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Synopsis

MaterialsWeek 2024 aims to bring together - for the first time - the numerous small and large Research and Innovation (R&I) communities that are driving advances in materials innovation manifested across diverse value chains and industrial markets.

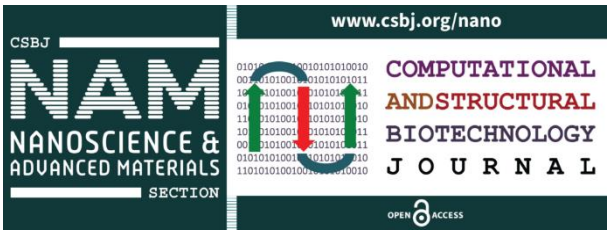
By addressing all materials application sectors and R&I communities concerned with the (re-)discovery, identification, improvement, handling, processing, manufacturing, (re-)use and recycling of materials, MaterialsWeek 2024 provides a cross-disciplinary meeting venue for communication and collaboration over and beyond traditional community boundaries. The aim of the meeting is to combine insights, theories, and methods from different fields to address complex issues. In addition, the meeting emphasises the fluidity of disciplinary boundaries and encourage the free flow of ideas and methods between different fields. This convergence aims to ultimately foster the best joint R&I approaches for meeting today's challenges and innovation requirements, including, but not limited to, more sustainability, circularity and resilience in materials' uses, higher reliability and efficiency in both R&I and sustainability assessment and safety testing of materials.

MaterialsWeek 2024 highlights and addresses all relevant R&I aspects along different materials innovation chains, including from up-stream pre-competitive basic research to end-of-life, highlighting and elaborating solutions to the challenges arising in the context of the overarching policies (e.g. EU Green Deal, Chemical Strategy for Sustainability (CSS), Chips Act, Circular Economy Action Plan (CEAP), Bioeconomy Strategy, Critical Raw Material Act, to name but a few), and their targets (e.g. the United Nations Sustainable Development Goals (SDGs), decarbonisation).

In bringing the R&I communities of energy materials, graphene, nanotechnology, bioeconomy, lightweight materials, smart materials and other innovative materials together into a single, solution-driven environment embracing all advanced materials, MaterialsWeek 2024 aims to establish an interdisciplinary, collaborative ecosystem to jointly advance materials R&I through:

- concepts, such as Safe-and-Sustainable- by-Design (SSbD), Industry Commons, Materials as a Service (MaaS),
- cross-cutting approaches, such as digitalisation, digital twinning, standardisation/harmonisation, FAIR (Findable, Accessible, Interoperable and Re-usable) and Open Data, and
- policy approaches, such as circularity, climate change prevention and adaption, sustainability, and resilience, and science-policy dialogue and translation.

In essence, MaterialsWeek 2024 aims to be a catalyst for innovative and sustainable materials development by fostering collaboration & sharing insights across diverse R&I communities.



The full paper proceedings of the MaterialsWeek 2024 will be published in a Special Issue in the journal *CSBJ – Nanoscience & Advanced Materials*.

Programme

Tuesday, 18. June 2024

Start	End	Title	Presenter
1. Materials Week 2024 – Welcome & Setting the Scene			
09:00	09:10	Welcome to MaterialsWeek 2024	Philippe Jacques & Steffi Friedrichs
09:10	09:20	Welcome to Cyprus	Demetris Skourides, Chief Scientist for Research, Innovation and Technology, Republic of Cyprus
09:20	09:40	**CHALLENGE**: The EU Strategy on Advanced Materials for Industrial Leadership	Jürgen Tiedje
09:40	10:05	Innovative Advanced Materials for Europe (IAM4EU) – A new EU Partnership to strengthen the EU's strategic cooperation with industry	Philippe Jacques
10:05	10:50	Panel Discussion: ***Green Future through Advanced Materials – Redefining Value Chains for environmental and economic Success***	Moderator: Steffi Friedrichs
10:50	11:10	Coffee/Tea Break	
2. Market Needs, Challenges & Opportunities for Materials R&I			
11:10	11:40	**CHALLENGE**: Polymer materials are essential – and so is change	Rolf Albach
11:40	11:55	SusChem as a Hub to support and monitor challenges and opportunities for sustainable supply chains	Karaoglanoglou Lazaros
11:55	12:10	An Open-Innovation Platform for knowledge-based management of materials modelling workflows for industrial data	Gerhard Goldbeck
12:10	12:25	Enhancing Collaboration and Innovation through DIGIPASS CSA and VIPCOAT Open Innovation Platform	Salim Beiouettar
12:25	12:40	Navigating Challenges and Embracing Innovation: Managing Partnerships and Ecosystems for Circular Materials in the Chemical Industry	Christian Seitz

12:40	12:55	Are Your R&D Plans Big Enough?	Liza Shvyndzikava
12:55	13:00	24/7 Poster Presentations	
13:00	14:30	Lunch Break	
3. Digital Transformation – Catalysing the Green & Digital Transition for Innovative Advanced Materials and Products			
14:30	14:55	Tbc	Victoria Petrova
14:55	15:05	DigiPass: Knowledge Valorisation for Innovative Advanced Materials Design and Development	Natalia Konchakova & Peter Klein
15:05	15:10	Session / Cooperation/ Collaboration	Natalia Konchakova & Peter Klein
15:10	15:20	Platform MaterialDigital: Enhancing Scientific Collaboration within the MSE Community	Jörg Schaarschmidt
15:20	15:30	PEPR DIADEM: Priority Equipment and Research Program on the development of innovative materials using artificial intelligence	Fernando Lomello
15:30	15:40	IRISS – the International ecosystem for accelerating the transition to Safe-and-Sustainable-by-design materials, products and processes	Emma Strömberg
15:40	15:50	The use of analytical research infrastructures to support industrial innovation	Ennio Capria
15:50	15:55	Magnetic Multiscale Modelling Suite	Thomas Schrefl
15:55	16:00	DECODE: Cloud-connected Labs of Future for Energy Materials	Kourosh Malek
16:00	16:05	Multiscale Characterisation and Simulation for Hydrogen Embrittlement Assessment: Development of an Open Knowledge Platform to Foster Capability Integration (HyWay)	Napat Vajragupta
16:05	16:10	SiToLub – Simulation Tools for the design of safe and sustainable Lubricants	Francesco Pagano
16:10	16:15	CHEMATSUSTAIN: Implementing Innovative Methods for Safety and Sustainability Assessments of Chemicals and Materials Particularly at Nano Level in the European Union	Jelena Barbir

16:15	16:20	AI-driven multiscale methodology to develop Transparent Wood as sustainable functional material using SSbD	Päivi Kivikytö-Reponen
16:20	16:40	Coffee/Tea Break	
16:40	16:45	Battery manufacturing digital twin design in view of requirements for the digital product passport	Martin Thomas Horsch
16:45	16:50	COST Action EuMINe – European Materials Informatics Network	Francesco Mercuri
16:50	17:05	24/7 Poster Presentations	
17:05	18:20	Round Table / Fishbowl discussion: Materilas Digitalization, Digital Materials & Product Passport	Peter Klein, Franz Pirker, Salim Belouettar, Natalia Konchakova
18:20	18:30	Collaboration actions/ Close Notes	all projects / participants
18:30		Conference Reception & Walking/Networking Dinner (& Poster Viewing)	

Wednesday, 19. June 2024

Start	End	Title	Presenter
09:00	09:20	**CHALLENGE**: The Need for International Test Methods for Industry, R&I and Regulation	Anke Jesse
6. Frameworks and Methodologies for Materials Safety & Sustainability			
09:20	09:35	PARC roadmap for nanomaterials – exploring how PARC can contribute most usefully	Iseult Lynch
09:35	09:50	NANOMESUREFRANCE: A Single Entry Point for Structuring the Nanomaterials Industry around Comparable and more Reliable Data	Georges Favre
09:50	10:05	Utilizing In vitro cytotoxicity data of advanced material in life cycle assessment and human risk assessment	Peter Wick
10:05	10:20	Making OECD Test Guidelines applicable for Nanomaterials and Advanced Materials – Activities by the Malta Initiative and MACRAMÉ	Elisabeth Heunisch

10:20	10:40	24/7 Poster Presentations	
10:40	11:00	Coffee/Tea Break	
11:00	11:20	The EC Safe & Sustainable by Design (SSbD) framework: Towards the improvement of its relevance, reliability and operability	Irantzu Garmendia Aguirre
11:20	11:35	Safe and Sustainable by Design Strategies for the H2020 SUNSHINE case studies	Arianna Livieri
11:35	11:50	Decision Support System for SSbD in the early innovation stages	Wouter Fransman
11:50	12:05	Challenges in Predictive Sustainability Assessment of Novel Lubricants following SSbD Principles	Jonas Hoffmann
12:05	12:20	Safe and sustainable by design roadmaps. A glimpse of the ASINA case studies	Furxhi Irini
12:20	12:35	Advances and challenges of Safe-andSustainable-by-Design: The case of high-entropy alloy coatings	Adamantia Kostapanou
12:35	12:50	Towards a nano-specific, quantitative based and human centric-SSbD Approach: Antibacterial nanocoatings case study	Massimo Perucca
12:50	13:00	24/7 Poster Presentations	
13:00	14:30	Lunch Break	
9. Infrastructure & Methods Requirements for Materials Innovation			
14:30	14:45	Chemical Nanoscale Analysis of Mesoporous Mixed IrOx-TiOy Thin Films	Vasile-Dan Hodoroaba
14:45	15:00	Chemical Analysis of Functionalized Graphene along the Production Chain	Loay Akmal Madbouly
15:00	15:15	Correlation between size distribution, morphology and chemical analysis of Graphene Family materials	Kerstin Jurkschat
15:15	15:30	SUNSHINE Safe and Sustainable by Design (SSbD) approach and e-infrastructure	Lisa Pizzol
15:30	15:45	Score System for a Multi-criteria Decision Analysis based on the SSbD framework for MCNM/HARN	Blanca Pozuelo Rollón

		Risk Management – The DIAGONAL Decision Support Tool Case	
15:45	16:00	Spectroscopic Approaches for Understanding Graphene Family Material interactions with Enzymes	Bashiru Ibrahim
16:00	16:20	24/7 Poster Presentations	
16:20	16:40	Coffee/Tea Break	
5. Digital Transformation – Towards a common Materials' Data Ecosystem			
16:40	16:55	Workflow for digital twin creation for secondary aluminium alloy in automotive parts	Eugen Gazenbiller
16:55	17:10	Normalised similarity assessment to inform grouping of advanced multi-component nanomaterials by means of an Asymmetric Sigmoid function	Georgia Tsiliki
17:10	17:25	Domain ontology for sharing data related to sustainable metallurgical and manufacturing industry	Jesper Friis
17:25	17:40	IUPAC International Chemical Identifier (InChI) – the compound identifier that makes molecule recognition FAIR	Gerd Blanke
17:40	17:55	How can we unambiguously refer to materials and their corresponding data?	Thomas E. Exner
17:55	18:10	Database generation workflow for supporting SSbD risk assessments	José Luis Vallés-Pardo
18:10	18:30	24/7 Poster Presentations	
18:30		Conference Day End	

