras

Accelerate materials development: Evolution/Revolution

Jan 2018: 55 scientists proposed the idea of MAPs: Mario Molina nobel laurate defined it a second revolution.

MAPs = self-driving autonomous materials laboratories: closed loop synthesis and characterization using robots --> high throughput experiments and calculations/artificial intelligence, to develop novel materials and devices



To be successful it is necessary to: build acceleration ecosystems: government, academy, industry; establish critical mass of platform development; leverage policy actions; mobilize infrastructures; training and education

Significant coordination is going on in Europe. Active platform developments: U. Liverpool, AFRL (AirForce research lab), U. Illinois, U. Glasgow, U. Toronto + Battery 2030 BigMap

Hardware providers are an integral part of the platform development

Accelerated simulation and modelling: complexity of computational perspective

Several examples of MAPs are being developed. MAPs have also safety implications: lower materials volumes, lower problems with toxic materials, 24/7 work. Ethics: remove human biases. IP: difficult issue.

Conclusion: conventional evolution science has been bolstered by MAPs; MAP ecosystem continues to be developed. Coordination and alignment at a global scale is needed.

Q. support implementation of new energy materials - MAP does not necessarily work out commercial aspects, but through the fast exploration of the phase space effective solutions are possibly found more quickly

Al serves 3 roles: 1. Explore large experimental space through efficient experimental planning, 2. Accelerate simulation and modelling and 3. Process large data sets. A MAP uses these 3 features to rapidly solve a materials problem that could include device performance as well. We are tackling a problem where we optimize a thermoelectric material and plan to build and test a TE module in the MAP

Q. Waste: quantity of material is really small, so actually waste is minimal

Jawad El Omari

Digital twins in the European battery supply chain:

Digital twin = digital copy of materials and components, their evolution (behaviour), including during production and transportation

Challenges: data fragmentation, human expert bottlenecks - key: machine readable identifiers

Marbel: manufacturing assembly modular reusable EV battery for environment friendly lightweight mobility - accelerate material and process development / e.g. welding process: materials digital twin modelling workflow: welding, precipitations, ...

How will the cell perform - where can I find my data - how much will the cell cost - BattMo physics based cell modelling framework (battery modelling toolbox)

Homogeneous data sources + physics based models (understanding)

Nico De Wispelaere

OCAS is developing accelerated melting, casting, rolling, thermal treatment and also characterisation: statistical analysis on metallography.

Metallurgy: link between composition/processing and properties. Plenty of parameters play a role, e.g., non-uniform rolling temperature. Variability is not simple to catch with models. By looking at the microstructure the correlation with properties is made.

Deep learning neural network transforms the image and puts it in a 2000 dimension space and classifies the steel, deducing its properties.

Supervised classification: model outperforms experts in classifying microstructures.





Problem: where to find images for training? Hidden in reports and publications (hand annotated) + curated image collection (additional info also useful, e.g. type of microscope, magnification, steel grade, grain size). Unsupervised clustering is successful \rightarrow embedded in standard procedures: sample \rightarrow metallography \rightarrow microstructural analysis \rightarrow data mining.

From microstructure picture to hardness: 7% error! Also C content is accurately predicted

Manuel Bauman

Sustainability is important because of climate change. The request for several materials will multiply by 6 to 18 by 2030: it is necessary to find potential alternatives, e.g., Al and Na instead of Cu and Li as cathod materials; Co-free cathods; materials with higher power density. Can indications be given from its start on which new technology is more sustainable?

Life cycle oriented sustainability assessment from low to high TRL is needed to identify the most sustainable research paths.

Challenge of sustainable assessment is that the sustainability of a technology decreases with increasing TRL, because the opportunities to change the basics decreases: early TRL does not know much of manufacturing and recycling, but these aspects need to be addressed from the beginning. This is difficult, though. Na batteries are now at medium TRL, how are they going to replace Li batteries? Expectation: 10 times less energy requirement from lab to high TRL and higher global warming counteract potential.