Thursday, 20. June 2024

Start	End	Title	Presenter
4. Digital Transformation – Computational Tools & Platforms for Materials R&I Acceleration			
09:00	09:30	**CHALLENGE**: Advanced Materials for a Sustainable Future through Digital Technologies	Mark Kozdras

09:30	09:45	Harnessing the power of automation and machine learning with a modular material acceleration platform – an illustrating example	Simon Stier
09:45	10:00	Advancing Material and Chemical Development through Innovative Computational Modelling in the PINK Project	Haralambos Sarimveis
10:00	10:15	Experimental synthesis of safer nanomaterials through computational modelling and design	Richard Harris
10:15	10:30	First Principles In Silico Characterisation of Advanced Materials and Bio-Nano Interface	Vladimir Lobaskin
10:30	10:45	Advancing Materials Development through Multiscale Modelling and Data-Driven approaches in the Safe and Sustainable by Design Framework	Andrea Lorenzoni
10:45	11:05	Coffee/Tea Break	
7. Sustainability & Circularity driven by Advanced Materials			
11:10	11:30	Sustainability & Circularity driven by 2D-materials	Sofia Öiseth
11:30	11:45	Circularity of MAX phases: from worn parts and broken samples to 2D functional materials	Grzegorz Kubicki
11:45	12:00	The Safe and Sustainable by Design Framework applied to Graphene-based Materials	Fiorella Pitaro
12:00	12:15	The reproducibility of green synthesized nanomaterials: a study comparing the antimicrobial effectiveness of green-produced ZnO vs. fossil-based particles	Benjamin Punz
12:15	12:30	Safe-and-Sustainable-by-Design for Advanced Materials – A case study on the agricultural use of imogolites	Veronique Adam
12:30	12:45	Sustainable value chains in an emergent context: The case of BIO-SUSHY coatings	Jesse de Pagter
12:45	13:00	24/7 Poster Presentations	
13:00	14:30	Lunch Break	
8. Materials Innovation for Resilience			

14:30	14:45	Safe by design assessment of a multi-component nanomaterial as anti-pest in food packaging	Andrea Brunelli
14:45	15:00	Approaches to Accelerating Materials Discovery: International Ecosystem Building	Anjuli Szawiola
15:00	15:15	Accelerating the development of new battery materials	Maha Ismail
15:15	15:30	Material Acceleration Platforms (MAPs), Standards and Workflows for reference data	Bastian Rühle
15:30	15:40	24/7 Poster Presentations	
15:40	16:00	Coffee/Tea Break	
10. MaterialsWeek Closing- & Awards-Ceremony			
16:00	16:05	Conference Summary and Look into the Future	Steffi Friedrichs
16:05	16:15	Poster Presentation Award 1 & 2	Gupta Udatha
16:15	16:25	Oral Presentation Award 1 & 2	Gupta Udatha
16:25	16:30	FAIR Competition Award	Iseult Lynch
16:30	16:40	Closing Remarks	Steffi Friedrichs
16:40		End of Conference	

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Conference Challenges

Climate Change, socioeconomic shifts and geopolitical developments impose existential threats to Europe and the world and are triggering an ever-growing number of policies and proposed strategic actions; these result in complex challenges for materials R&I to support all needs of the major materials innovation markets.

A selection of high-level speakers highlights R&I as well as regulatory requirements in the form of 'Conference Challenge' presentations during the MaterialsWeek 2024.

Conference delegates are then invited to further address these challenges in their discussions and their oral and poster presentations, in order to develop collaborative ideas on how to tackle the increasing complexity of interdisciplinary materials R&I to build sustainable value chains of the future.

Detailed Programme

Date	Start	End	Title	Presenter
18 June	09:20	09:40	The EU Strategy on Advanced Materials for Industrial Leadership	Jürgen Tiedje
18 June	11:10	11:40	Polymer materials are essential – and so is change	Rolf Albach
19 June	09:00	09:20	The Need for International Test Methods for Industry, R&I and Regulation	Anke Jesse
20 June	09:00	09:30	Advanced Materials for a Sustainable Future through Digital Technologies	Mark Kozdras

Oral Presentations: Conference Challenges

Polymer materials are essential - and so is change

Rolf Albach[1]

Sustainability is a licence to operate but green is not enough: the reason for growth of polymer materials is the long-term low-weight performance and adaptability. The transformation of the industry is outlined for discussion.

[1] German Chemical Society, Frankfurt am Main, Gemany, r.albach@go.gdch.de

The Need for International Test Methods for Industry, R&I and Regulation

Anke Jesse[1], Laura Gross[1] Elisabeth Heunisch[2], Thomas Kuhlbusch[2]

1. Introduction

Appropriate, clear and enforceable legislation is a key factor to push innovation and support long-term investments. Legislation has to keep pace with innovative developments to enhance citizens' trust in innovation. This also includes having appropriate, recognised methods in place for determining legally required safety data. Internationally standardised and harmonised test methods are a prerequisite to build people's trust in safe innovation. OECD Test Guideline (TGs) are internationally accepted test methods, help overcome global trade barriers and, hence, increase the competitiveness of European industry. The Malta Initiative

In the Malta Initiative representatives of European countries, several Directorates-General of the European Commission, the European Chemicals Agency (ECHA), authorities, research institutions, NGOs, universities and industry work together on a voluntary and self-organised basis, hence without an official mandate. They work together to find possibilities for developing and amending the measurement and test methods required to enforce legislation (particularly in the field of chemicals). In order to make REACH enforceable for nanomaterials, the Malta Initiative committed itself in a first step to facilitating projects in which OECD Test Guidelines (TGs) are amended or developed for nanoscale substances. Other legislative areas, such as European regulations on biocides, cosmetics and plastic food packaging also refer to some extent to the OECD TGs when it comes to safety assessments for nanomaterials and thus benefit from the amendments.

The Malta Initiative started 2017 on Malta during the Maltese EU Council Presidency. It asked the EU Directorate-General for Research and Innovation (DG RTD) to politically and financially support the development and amendment of the OECD TGs and Guidance Documents (GDs) to ensure that nano-specific issues are addressed. To achieve this, several projects were put to tender within the framework of Horizon 2020, the 8th EU Framework Programme for Research.

2. The Malta Initiative Position Paper

The Malta Initiative Position Paper highlights that a strong European financial support is needed to support the validation and harmonisation of test methods and to coordinate the efforts towards OECD Test Guideline development. Experience has shown that

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[2] Federal Institute for Occupational Safety and Health, Germany

adaptation and development of test methods require intensive effort (in terms of time, human and financial resources), which individual researchers, industrial actors or EU Member States cannot undertake alone. The experiences of the Malta Initiative show that a coordinated effort leads to successful and efficient TG development. Furthermore, a coordinated approach can be more effective and help avoiding duplication of work.

3. Conclusions

To support safe and sustainable innovation, help overcome trade barriers and make legislation enforceable we need a European Test Method Strategy, which includes (a) funding of researchers for the development, validation and harmonisation of test methods, and (b) an international platform for collaboration and exchange between stakeholders.

Advanced Materials for a Sustainable Future through Digital Technologies

Mark S. Kozdras[1]

Materials Week 2024 embodies key concepts of Safe and Sustainable by Design (SSbD), Industry Commons and Materials as a Science (MaaS). These are core tenets of a novel way of developing new materials for a sustainable future in Europe and globally. Digitalization plays a critical role in realizing practical materials solutions for that future. Yet, digitalization has diverse forms, some of which are elaborated in this conference session on Materials Tools & Platforms for R&I Acceleration. The emerging premise is that Materials Acceleration Platforms (MAPs), autonomous or self-driving materials laboratories, have considerable merit in accelerating the discovery and development of novel materials and devices, embedding sustainability principles, and reaching and engaging developed and developing nations. The deployment of advanced methods including artificial intelligence, robotic automation and computational simulation and modeling will extend our capabilities beyond conventional scientific processes. And, it will do it on an accelerated time scale. The fact is that climate mitigation, geopolitical realities and scarce resources are driving us to find higher performing alternative materials for a broad set of applications. Digitally enhanced research and technology infrastructure is needed to make credible impact in health, pharma, energy and electronics, and these sectors will benefit from investment in accelerated materials discovery.

[1] Natural Resources Canada, Ottawa, ON, Canada, mark.kozdras@NRCan-RNCan.gc.ca

Session 1: Materials Week 2024 - Welcome & Setting the Scene

Leading public and/or private decision-makers will highlight Europe's current and future mix of policies pertaining to the role and use of materials in their diverse and complex value chains. By way of outlining the role of and expectations from materials R&I in the context of the relevant policies (e.g. Green Deal, Plastics Action Plan, Chips Act, Critical Raw Materials Act, Chemicals Strategy for Sustainability), the speakers will set the scene for the three-day MaterialsWeek 2024 Programme, and its diverse session topics.

Detailed Programme

Start	End	Title	Presenter
09:00	09:10	Welcome to MaterialsWeek 2024	Philippe Jacques & Steffi Friedrichs
09:10	09:20	Welcome to Cyprus	Demetris Skourides, Chief Scientist for Research, Innovation and Technology, Republic of Cyprus
09:40	10:05	Innovative Advanced Materials for Europe (IAM4EU) – A new EU Partnership to strengthen the EU's strategic cooperation with industry	Philippe Jacques
10:05	10:50	Panel Discussion – challenges and solutions to accelerate the time-to-market of green technologies enabled by advanced materials	Moderator: Steffi Friedrichs

Session 2: Market Needs, Challenges & Opportunities for Materials R&I

This session highlights the various, and very complex, value chains in which R&I for materials already plays an important role today or will play an increasing role in the future. As the demand for advanced materials continues to grow across industry sectors, there is a pressing need for materials research and innovation to address the evolving market needs.

Key challenges in materials R&I, that represent and require a "mindset shift", include not only the change towards designing materials and processes for recycling, the switch to alternative raw materials from recycling processes, the innovative substitution of unsafe, unsustainable materials and a convergence of disruptive technologies (incl. Artificial Intelligence, Machine Learning).

Speakers from both the public and private sector introduce the Market Needs, Challenges and Opportunities pertaining to materials R&I, and describe their projects', organisations' or initiatives' contribution to meeting these challenges.

Detailed Programme

Start	End	Title	Presenter
11:40	11:55	SusChem as a Hub to support and monitor challenges and opportunities for sustainable supply chains	Karaoglanoglou Lazaros
11:55	12:10	An Open-Innovation Platform for knowledge-based management of materials modelling workflows for industrial data	Gerhard Goldbeck
12:10	12:25	Enhancing Collaboration and Innovation through DIGIPASS CSA and VIPCOAT Open Innovation Platform	Salim Beiouettar
12:25	12:40	Navigating Challenges and Embracing Innovation: Managing Partnerships and Ecosystems for Circular Materials in the Chemical Industry	Christian Seitz
12:40	12:55	Are Your R&D Plans Big Enough?	Liza Shvyndzikava
12:55	13:00	24/7 Poster Presentations	

Posters

S02_P01	Navigating challenges: the use of advanced materials in medical devices	Susanne Resch
S02_P02	AMULET Technology Roadmap	Marine Viale

Oral Presentations: Session 2

SusChem as a Hub to support and monitor challenges and opportunities for sustainable supply chains

Karaoglanoglou Lazaros[1], Ioanna Kostopoulou[2], Stelios Bikos[3], Antonis Kokossis[2]

1. Introduction

The present paper will provide an overview of SusChem GR's initiatives and highlight its role as a hub for supporting and monitoring challenges and opportunities in sustainable supply chains for materials and products generation. SusChem is the European Technology Platform for Sustainable Chemistry which operates as a forum that brings together industry, academia, governmental policy groups and the wider society. It aims to implement the vision for a competitive and innovative Europe, where sustainable chemistry and biotechnology collectively will provide solutions for the future generation of process and products. This vision is pursued through priority areas, led by industries, including Resource and Energy Efficiency, Water Use and Management, Raw Materials, Smart Cities, Enabling Technologies, and Education.

2. SusChem GR [1]

SusChem GR, which was founded in 2016 by the National Technical University of Athens (IPSEN Unit), is one of the 17 National Technology Platforms, which are members of SusChem ETP. During its lifetime, it brought together national stakeholders and fostered a two-way communication at the European level; by promoting Greek priorities in the European research agenda for sustainable chemistry; and by advancing the national strategy for sustainable chemistry according to the European vision. Its members include the Hellenic Association of Chemical Industries, the Centre for Renewable Energy Sources, the Greek Association of Environmental Protection Companies, the Association of Greek Chemists, the Hellenic Association of Chemical Engineers, the Panhellenic Union of Bioscientists, the Hellenic Coatings Association and the General Consumers' Association of Greece.

SusChem GR actively has been supporting and encouraging SMEs to participate in EU projects and provide training and education services. It is also responsible for exchanging information within the SusChem network, other Member States, the EU Commission and any other organisation that may be of interest to the SusChem activities.

[1] National Technical University of Athens; School of Chemical Engineering; Industrial Process Systems Engineering Unit; lkaraog@chemeng.ntua.gr
[2] National Technical University of Athens; School of Chemical Engineering; Industrial Process Systems Engineering Unit
[3] SusChem GR; https://suschem-gr.org

3. SusChem GR as partner of IRISS Project [2]

“IRISS – International ecosystem for accelerating the transition to Safe-and-Sustainable-by-Design (SSbD) materials, products and processes”, is a three-year project, started in June 2022. It is funded by the EU’s framework programme for research and innovation, Horizon Europe. Within the project duration a permanent structure will be built for long-term operation of established expert’s network with the involvement of wider communities. SusChem GR as one of the 4 NTPs attending as partners to the project, and as a regional hub, coordinates the dissemination activities for South-West region; communicates the current SSbD related initiatives in the region; contributes to the identification of the information, training and education gaps and overall, supports the integration of the SSbD framework into the roadmap of the Chemical Industry and the national research and innovation policy agendas. Moreover, it fosters the establishment of a sustainable network for long-term collaboration among network members, extending engagement to partners beyond the consortium, both during and beyond the project's duration. Additionally, the priority value chains at both national and project levels has already been identified, and an action plan has been developed to communicate the SSbD concepts relevant with these value chains to national stakeholders and to explore the crucial issues for each value chain.

4. SusChem and Sustainability Section of European Federation of Chemical Engineering (EFCE)

Sustainability has been identified by EFCE, as a driving force to develop new business models that promote interactions in the context of circular economy. Chemical engineering emerges as a core discipline to scale up lab chemistry into industrial-scale processes, to screen processes for overall economic viability, to upscale waste to valuable feedstocks, and to target material and energy efficiency using a wide variety of technologies in process, energy, and systems integration. To that purpose, EFCE has prepared the formation of a new section with a vision to promote the rebuilding of industry, using a systemic and holistic approach and addressing the critical challenges of sustainable development as a coordinated working party. SusChem infrastructure and network is expected to play a key role in the activities of the Section, bringing the state-of-the art view of Chemical Industry on the sustainability challenges and contributing to the exchange of knowledge and experiences.

5. Conclusions

SusChem NTPs are anticipated to play a pivotal role in the transition toward Safe-and-Sustainable-by-Design innovation, addressing a societal imperative by ensuring a toxic-free environment and resource preservation. Considering the complexity inherent in adopting a system and lifecycle approach for this transition, SusChem NTPs can serve as catalysts between industry, academia, and policymakers, providing access to the essential tools, knowledge, and networking capabilities necessary for decision making to address this challenge.

6. References

[1] https://suschem-gr.org/

[2] https://iriss-ssbd.eu/

[3] https://efce.info/Section_Sustainability.html

An Open-Innovation Platform for knowledge-based management of materials modelling workflows for industrial data

Gerhard Goldbeck[1], Otello M Roscioni[1], Jesper Friis[2], Francesca Lønstad Bleken[2], Owain Beynon[3], Adham Hashibon[3], Louis Ponet[4], Michael Noeske[5]

1. Introduction

Understanding the properties of complex materials through materials modelling has been the drive for intense research in the field of numerical simulations for almost 100 years [1]. The advances made in computer hardware and simulation software now allow capturing the behaviour of materials down to any desired/required level of interactions (continuum, mesoscopic, atomistic or electronic) and at scales extending from nano- to macroscopic. Modern computational materials science relies heavily on automated complex numerical procedures, involving multi-step processes and on the integration of different simulation software. While workflow managers exist to automate, execute, and track materials modelling workflows, a steep learning curve still exists for utilising materials modelling effectively. Moreover, multi-model/multi-scale simulations coupling or linking different models and operating at different length and time scales require a level of expertise that is rarely mastered by a single individual. Finally, reproducibility of numerical simulations and validation of modelling strategies are often poorly addressed in the published literature, e.g. by lack of a standard format for sharing technical details. Therefore, the need arises to better manage, document and retrieve workflows, exposing the physical predictions to end-users without prior knowledge of theoretical models or specific software.

2. The OpenModel platform

The Open-Innovation Platform developed in the OpenModel project [2] addresses the challenges of managing materials modelling workflows by using semantic technologies for storing, documenting, retrieving, and executing them. An ontology-based simulation platform has been developed, which includes a workflow ontology, a big-data curation database, integration of third-party software, and a workflow runner/executor. The OpenModel platform delivers accurate, validated, and traceable simulation workflows and uses ontologies to formalise the knowledge required to use materials modelling. On top of that, a semantic description of input and output datasets delivers Findable, Accessible, Interoperable, and Reusable (FAIR) data which are fundamental for the digitalisation of industry. Validation and verification of materials workflows are performed with dedicated software, and the results attached to the workflows as

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metadata. In this way the platform ensures the consistency of numerical predictions and the robustness of materials models.

3. Workflow Builder

The OpenModel software stack includes a semantic-based workflow builder that describes workflows as tasks exchanging datasets. This information is stored in a knowledge base and retrieved using high-level queries. It enables end-users to initiate computations without detailed knowledge of computational implementations. In case of conflicting requirements, an algorithm prioritises and supports selection among potential workflows. The exchange of data between tasks is provided by pipelines based on semantic mapping schemas plus parsing and serialisation plugins. By storing workflows and datasets semantically in a knowledge base, new simulation workflows can be obtained as the builder can infer connections between heterogeneous tasks, providing new insights into complex problems. The builder utilises the Elementary Multiperspective Material Ontology (EMMO) [3] as a conceptual framework for describing workflows at various levels of detail.

4. Workflow Management

The materials modelling workflows are executed using the AiiDA [4] Python infrastructure. The validation and verification services assess the logical consistency and integrity of workflows, ensuring accuracy in physical predictions by comparing simulation outputs to reference data. This approach enhances the creation of reliable and reproducible materials modelling workflows, crucial for informed decision-making in industrial contexts and for FAIR datasets creation from simulation outputs, which can be used to interpret experimental data or for machine learning applications. By embracing semantic technologies and FAIR principles, OpenModel facilitates seamless integration and sharing of materials modelling data, contributing to the advancement of digital economy principles and Industry 5.0 initiatives.

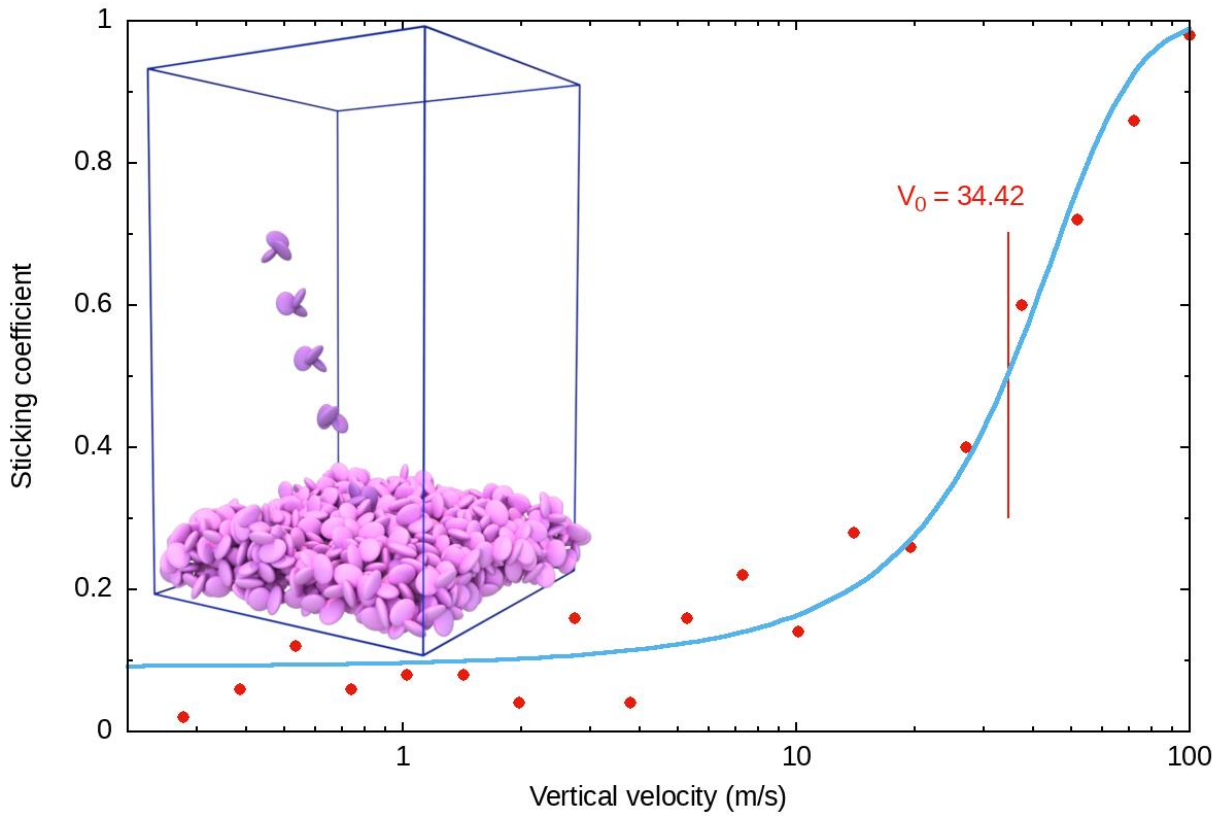

Figure 1: Extracting physical observables from molecular simulations involves setting up materials models, executing specialised software, and post-processing the resulting data. Managing these complex workflows and connecting them to metadata describing their physical accuracy and numerical consistency are among the objectives of the OpenModel project.