Analysis of 42 cathode active materials with indicators cost, carbon footprint and criticality: Co and Ni (and V) provide the highest share of carbon footprint; correlation also with cost and criticality. But there is high uncertainty due to assumptions.

Na batteries do not perform much better than Li in terms of global warming, but way better in terms of abiotic depletion, while the cost of recycling may be too high. But then results may be overturn by looking at higher level, they depend not only on the material, but on the analysis at cell level and device level. Change even more if the entire storage system is looked at.

Q. There are uncertainties in assessing the sustainability of a low TRL technology, and there are evolving methodologies: will the improvement of the methodology reduce the uncertainties, or are they intrinsic to the low TRL starting point?

A. Improved methodologies should reduce uncertainties, but these uncertainties cannot be completely removed at low TRL.

14th March

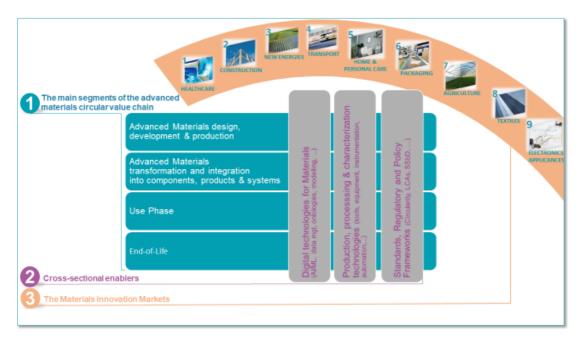
Fabrice Stassin

AMI2030 started in 2021 talking with Mariya Gabriel within a small group that produced the Manifesto and then towards a Roadmap and a Strategic Agenda.

AMI2030 roadmap has 3 pillars: materials digitalisation (merge theory and experiments), production and processing (energy consumption reduction, more efficient processes), identification of priority areas: blues sky research brought to the market

9 markets: healthcare, construction, energy, transport, home & personal care, packaging, agriculture, textiles, electronics

Focus on activities addressing needs and challenges common to many innovation markets, initially focus on a couple of them, but with cross sectoral applicability in mind



Pictorial description of the Strategic Agenda:

Core of AMI: from TRL 3 to TRL 8

Activities aiming at market, regulatory and societal uptake: regulation and policies, certification and standardization, education and training, etc.

Several initiatives already exist on which AMI can grow.

High level actions:

• Leverage on game-changing technologies for the fast development of scalable advanced materials solutions





- Develop advanced materials technologies with low environmental footprint and circular business models
- Support innovation uptake and access to infrastructures and services
- Contribute to an efficient implementation of key regulations, norms and standards supporting the design, development and uptake of advanced materials
- Education & Skills (Knowledge management)
- Paving the way towards an European advanced materials Innovation Eco-system
- International cooperation strategy

General objectives: boost industrial competitiveness, reinforce EU sovereignty and autonomy in key areas, support the green deal and digital age.

Francesco Matteucci

EIC is the pillar III of HEU, innovative Europe: it designs the work-programme and implements it. Pathfinder: ideas from previous projects eg in ERC; transition: no topic prescription or according to challenges; accelerator: work contentwise with the projects to accelerate innovation looking for interproject interactions --> clustering of projects, identify emerging challenges, EIC ambassador by networking with other programmes

Portfolios: renewable hydrogen, energy storage, solar conversion technologies, ocean technologies, sustainable materials, climate and environment

Sustainable materials: think of reuse and recycling, second life of materials and components, since the beginning

Currently difficult to establish collaboration between projects inside EIC and especially outside it

Strong emphasis on hydrogen production through renewables and batteries within the EIC.

Strong emphasis on looking for collaboration.

Q. Are nuclear materials included in the portfolio of EIC?

<u>Matteucci</u>: no clear answer, it has to be discussed - <u>Bourg</u>: nuclear energy materials can be addressed concerning CRM (supply), without entering the technology.