5. Conclusions

The OpenModel project has developed an Open-Innovation Platform which enables a knowledge-based approach to materials modelling workflows for industrial data. By leveraging semantic technologies, the project enables efficient management, validation, and sharing of simulation workflows, ultimately bridging the gap between industrial challenges and actionable results. Through the creation of FAIR datasets and adherence to best practices, OpenModel fosters a collaborative environment promoting innovation and informed decision-making in materials science and the manufacturing industry.

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Enhancing Collaboration and Innovation through DIGIPASS CSA and VIPCOAT Open Innovation Platform

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1. Introduction

In the era of digitalisation and Industry 5.0, the innovation paradigm has evolved to embrace collaborative frameworks that transcend traditional boundaries [1]. By showcasing VIPCOAT's developments towards Industry 5.0 through Quadruple Helix Open Innovation [2,3], this presentation aims to inspire and inform industry stakeholders, policymakers, researchers, and practitioners on the potential of collaborative ecosystems to drive technological advancement and sustainable development in the protective coatings industry and materials modelling and design more broadly.

2. Ontology-driven Open Innovation: Collaborative Pathways in Materials Science and Manufacturing

Ontologies serve as structured representations of knowledge, facilitating interoperability and semantic understanding among diverse stakeholders [4]. Incorporating ontological constructs into open innovation processes, this approach aims to streamline knowledge sharing, enhance data interoperability, and catalyse cross-disciplinary collaboration [5]. Significant advancements have been made in developing ontologies across diverse domains encompassing coating, physical entities and processes, business-related data, translation processes, and workflows. Key achievements include: i) the development of ontology tools facilitating ontology generation and updates, ii) the representation of physical entities and processes through knowledge graphs, and iii) the integration of business-related data into a Materials-based Business Case Ontology. Notable contributions include the harmonising the BPMN ontology with the EMMO, yielding a more comprehensive framework for workflows modelling, and the of a Translation ontology tailored to address intricate relationships within B2B2B environments. [6].

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3. Ontology-Based Translation and Decision-Making in the VIPCOAT Open Innovation Platform

The VIPCOAT architecture and platform facilitate group decision-making techniques and improve translation procedures in a business-to-business (B2B2B) setting. VIPCOAT simplifies commercial decision-making, translation procedures, and open innovation by fusing BPMN standards with ontology-based workflows and serious gaming principles.

4. Collaboration and Innovation through the VIPCOAT Open Innovation Platform.

VIPCOAT draws from open innovation, interoperability principles, and an open simulation platform, providing a structured approach that facilitates seamless integration and communication among disparate systems, enabling more efficient and effective collaboration. A critical component of the OIP is the integration of Business Process Model Notation (BPMN) workflows, powered by the Camunda engine, to support the innovation process from idea generation to project execution. This integration enhances transparency, efficiency, and collaboration across diverse stakeholders by providing standardised processes accessible to all users. Moreover, the event-driven workflow execution system, coupled with publish-subscribe patterns, ensures flexibility and scalability in managing complex workflows. By incorporating the Quadruple Helix Model, roles for stakeholders from different sectors are defined, optimising teamwork, and identifying potential bottlenecks in the innovation process proactively. Implementing custom BPMN and DMN editors, along with execution procedures, empowers users to create and deploy their applications seamlessly. Additionally, efforts have been made to ensure data interoperability through metadata standardisation and mapping to ontological concepts. This facilitates semantic interoperability, enabling meaningful data exchange and integration across different platforms and domains [7].

Figure 2: Web-page summarizing collaboration contributions and Simple BPMN workflow behind the process of project creation.

5. Conclusions

In conclusion, the emergence of collaborative frameworks in the era of digitalisation and Industry 5.0, exemplified by VIPCOAT's OIP, highlights the transformative power of Quadruple Helix Open Innovation. Through the integration of ontology-driven approaches, significant strides have been made towards enhancing knowledge sharing, interoperability, and collaborative decision-making in the protective coatings industry and beyond.

6. Acknowledgements

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Navigating Challenges and Embracing Innovation: Managing Partnerships and Ecosystems for Circular Materials in the Chemical Industry

Christian Seitz[1]

In today's rapidly evolving business landscape, traditional chemical and material producers like BASF are facing an array of challenges. These challenges arise from legislative pressures, escalating raw material and energy prices, and ever-increasing customer expectations. To navigate this challenging environment, innovation has become the key to success. However, for an established player like BASF, the focus lies on process innovations as a means to adapt and thrive.

One promising avenue for innovation lies in the development of technologies for circularity. These technologies enable the establishment of new raw material sources and the closure of material loops, contributing to a more sustainable and efficient production process. In this context, BASF has recognized the importance of forming new partnerships and ecosystems that include recycling companies and regulators. These collaborations are essential for harnessing the potential of circularity and overcoming the challenges that come with it.

This presentation aims to shed light on the significance of effectively managing these newly emerging partnerships and ecosystems. By delving into current examples from BASF's innovation pipeline, the contribution will highlight the strategies and approaches employed by the company to address the challenges of the evolving business landscape. The examples will showcase the successful integration of circularity technologies, effectively leveraging partnerships, and navigating regulatory frameworks.

Furthermore, the presentation will touch upon additional aspects that can be incorporated, such as the role of digitalization in enabling circularity, the importance of stakeholder engagement, and the potential economic benefits that can be derived from circular business models. By examining these key aspects, the presentation aims to provide valuable insights and practical lessons for other stakeholders in the materials arena.

The contribution will emphasize the significance of effectively managing these partnerships and ecosystems using three current examples from BASF's innovation pipeline.

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Are Your R&D Plans Big Enough?

Liza Shvyndzikava[1]

1. Introduction

The advanced materials market is expected to significantly grow over the next 5-8 years. The opportunities are there, but are the European companies ready to take them? Research shows that the European industry is behind in terms of investments, start-ups, and patents.

There are a number of technical challenges that the advanced materials market faces, but without solving the problems listed above, it would be difficult to overcome the technical challenges and keep the leading innovation position in the market.

The goal of my presentation is to bring attention to opportunities, show underlying challenges of the advanced materials market, and share potential ways to solve these challenges.

2. Current State of the Advanced Materials Market, Its Trends and Challenges

To give some examples of advanced materials market growth, according to Statista, the global market size for composites was 86.4 billion U.S. dollars in 2020 and will amount to 145 billion U.S. dollars in 2028. BCC Research claims that the global market for advanced aerospace materials is expected to grow from $26.4 billion in 2023 to $39 billion by the end of 2028. According to the European Commission, global demand for batteries is set to increase 14-fold by 2030. Revenue in the semiconductors market is projected to reach US$613bn in 2024, it is expected to show an annual growth rate (CAGR 2024-2027) of 6.3%, resulting in a market volume of US$736bn by 2027.

While the markets of various advanced materials are growing, there is also a number of existing technological challenges that need to be solved to secure a sustainable and prosperous future:

1) process optimisation
2) decarbonisation
3) mass customisation
4) zero defect production
5) circular economy
6) multi-materials processing
7) new materials processes.

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3. The European Advanced Materials Industry and Challenges It Faces

The European Union and its companies have all the chances to utilise the opportunities as they have the highest share of innovation leaders (41.9%), followed by China with 17.4%, and Japan with 11.5%. The US has only 4.5% of innovation leaders in this area. Another advantage for the EU is coming from a balanced industry ecosystem in advanced materials with a share of 13.7% resident companies.

However, the US takes a lead in the biggest and the most diverse start-up ecosystem, both in terms of the share of start-ups (around 50%) in advanced materials, and in terms of the share of capital raised (69.7%). The EU accounts only for 18.6% of start-ups, which is less than half of that of the US, and only 6.3% of raised capital. This is a big issue for the EU because start-ups may offer more radical innovations, they are usually more agile and responsive to disruption in the market.

Another challenge lies in the fact that the EU industrial R&I investments on advanced materials are not even half of those in the United States of America (EUR 19.8 billion investment in 2020 compared to EUR 50.3 billion).

There's also a rising gap in patents: the EU accounts for 15% of patents in advanced materials while the US has 28% and Japan—24%. The patent trend is rising in the US, China and Japan, but it remains stable in Europe.

Another important factor among many others acknowledged by the European Commission is the gap between groundbreaking research and industrial application which influences collaboration and strategic alignment, preventing the integration of advanced materials into industries.

All these factors combined pose a threat to the leading positions of European companies in the advanced materials market.

4. Insufficient Investments

The U.S. has a more developed capital market and a more specialised banking sector. VCs in the US tend to risk more and they also have stronger relationships with corporates. It allows American companies to be more efficient with investments.

It is difficult for the EU to compete with the quantity of the US investments due to certain peculiarities. That means the European companies need to find other ways to overcome the problem of limited financial resources:

- taking a more agile approach to innovation management;
- decreasing a level of bureaucracy and decentralising innovation;
- supporting start-ups and spin-offs that are able to develop radical innovations needed by the market;
- taking a more proactive approach in fostering innovation and relying less on the government, regulations and their initiatives;
- taking novel approaches to develop innovations and collaborate with other organisations.

5. Collaboration as the Solution

One of the solutions to the problem of limited resources is collaboration with other entities. However, willingness to collaborate should come from all stakeholders to be truly effective.

The European Union government is paying a lot of attention to the question of cooperation between the industry, academia and other players. AMI2030 is a great example of an initiative designed to unite organisations from various European countries.

Yet, this should not be the only solution. Collaboration should happen not only on the macro level, but also on the micro level. Keeping in mind the gap between groundbreaking research and industrial application, it is important to build bridges between enterprises and universities, and the initiative should be taken from both sides.

The companies might work towards:

- creating more industry-focused research centres at the universities;
- investing more into collaboration with students that might later become their employees;
- working with smaller, more applied universities across Europe and other countries that are not included in Top 100 universities;
- popularising science and making it more appealing to the younger generation;
- supporting university spin-offs.

Universities also need to move towards the industry and their challenges, as universities are also a part of the market economy. Losing market share leads to decreasing profits and taxes, which academia will also feel as cuts in programs and grants.

One of the main missions of Disruptiv is supporting collaboration between academia and the industry, to foster innovation and creativity, help the different parties in the process understand each other and find reliable partners by utilising novel approaches and frameworks.

6. Conclusions

The advanced materials market offers big opportunities in its growth and perspectives while also setting challenges that have to be solved. However, for the European industry to succeed and keep its leading innovation position, it is important to overcome other problems such as insufficient investments and the gap in research.

With limited resources, it is time to unite for all the stakeholders, including industry, academia and the government and become proactive in solving the challenges we face. At the end of the day, it is for our own benefit to be able to utilise the opportunities the market gives. The data suggests that European firms need to step up or their R&D in advanced materials risks being insufficient to maintain market share.

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Poster Presentations: Session 2

Navigating challenges: the use of advanced materials in medical devices

Susanne Resch[1], Julia Voglhuber-Höller[1], Andreas Falk[1]

1. Introduction

Advanced materials and its subgroup of nanomaterials enable the improvement and optimization of medical devices through targeted use. The special effects that these materials produce on the surface of certain products open up new possibilities for better treatment of patients. Still, the associated potential risks by using new, advanced materials should be controlled appropriately.

While medical devices are generally highly regulated (e.g., through the Medical Device Regulation (MDR) [1] in the European Union), the incorporation of advanced materials can generate risks and safety concerns (both for humans and the environment) that need to be addressed in order to achieve a predominantly beneficial use of advanced materials in medical devices and fully exploit their innovative potential.

2. Methods

Based on desk research, experts' interviews and workshops, the relevance of the MDR for advanced materials and nanomaterials was determined and gaps were identified. In addition, the relationship and links to other relevant guidance documents (e.g. ISO/TR 10993-22) were elaborated.

Next, safety concerns of selected advanced materials in medical devices were investigated along the value chain and the real-life applicability of the MDR was evaluated. The specific use cases were based on medical devices with antimicrobial and/or filtering effect, namely: (i) face masks made from antimicrobial textiles with silver nanoparticles, (ii) personal protective equipment based on textiles with an antiviral effect using zinc-oxide nanoparticles, and (iii) wound dressings with improved wound healing through advanced materials.

In addition, the potential added value of the Safe-and-Sustainable-by-Design (SSbD) concept to these use cases was investigated.

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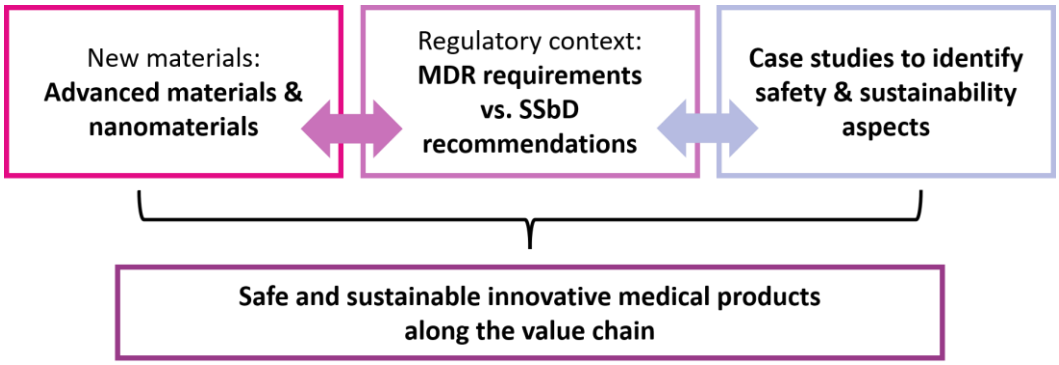

Figure 3: Methodological approach to evaluate the potential role of advanced materials in medical devices, their regulatory requirements as well as pre-market SSbD considerations to ultimately achieve safe and sustainable medical products along their value chain.

SSbD is aimed at developing safer and more sustainable substances via an iterative approach initiated in the early phases of innovation. The concept focuses on chemical substances and materials and covers their entire life cycle. It also incorporates safety and sustainability aspects into processes and related end products to ensure the protection of human health and the environment in all life cycle phases while balancing socio-economic aspects. The designated task for SSbD is to support achieving the objectives set in the European Green Deal. The SSbD framework [2] published by the European Commission's Joint Research Centre in 2022 describes the holistic approach in five steps, focusing on chemicals and materials; ultimately, the concept can be applied to R&D&I in all sectors, including the medical sector and medical devices.

Putting SSbD into practice by designing advanced materials as safe and sustainable as possible requires tools and models that enable the assessment of material properties such as reactivity, inflammatory and cytotoxicity potential. The HARMLESS SSbD framework builds on three pillars: (i) safer materials and products, (ii) safer production processes and safer use, and (iii) end-of-life. It is a stage-gate model with an implemented life cycle thinking approach that takes into account safety and sustainability, including design principles and different tools. It evaluates the safety, sustainability and functionality of the advanced material in the ideation and business phase, the lab phase as well as the pilot phase. As pre-market approach, it supports implementing SSbD in early innovation phases. The potential impact of the HARMLESS SSbD framework was assessed with a medical device use case and lessons learned for its applicability in this sector could be derived.

3. Conclusions

There is a need to investigate both benefits and risks associated with advanced materials in medical device development, not only to protect patients but also in a wider context to ensure the safe and sustainable use of new, advanced materials with (at least partly) unknown properties. The challenge lies in appropriate regulation that protects human health and the environment while not hindering innovation and market access, especially in Europe. The SSbD framework as a pre-regulatory approach supports a holistic design approach that emphasizes not only functionality but also safety and sustainability in the early innovation phase. However, it remains to be determined how the medical device market can benefit from this innovative approach and to what extent

it can complement regulatory requirements without placing additional burdens on the medical device development process.

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5. Acknowledgements

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AMULET Technology Roadmap

Marine Viale[1], Indira Altynbekova[1], Alexander Moreno[1], Emma Arussi[1], Aitor Hornés[1]

1. Introduction

The tremendous increase in anthropogenic CO2 emissions arose after the Industrial Revolution until our days are bringing undesired climate changes at a rate steeper than predicted. European Climate Law includes a set of measures targeting net greenhouse gas emissions reductions of at least 55% by 2030, compared to 1990 levels, aiming to make Europe climate neutral by 2050. These changes will involve the radical transformation of multiple value chains, from material development to the product's End-of-Life. In this context, advanced lightweight materials are central in driving the green and digital transition, recognized as critical enablers for nine key Materials Innovation Markets that address societal needs sustainably.

The Advanced Materials & manufacturing United for LightwEighT (AMULET) project (HORIZON 2020) aims to exploit the innovation potential of SMEs through a cross-sectoral, funded knowledge exchange to create new value chains by fostering the penetration of advanced lightweight materials (i.e., polymer-based composites (PBC), metallic alloys and ceramic matrix composites (CMC)) in different fields and sectors: automotive, aerospace and aeronautics, energy, and building.

AMULET's technology roadmap aims to inform decision-makers about the drivers, challenges and innovations related to lightweight materials in four different industrial sectors. This information will provide relevant technological insights about the developments being made in these sectors, allowing the elaboration of better policies as well as providing recommendations on which developments are more suitable to be prioritized.

The technology roadmap was developed using information from four sectoral workshops involving over 50 stakeholders covering various stages of the value chain. This data was completed with detailed bibliographic research.

2. The Automotive sector

The recent EU legislation, including the EU Climate Law, Fit for 55, and the EU Green Deal, underscores the global push to cut CO2 emissions and enhance resource efficiency. In the automotive sector, lightweighting has gained prominence to meet the ambitious target of 60 gCO2/km by 2030. Advanced lightweight materials offer a solution, showing promise in mitigating these additional aspects and even optimizing CO2 emissions for ICEs vehicles.

Studies indicate that a 10% weight reduction leads to a 14% improvement in electric range and a 6-8% decrease in CO2 emissions and fuel consumption. Transitioning to eco-

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friendly automotive sectors requires sustainable practices, with lightweight materials to extend range, enhance safety, and improve energy efficiency.

The automotive industry faces challenges in adapting to this transition, necessitating eco-design strategies and adjustments in manufacturing processes to incorporate renewable, bio-based, and recycled materials. Innovations such as thermoplastic materials, embedded sensors for predictive maintenance, and design-for-disassembly contribute to sustainability. Circular strategies like recyclable polymers and bio-based materials facilitate the use of secondary materials.

3. The Aerospace sector

In response to the escalating demand within the aviation industry for advanced lightweight materials, several drivers are at play, including the need for high-performance materials, adherence to fuel efficiency and emissions standards, capacity as well as maintenance cost optimization. Even a minor reduction in an aircraft's weight has the potential to yield reductions in fuel consumption and the associated CO2 emissions.

However, challenges persist, including supply chain vulnerabilities for critical raw materials and energy usage in manufacturing processes. Standardizing testing and certification for new materials in safety-critical components involves significant time and cost, impacting technology adoption.

Despite these challenges, material science is advancing with vigour. Nanotechnology is rapidly advancing, with nanocomposites growing at a 25% annual rate, enhancing aircraft components' durability and functionality. Multifunctional composites improve aircraft efficiency, while advanced modelling tools streamline design optimisation. Substituting thermoset materials with carbon fiber composites reduces structural weight and long-term costs. Graphene-related materials (GRMs) exhibit versatility in constructing lightweight, robust, electrically and thermally conductive structures, with the potential for self- healing and a remarkable 70% weight reduction.

4. The Energy sector

Energy is in the spotlight due to its key role in the transition to a zero CO2 emission society. The electrification of industrial and transport sectors is increasing the demand by an average of 2.4% per year. This concern extends beyond just considering CO2 emissions and encompasses the materials that will be used for the transition.

Wind turbine technology demonstrates this where PBCs constituting 16% of a wind turbine generator's weight have enabled the development of larger and more resilient blades (e.g., GE Haliade X). Nonetheless, the recycling and circularity of these composites present intricate challenges. Consequently, there's a growing trend towards the development of biodegradable materials. Affordable lightweight materials are essential to challenge existing technologies and align with Sustainable Development Goal 7, focusing on "affordable and clean energy."

An efficient value chain, prioritizing both cost and emission reduction, is essential. Streamlining manufacturing through local regulations and optimised transport networks in Europe is instrumental in addressing this challenge. Expanding beyond

energy generation, the effective storage of surplus energy, a critical aspect in the era of renewable energies, is vital.

5. The Building sector

The construction sector is known for its energy-intensive nature, demanding vast amounts of raw materials and natural resources. Additionally, the sector generates considerable waste and often operates inefficiently in terms of energy. In response, the industry is placing a higher emphasis on sustainability, focusing on life cycle assessments, minimising environmental impacts, and using recyclable, energy-efficient products.

However, challenges remain, like recycling difficulties, reliance on distant raw materials, and adapting to climate change. Research suggests solutions such as designing recyclable products, localising material sourcing, and introducing self-healing materials to mitigate greenhouse gas emissions and improve sustainability.

Regulatory requirements for the construction sector are also indispensable, addressing issues from energy inefficiency to safety requirements. The materials cost is comparably high and can be reduced with the use of lightweight materials. The durability and performance of construction materials are important for extending building lifespans and reducing repair and replacement frequency. Lightweight materials offer speed and efficiency in construction, saving labor and transportation costs, and enabling innovative designs.

6. Conclusions

Innovative lightweight materials are paving the way in diversifying innovative advancements globally at a phenomenal pace. These materials are part of the solution to the global challenges offering higher performance during use, lower cost, resource, and energy efficiency considering the end-of-life performance. Global trends toward CO2 reduction and resource efficiency have significantly increased the importance of this topic over the last years.

Advanced lightweight materials are crucial for realising sustainable growth of all four sectors under study: automotive, aviation, energy and building. AMULET's technology roadmap emphasises the relevance of advanced lightweight materials to contribute to Europe's competitiveness by increased sustainability standards and provides first-hand information to decision-makers.