Massimo Celino

Italian energy materials acceleration platform, IEMAP. Framework: mission innovation - doubled funding for: hydrogen demo valley, smart systems and intelligent microgrids, and IEMAP.

IEMAP: computational laboratory for electrochemical storage, low and high temperature electrolytes, PV labs \rightarrow materials for batteries, electrolizers and PV

Data generation, storage, format, analysis: all is looked at appropriately

Example of DFT calculations and then AI to find the best compositions for given property.

Focus on: recyclability of PV cells, low CRM or CRM-free catalysts

Stéphane Bourg

Critical raw materials EU expert network - Motivation: population + energy and materials request + CO2 emissions are growing exponentially

2011, 1st EU CRM list in order to identify supply

Highest CRM risk technologies: motor traction and wind turbines, then batteries and fuel cells. The more solar panels in EU, the heavier the dependence on China, as all are produced there. Even when CRM are not mined in China (eg Africa, S. America) they first go to China for refining and transformation (Co, Li, ...). Difficult for the EU to become independent of China, but the level of dependency on one country in this case can be higher than it is now for fossil fuels!

Even if all Cu used from the bronze age was recycled, it wouldn't be enough to meet the needs foreseen between 2050 and 2070; in a market that grows 15%/year, even recycling all end of life components from 15 yrs before enables only a 12.5% of needs to be met \rightarrow recycling does not solve all pbs, currently EU focuses on that; moreover China recycles. Too.

Strategy to be adopted is strongly material dependent.

Conclusions:

- EU is a poor producer of CRM
- There is almost no EU industry transforming CRM into energy technologies
- We have to secure our supply chains (and not our supply)
- It will mainly rely on primary production, but we need to develop recycling at the right level
- We are globally responsible for the impacts of the raw materials production

Marcel Meeus

Description of EMIRI and how its technology roadmap has been built for hydrogen.

EMIRI's focused on: batteries, hydrogen, solar and wind, low carbon indistries, lightweight materials for mobility, buildings. Drivers: decarbonisation, sustainability/circularity, competitivity/autonomy, digitalisation.





A group of experts from various organisations has been set up. For each technology, e.g. alkaline electrolysis, the group provided technology description, identified and ranked the technology challenges, and defined quantitative targets to be reached overtime (technology sheets).

Eibar Flores - Semantic technologies to scale up battery materials

By 2030 energy storage with batteries is supposed to increase 14x especially for auto motion \rightarrow it is a materials challenge: materials with more energy per gram and lower cost (reduce by 40%) + challenges related with CRM + performance of materials in terms of efficiency to release Li and lifetime --> Bigmap project

Data highways are needed - <u>semantic technologies are ways to help machines to understand</u> <u>data</u>: standards, ontologies and knowledge bases (databases that use resources from different geographical domains). Ways of connecting resources for any kind of applications.

Semantic technologies = define controlled vocabularies that enable the machine to identify what a human expression corresponds to and thus where to look for relevant data and also how to connect data and so extend the network

Semantic is very specific for a given technology (has to be developed by experts for each technological ambit): example of batteries has been provided

Eugenia Zugasti

Good summary of the direction in which materials for solar should evolve.

EU-SOLARIS ERIC as example of single entry point installation to research and qualify materials for CSP

Panel discussion:

3 questions were asked to each panellist:

- 1. What are the key breakthroughs in the materials development you foresee in the coming 10 years?
- 2. What are the most important materials R&D areas to support/accelerate the material development?
- 3. How can we best set up concrete cross-cutting joint actions to reach real synergies at European and international level?