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Session 3: Digital Innovation - Catalysing the Green & Digital Transition for Innovative Advanced Materials and Products

This Session is organised by the Horizon Europe DigiPass CSA, whose overarching goal is to support EU materials communities on their transition towards a green and digital future, irrespective of their current digital maturity level. The aim of DigiPass is to elevate the digital maturity of these communities by providing clear guidance and tools supporting the implementation of digitalised circular business models that rely on safe and sustainable Innovative Advanced Materials (IAM) and product manufacturing. This objective builds upon the Advanced Materials Initiative 2030 (AMI2030) and the up-coming partnership on Innovative Advanced Materials for EU (IAM4EU).

The main objective of the session is to initiate collaboration among different ongoing EU-wide and national projects and initiatives focused on digitalisation of IAM´s development and manufacturing. The session aims to foster homogenisation and standardisation within the IAM ecosystem as a necessity for the introduction and utilisation of open innovation processes and Digital Materials and Product Passports (DMP, DPP) for a diverse range of industrial applications.

Specific objectives of the session are to delve into the needs, requirements, and challenges pertaining to:

- Requirements on an EU-wide federated digital platform supporting DMP/DPP utilization and to facilitate the design and manufacturing of IAMs.
- Identification of common themes and scientific/technical interests shared among ongoing EU projects that align with the objectives and vision of the DigiPass CSA initiative.
- preparation of an initial action plan on the collaboration of DigiPass and related projects and initiatives.

Presentations and posters will also cover the following topics:

- Digitalisation of workflows in materials R&I along value chains,
- Digital Materials and Digital Product Passports (DMP/DPP),
- Data-handling, -storage, – management (e.g. Industry Commons)
- Circular business models.

Detailed Programme

Start	End	Title	Presenter
14:30	14:55	tbc	Victoria Petrova
14:55	15:05	DigiPass: Knowledge Valorisation for Innovative Advanced Materials Design and Development	Natalia Konchakova & Peter Klein
15:05	15:10	Session / Cooperation/ Collaboration	Natalia Konchakova & Peter Klein

15:10	15:20	Platform MaterialDigital: Enhancing Scientific Collaboration within the MSE Community	Jörg Schaarschmidt
15:20	15:30	PEPR DIADEM: Priority Equipment and Research Program on the development of innovative materials using artificial intelligence	Fernando Lomello
15:30	15:40	IRISS – the International ecosystem for accelerating the transition to Safe-and-Sustainable-by-design materials, products and processes	Emma Strömberg
15:40	15:50	The use of analytical research infrastructures to support industrial innovation	Ennio Capria
15:50	15:55	Magnetic Multiscale Modelling Suite	Thomas Schrefl
15:55	16:00	DECODE: Cloud-connected Labs of Future for Energy Materials	Kourosh Malek
16:00	16:05	Multiscale Characterisation and Simulation for Hydrogen Embrittlement Assessment: Development of an Open Knowledge Platform to Foster Capability Integration (HyWay)	Napat Vajragupta
16:05	16:10	SiToLub – Simulation Tools for the design of safe and sustainable Lubricants	Francesco Pagano
16:10	16:15	CHEMATSUSTAIN: Implementing Innovative Methods for Safety and Sustainability Assessments of Chemicals and Materials Particularly at Nano Level in the European Union	Jelena Barbir
16:15	16:20	AI-driven multiscale methodology to develop Transparent Wood as sustainable functional material using SSbD	Päivi Kivikytö-Reponen
16:40	16:45	Battery manufacturing digital twin design in view of requirements for the digital product passport	Martin Thomas Horsch
16:45	16:50	COST Action EuMINe – European Materials Informatics Network	Francesco Mercuri
16:50	17:05	24/7 Poster Presentations	
17:05	18:20	Round Table / Fishbowl discussion: Materilas Digitalization, Digital Materilas & Product Passport	Peter Klein, Franz Pirker, Salim Belouettar, Natalia Konchakova
18:20	18:30	Collaboration actions/ Close Notes	all projects / participants

Posters

S03_P01	Ensuring regulatory Alignment in the R&I of Innovative Materials	Steffi Friedrichs
S03_P02	CHIASMA – Accessible Innovative Methods for the Safety & Sustainability Assessment of Chemicals & Materials	Tommaso Serchi
S03_P03	INSIGHT – Integrated Models for the Development and Assessment of High Impact Chemicals and Materials	Dario Greco
S03_P04	PINK – computational approaches for industry-ready Safe-and-Sustainable-by-Design	Thomas E. Exner
S03_P06	Multidimensional Integrated Quantitative Approach To Assess Safety And Sustainability Of Nanomaterials In Real Case Life Cycle Scenarios Using Nanospecific Impact Categories	Massimo Perucca
S03_P07	SSbD4CheM: Safe and Sustainable by Design framework for the next generation of Chemicals and Materials	Panagiotis D. Kolokathis
S03_P08	An SSbD integrated impact assessment framework for advanced materials developed by SUNRISE	Lisa Pizzol
S03_P09	Development of PFAS-free coatings in a safe and sustainable by design (SSbD) approach- the PROPLANET project	Eleonora Longhin
S03_P10	The interlinked SUNSHINE Trusted Environment and Foresight Framework as a tool for detecting emerging trends in AdMa Innovation	James Baker
S03_P11	Tackling Innovation Challenges in an Industry 5.0 context with an Ontology-based Open Translation Environment	Gerhard Goldbeck
S03_P12	Bridging the Gaps in Nanosafety for Animal-Free Prediction of Adverse Outcomes	Vladimir Lobaskin
S03_P13	Ontology-based Decentralized Sharing of Industry Data in the European Circular Economy	Mikael Lindecrantz
S03_P14	openLCA and OpenSemanticLab – Build a Digital Bridge between Material Science and Life Cycle Assessment (LCA)	Simon Stier

Oral Presentations: Session 3

DigiPass: Knowledge Valorisation for Innovative Advanced Materials Design and Development

N. Konchakova[1], S. Belouettar[2], F. Pirker[3], P. Klein[4]

1. Introduction

The twin green-digital transition is a cornerstone of the European strategy. This transition should lead to a circular, sustainable, and net-zero-emission European economy that works for people. Advanced materials are the source of prosperity and form the backbone of a systematic approach to innovative products in-line with the European strategy as greatly analysed in the Materials 2030 Manifesto [1] and presented in the Communication of the Commission on Advanced Materials for Industrial Leadership [2].

DigiPass CSA project, started in April 2024, supports the twin green-digital transition accelerating digitalization processes in materials manufacturing through enhancing the digital maturity of industrial stakeholders and through harmonization of data and knowledge exchange using digital environments / platforms [3]. DigiPass promotes the exchange of digital material data between industry and research institutions, laying the foundations for a digital material and product passport [4].

Figure 4: DigiPass Logo and Slogan.

2. Digitalisation of Advanced Materials

The overarching objective of the DigiPass CSA project consists in enhancing the digital maturity of the European communities that develop materials and intermediate products by harmonizing and synergizing collected materials data sources and digital infrastructures. The project develops recommendations and clear routes toward digitalized circular business models. The overarching key result of DigiPass is to create a sustainable platform which includes support for Digital Materials & Product Passports and for collaborative innovation-by-design processes in a circular economy served by advanced materials. A business model for operating such a platform completes the overarching objective.

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Accelerating the design, development, and production of safe and sustainable chemicals and materials, as they are necessary for innovative products, calls for a collaborative approach involving different stakeholders to advance circularity of the European economy at large. However, the stakeholder groups involved in product innovation based on advanced materials are today at heterogeneous levels of digital maturity. Digital Materials & Product Passports will create a coherent framework and minimum digital maturity across advanced materials and manufacturing in Europe. In addition, DigiPass will enable interoperability of data exchange and standardization of advanced materials data at all maturity levels.

3. Demonstration by industrial use cases

DigiPass will provide 4 demonstration cases for different industrial sectors:

- Advanced Composite Materials
- Advanced Materials for Renewable Energy Sources
- Health & Safety of Advanced Nanomaterials
- Innovative Materials for Pre-painted Metals

Partners from academia and industry, including industrial associations are working together to increase the competitiveness of European companies and boost their productivity. Digital materials and product passport contains all relevant information about the material, its origin, processing and environmental impact on all stages of its lifetime. At the end of its life, the collective product information will enable recycling companies to process materials more effectively, resulting in more sustainable solutions and helping minimise the material's overall environmental impact [4]. The ideal scenario will be provided for each demonstration case as a success user story.

4. Collaboration among Stakeholders and Projects.

DigiPass collaborates with projects and national initiatives working on digital aspects of materials design and development, in particular with the Materials Commons infrastructure components [5], EOSC, Platform MaterialDigital, Diadem [2], some EU funded projects like BIG-MAP, and CIRPASS-2.

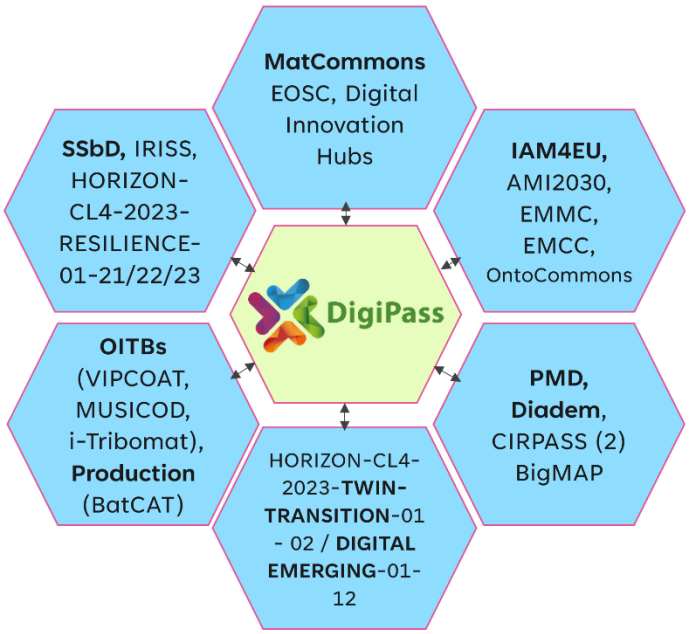

Figure 2: DigiPass focused collaboration environment.

Moreover, the SSbD projects lead by IRISS CSA and EU projects funded under following topics:

HORIZON-CL4-2023-TWIN-TRANSITION-01-02,

HORIZON-CL4-2023-RESILIENCE-01-21,

HORIZON-CL4-2023-RESILIENCE-01-22,

HORIZON-CL4-2023-RESILIENCE-01-23,

HORIZON-CL4-2023-DIGITAL-EMERGING-01-12

are in the focus of establishing collaborations with DigiPass. A schematic representation of the DigiPass cooperation network is presented in Figure 2.

DigiPass CSA is aiming to take on board all materials development communities. We are open for cooperation with any projects and stakeholders. Please contact us and register at the project homepage as a stakeholder to receive information about the project development and on-going actions [3].

5. Conclusions

Accelerating the materials innovation cycle calls for a collaborative approach involving different stakeholders in a circular economy to support manufacturing, durability, repair and overhaul, reuse, and recyclability of products. These requirements set the stage for all materials development communities in Europa and need to get implemented as targets in materials and product innovation processes as soon as possible [6]. The long-term vision of the DigiPass CSA is to enable industry to know their products in a systemic sense as entities in a circular economy.