Mark Kozdras

1. Key breakthroughs \rightarrow equipments from providers that can be used to make MAPs

2. Materials R&D \rightarrow power train, high conductivity cables, electrical steels, higher performance, use of aluminum

3. Xcutting joint actions \rightarrow intense access to HCP, data made available to people, as well as CPU and GPU

Fabrice Stassins

1. Solid state batteries coming to the market with lower consumption in CRM, higher efficiency PV, catalysis, recycling of plastic

2. AI, models, understanding, acceleration of materials testing in small quantities, fast methodologies to assess safety and sustainability

3. Align agendas and priorities, pull resources and assets, increase funding in the EU

Luca Giovannelli

1. Breakthroughs: emphasis on other dimensions of the Green Deal, more sustainability and circularity embedded in technologies, consider what happens after decommissioning

2 Data driven and mechanistic models, targeting goals of performance and sustainability

3 Already trying to work to make programmes more compatible to make it easier to collaborate through projects

Massimo Celino

1. Digitalization technologies (cloud technologies) to be used for materials for energy

2. Data management crucial point: standards, interoperability, etc etc

3. E&T, attract young people with specific expertise on materials and digital technologies, good programmers for new generation of numerical codes, coordination among centres, data spaces, support for communities to increase them around these technologies

Francesco Matteucci

1. Computational materials science, lifecycle design thinking and supply chain (clean mining, sea mining)

2. Reduce CRM, new storage materials, low C cement, alternatives to fertilizers, new semiconductors (little interest from corporates on the latter)





3. Training of innovation managers and new capabilities on computational materials science, open innovation test-beds (innovators and scientists working together to scale up), need to interact more, policy makers to make decision based on data and numbers

Eibar Flores

1. High throughput materials discovery centres, research as a service concept, large centres offering campaigns like synchrotrons do today, exploring compositional spaces to do datadriven research

2. Electrochemical storage, complex problem with political support, so pushing the boundaries for new techniques also for other materials and applications

3. Controlled vocabularies as technical solutions to structured data to make data-driven decisions: datasets, metadata, equipments, all connected to ask for critical research questions

Lorenzo Malerba

1. Develop capability (with whichever means, computational and/or experimental, or mixed) to deduce long term materials performance from initial composition, microstructure/architecture, for given conditions. This would be a real breakthrough.

2. Develop models that combine and blend data-driven approaches with physical approaches, to avoid the danger of the "black box" effect of purely data-driven science; be able to make deductions from scarce data ("few-shot learning" - in the field of nuclear materials there is a problem of small data rather than big data)

3. Break the silo way of working, which makes it difficult for EIC projects to collaborate outside EIC and for Euratom to collaborate outside Euratom. Join funds whenever it avoids duplication or overlap.

Discussion:

Kalle Nilsson, summary - Commonalities throughout technologies concerning materials are clearly seen: replace materials when they use CRM, increase sustainability, recycle, rely on data-driven. The latter, however, implies good quality of data, abundance of data. Everything needs to be accelerated, but we also need hardware, can this be accelerated? Break silos. Train and educate to new technologies.

Fabrice Stassin - it is important to accelerate materials development, but also industrial upscaling: materials need to be evolutionary in kind, but revolutionary in performance, otherwise the production chain has to change too much.

Francesco Matteucci - The community that is able to develop materials should also be able to interact, although this requires effort.

Eibar Flores - Whart are discovery centres? MAPs do not need to be in the same geographical position if they are connected, the key is to connect high throughput facilities through networks of data.

Mark Kozdras - IP (intellectual properties) are an issue: researchers vs industries, MAPs are developed by researchers, but the technologies coming out of them can be independent of the creators and proprietary.

Sketch of EERA white paper on energy materials: start from the opportunities the workshop opened for the CEP on NM and for AMPEA, then discuss the limits of the new materials science approaches that are being pushed forward.













edf

RØD



Narodowe Centrum Badań Jądrowych National Centre for Nuclear Research ŚWIERK instytu kategorii A+, JRC colaboration partner





sck cen



CVŘ CHTrum výzkumu Řež







ORIENT



This project has received funding from the Euratom research and training programme 2019/2020 under grant agreement No. 899997