6. Acknowledgements

The authors acknowledge funding from the Horizon Europa programme of the EU by Grant Agreement No. 101138510, DigiPass CSA project, and UKRI funding under Grant Number 10100819-DigiPass.

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Platform MaterialDigital: Enhancing Scientific Collaboration within the MSE Community

Jörg Schaarschmidt[1], Tilmann Hickel[2,3], Wolfgang Wenzel[1], Platform MaterialDigital Consortium[1,2,3,4,5,6]

1. Introduction

The 'Platform MaterialDigital' (PMD)[1], supported by the German Federal Ministry of Education and Research (BMBF), focuses on creating a prototypical infrastructure for the digital representation of materials science and engineering. The core of the PMDs approach is enabling digitalization in this field through decentralized data servers, standardized data schemas, and digital workflows. These different aspects are addressed within the platform's focus areas IT architecture, semantic interoperability, and workflows and disseminated via the working group of the focus area community interaction.

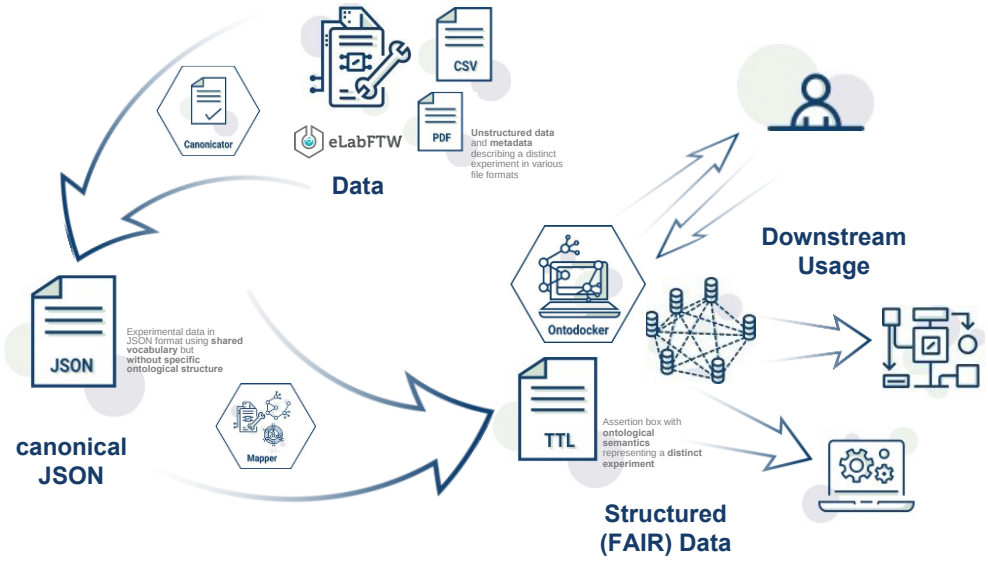

Figure 5: The platform MaterialDigital (PMD) aims to provide prototypical solutions for all processes involved in the digitalization of materials science including acquisition, structuring, storage, and processing of data. The depicted PMD data acquisition pipeline showcases the different concepts involved, including the PMD core ontology [2], in the transformation of raw data to is FAIR-compliant structured data within the context of MaterialDigital.

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[5] Leibniz-Institut für Werkstofforientierte Technologien (IWT), Bremen
[6] FIZ Karlsruhe – Leibniz-Institut für Informationsinfrastruktur, Karlsruhe

2. Scientific Workflows within MaterialDigital

With the first funding phase nearing its end, the PMD is entering a pivotal phase. The initial projects, primarily driven by academic research, have set a robust foundation. The ongoing transition marks the beginning of the second funding phase, now spearheaded by industry-led projects. These new endeavors aim to extend the reach and influence of PMD in the materials science community. At the heart of PMD's strategy to streamline data processing steps and simulation tasks are the workflow frameworks pyiron [3] and SimStack [4], reflecting the platform's emphasis on scientific workflows. The respective working group focuses on the various challenges involved, including the integration of semantic data and the semantic description of workflows. It Furthermore develops and provides the MaterialDigital Workflow Store [5] as an important tool to spread established workflows and encourage standardization across the community.

3. Conclusions

The Platform MaterialDigital represents a pioneering effort to harness the potential of digitalization in materials science and engineering. By fostering a collaborative ecosystem that bridges academia and industry, the PMD aims to streamline scientific workflows and enhance data interoperability. The transition to industry-led projects signifies a maturation of the PMD's objectives, ensuring that the platform remains at the forefront of innovation and application in MSE. The emphasis on standardized data schemas, decentralized data management, and the integration of semantic workflows underscores the platform's commitment to establishing a comprehensive digital infrastructure. As the PMD moves forward, its continued evolution and the expansion of the MaterialDigital Workflow Store are pivotal in realizing a unified, efficient, and highly collaborative materials science community. By harnessing the collective expertise of the MSE community, the PMD stands not only to enhance scientific collaboration but also to drive forward the development of new materials and technologies. In doing so, it underscores the transformative potential of digitalization in advancing both research and industry.

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[3] *J. Janssen, S. Surendralal, Y. Lysogorskiy, M. Todorova, T. Hickel, R. Drautz, J. Neugebauer;* **pyiron: An integrated development environment for computational materials science** Computational Materials Science 163 (2019) 24 - 36
[4] *C. Rego, J. Schaarschmidt, T. Schloeder, M. Penaloza-Amion, S. Bag, T. Neumann, T. Strunk, W. Wenzel*; **SimStack: An Intuitive Workflow Framework**. Frontiers in Materials 9 (2022) 877597
[5] https://workflows.material-digital.de

PEPR DIADEM: Priority Equipment and Research Program on the development of innovative materials using artificial intelligence

Fernando Lomello[1], Lucie Bard[2], Mario Maglione[2], Frédéric Schuster[3]

To foster the rapid research and market entry of more efficient, sustainable materials derived from non-critical and non-toxic resources is a major challenge. To this aim, a nationwide program has been launched in France in 2021. This exploratory Priority Equipment and Research Program (PEPR) DIADEM is focussed on the Development of Innovative Materials Using Artificial Intelligence). Through the orchestrated synergy of scientific endeavours powered by artificial intelligence (AI), PEPR DIADEM aims to speed up the innovation chain "from concept to fruition," thereby fundamentally reshaping the approach to Materials Science in a sustainable manner. This global approach is similar to some undergoing projects, worldwide.

Addressing contemporary and future societal challenges across energy, transportation, digitalization, and healthcare necessitates the rapid discovery of novel materials, spanning from metallic alloys to functional nanostructures. Given the pressing timelines outlined in the Green Deal framework, there is an urgent call for accelerated development in this domain. Fortunately, the requisite technologies, including rapid synthesis and characterization tools, automation, digital simulations, data management capabilities, AI, additive manufacturing, and thin films engineering, are readily available to meet these challenges head-on.

Led by the CNRS and the CEA in collaboration with seven academic partners, PEPR DIADEM aims to expedite the discovery and integration of materials while addressing environmental and societal concerns. Endowed by France 2030 with a budget of €85M, the program seeks to facilitate the design and market entry of superior and sustainable materials, with a strong emphasis on leveraging AI. This funding is initially allocated to establish a network of four cutting-edge platforms across France, strategically distributed and meticulously coordinated under the banner of the DIADEM DISCOVERY HUB. These platforms integrate high throughput synthesis, combinatorial formulation, automatized shaping, broadband characterization, and digital tools for multi-scale modelling, data mining, supervised learning, and AI adaptation.

Seventeen targeted projects aim to establish this unique network and demonstrate its effectiveness in accelerating the discovery of innovative materials. Additionally, three calls for projects, open to the extensive French materials community comprising approximately 4000 researchers and engineers, have been launched from 2023 and extended up to 2025. Interaction with existing infrastructures and research networks is a key criterion for project selection and co-funding by companies and international partners is strongly encouraged. The openness of the DIADEM DISCOVERY hub to

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[3] Université Paris-Saclay, CEA, Cross-Cutting Program on Materials and Processes Skills, 91191 Gif-sur-Yvette, France

various partners will be a key indicator of its global success, with approximately 30 projects set to be selected through an international panel across the three rounds of calls.

A dedicated program for the training of scientists, both novice and experienced, complements this framework, with international cooperation, such as co-supervision of PhDs, playing a crucial role. PEPR DIADEM leverages existing infrastructure such as the SOLEIL and ESRF synchrotron facilities and collaborates with the recently established "AI for sciences and sciences for AI" centre by CNRS. International cooperation is central to DIADEM's mission, both in research and development and in training. At the European level, DIADEM aligns with initiatives such as IAM4EU and AMI2030.

The DIADEM DISCOVERY HUB project builds upon platforms initially dedicated to key material classes, crucial for accelerating the materials identification cycle from two decades to a range of four to ten years. These platforms ideally encompass:

1. Combinatorial and/or high-throughput synthesis and shaping of materials: Leveraging various robotized synthesis and additive manufacturing techniques to swiftly develop novel material compositions, including metallic, inorganic, and potentially bio-sourced polymer matrices. Thin film engineering plays a significant role in achieving desired performance outcomes, with special emphasis on synthesizing new architectured materials, composites, hybrids, and bio-inspired constructs.
2. High-throughput chemical and structural characterization: Utilizing cutting-edge facilities such as the SOLEIL and ESRF synchrotrons, advanced TEM, and fast chemical mapping methods such as LIBS, to assess usage properties; in situ and operando characterizations are crucial for broadening and expediting data acquisition, particularly under extreme conditions.
3. Digital simulation of materials and processes: Employing multiscale simulation tools, including AI approaches, seamlessly integrated into workflows to enable automated and high-throughput calculations.
4. Databases for storage, management, and AI-driven exploitation: Structuring resulting data into databases and developing AI tools to enhance data exploitation, crucial for facilitating a productive dialogue between data and material sciences. The digital platform DIAMOND is the green part of figure 1, binding the entire experiment-oriented platform. This raises the challenge that all similar projects are facing, which is the necessary dialog between data and material sciences.

The interplay among these platforms holds the potential to revolutionize innovation in materials science, driving sustainable solutions to address global challenges.

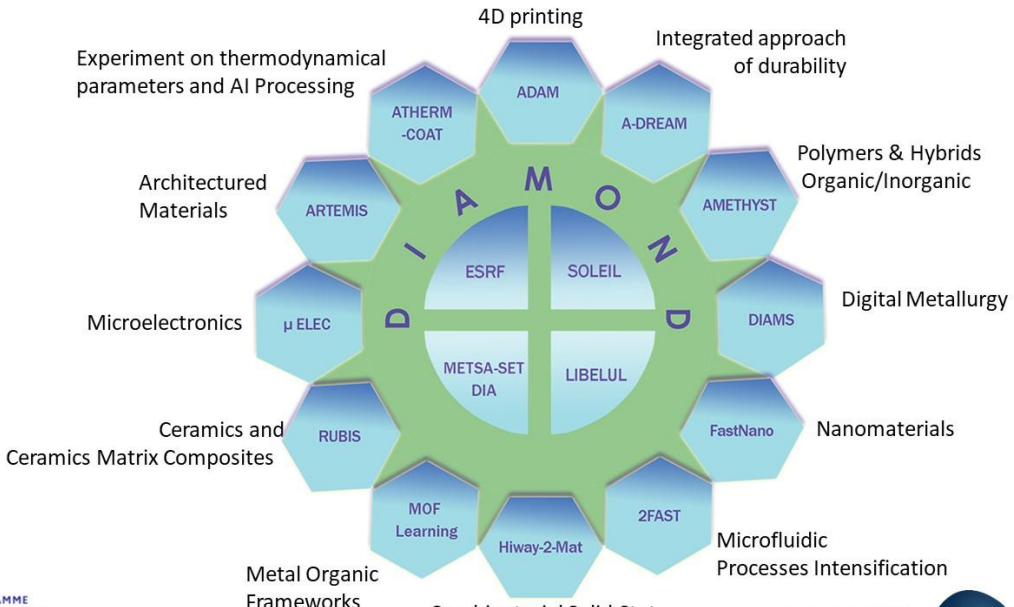

Figure 6: Actual seventeen targeted projects of PEPR DIADEM more details at https://www.pepr-diadem.fr/en/

IRISS - the International ecosystem for accelerating the transition to Safe-and-Sustainable-by-design materials, products and processes

Emma Strömberg[1]

1. Introduction

The IRISS project aims to connect, synergize and transform the SSbD community in Europe and globally towards a life cycle thinking where there is a holistic integration of safety, climate neutrality, circularity and functionality of materials, products and processes throughout their lifecycle to meet the EU Green Deal, EU Chemicals Strategy for Sustainability, and UN SDGs.

One of the main goals is to build an EU-led permanent network though development of a state-of-the-art SSbD ecosystem that is supportive for the uptake of SSbD strategies by all stakeholders in the society, facilitating implementation of the EU SSbD framework. The project offers a platform for knowledge sharing towards a common understanding and implementation of the SSbD concept. The engagement of a broader community is achieved through the international dissemination activities. In addition, IRISS is committed to engage multiple stakeholders with different roles in the society in dialogues, co-creation and cooperation on SSbD as an enabler for resilience and competitiveness.

The project is also developing broadly supported overarching and value chain specific SSbD roadmaps targeting scientific research needs; skills, competences and education needs; knowledge and information sharing needs. The IRISS project enables to facilitate adaptation to new requirements for design and production processes that will lead to technological development. The project contributes to both policy understanding and exchange of experience between different value chains and sectors, highlighting the challenges and opportunities the SSbD concept entails. The value chains are assessing the challenges and providing solutions through specific roadmaps, which describe innovation proposals for SSbD products. The knowledge exchange and dissemination of case study results facilitates faster uptake within the market, supporting SSbD implementation, with emphasis on SMEs. The collaboration with the PARC partnership and both Horizon 2020 and Horizon Europe projects ensures the knowledge transfer needed for the implementation of the SSbD concept. The developed roadmaps will assure the companies' integration of SSbD at the forefront as well as creating regulatory feedback.

Funded by the European Union

The project receives funding from the European Union's HORIZON EUROPE research and innovation programme under grant agreement n° 101058245. UK participants in Project IRISS are supported by UKRI grant 10038816. CH participants in Project IRISS receive funding from the Swiss State Secretariat for Education, Research and Innovation (SERI).

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The use of analytical research infrastructures to support industrial innovation

Ennio Capria[1]

1. Introduction

Analytical Research Infrastructures (ARIs, (among which synchrotrons sources like the ESRF), may contribute and already contribute to industrial innovation, supporting R&D and QA activities of SMEs and LCs. They are definitely supporting industry in new material development and in the optimisation of processes and products. This is indeed part of their mission and they have dedicated resources for this. Furthermore, they are often active at the core of dedicated ecosystems (like the one of Grenoble). This can allow them to make available a know-how that can go far beyond the simple deployment of our instrumentation.

2. Analytical Research Infrastructures supporting accelerated discovery of new materials

Today, these large scale research infrastructures, are organised in the framework of ARIE (Analytical Research Infrastructures of Europe (www.arie.eu). If we think about the opportunities related with the deployment of these ARIs there is a quite low hanging fruit to be harvested. This is represented by the deployment of streamlined routine services capable to run high throughput standardised experiments, where large lots of similar samples need to be characterised in an automatic fashion. These novel routine services need new pipelines to be consolidated going from the data acquisition, to the data reduction, to the data analysis. These systems will be capable to produce huge datasets capable to feed AIs in a feedback loop between sample production, characterisation and modelling with the results to accelerate the discovery of new material and a more rational design of new products (see fig.1).

3. Overcoming the barriers to entry

Unfortunately, today, when one thinks about ARIs supporting industry, often only considers their contribution to the scientific excellence pillar, where a lot can be done, for sure, in collaboration with industry, in the pre-competitive phase of the product development. Nonetheless, it already exists a proof of evidence that, by considering ARIs as potential business partners for industrial projects at higher TRL/MRL, could result in an incredible acceleration in material discovery and new product design. Nonetheless, in order to happens, this would need external stimulation, because this activity falls somehow beyond the core business of these facilities and industry would be a fast follower indeed, but would not take the initiative, due to a perceived lack of specific competences.

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4. A core business for Pillar II

Some of the tools made available in pillar II demonstrated very effective in the definition and the deployment of these new services. In particular, in the context of the calls supporting characterisation, the projects EASI-STRESS, NanoMECommons and AddMorePower, demonstrated the viability of this concept. New services have been developed exploiting the unique capabilities available at the European Synchrotron (ESRF), always in compliance with the data exploitation frameworks developed by the European Material Characterisation Council (EMCC) and Modeling Council (EMMC).

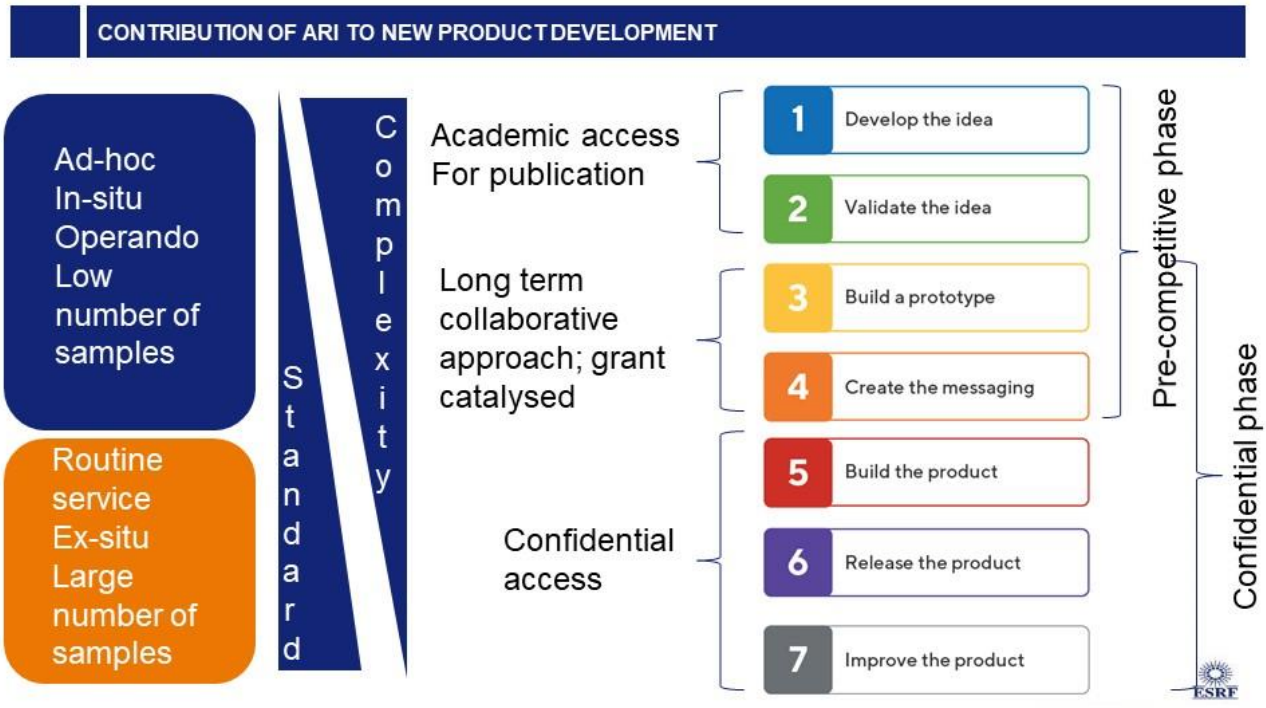

Figure 7 Contribution of ARI to the New Product Development]

5. Conclusions

In conclusion, there is a strong evidence that whatever strategy would be defined to support advanced material based industrial innovation, it would receive enormous benefits if these considerations will be taken on-board.

Magnetic Multiscale Modelling Suite

Thomas Schrefl[1], Thomas G. Woodcock[2], Heike Herper[3], Nora Dempsey[4], Hans Fangohr[5], Andreas Marek[6], Gotthard Rieger[7], Stefan Tibus[8]

1. Introduction

Magnets are crucial for many of today's technologies, from the motors that power electric vehicles to computers, smartphones and the generators in wind turbines which help to reduce global warming. The EU demand for rare earth metals, used in wind turbines and electric vehicles is expected to increase six to seven-fold by 2050 [1]. The EU relies almost exclusively on imports for rare earth elements used in high-performance magnets. Substitution of critical raw materials and recycling are facilitated by computational materials design. The project entitled MAgnetic Multiscale MOdelling Suite (MaMMoS) is funded under the umbrella of the call Adaptive multi-scale modelling and characterisation suites from lab to production (HORIZON-CL4-2023-DIGITAL-EMERGING-01-12) and aims at the development of an open-source software platform for magnetic materials modelling.

2. Multiscale simulations and artificial intelligence

The macroscopic properties of magnets arise from the interaction of phenomena at different length and time scales. This often limits the application of numerical methods for magnetic materials development. The goal of MaMMoS is the design and optimisation of magnetic materials and devices based on multiscale modelling, characterisation, and numerical optimisation. To achieve interoperability between software and analysis tools, we will establish a domain ontology for magnetic materials. We aim to create standards for linking simulation software for magnetic materials from first principles simulations and micromagnetics to device level simulators (see Figure 1). MaMMoS will use artificial intelligence (AI) to fuse modelling and characterization data. AI methods will identify and correct systematic errors in the simulation data, enabling more accurate predictions. Moreover, AI models can fill gaps where measurements are not available. AI models can also serve as a surrogate in multi-objective optimisation. Optimisation will guide further experiments or simulations, reducing the development time. In MaMMoS, we will apply this approach to speed up the development of permanent magnets with reduced critical elements for electric machines and to optimise the layout of magnetic field sensors for high linearity range. The MaMMoS software will be validated against benchmarks defined according to the industrial

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requirements for electric machine and sensor design. The multiscale magnetic materials modelling suite will be made open source to enable easy access to high-end simulation tools. Interoperability will facilitate data sharing and reuse among researchers and industries. Interpretable machine learning will reveal insights into the physics and chemistry of magnetic materials and guide the discovery of new materials.

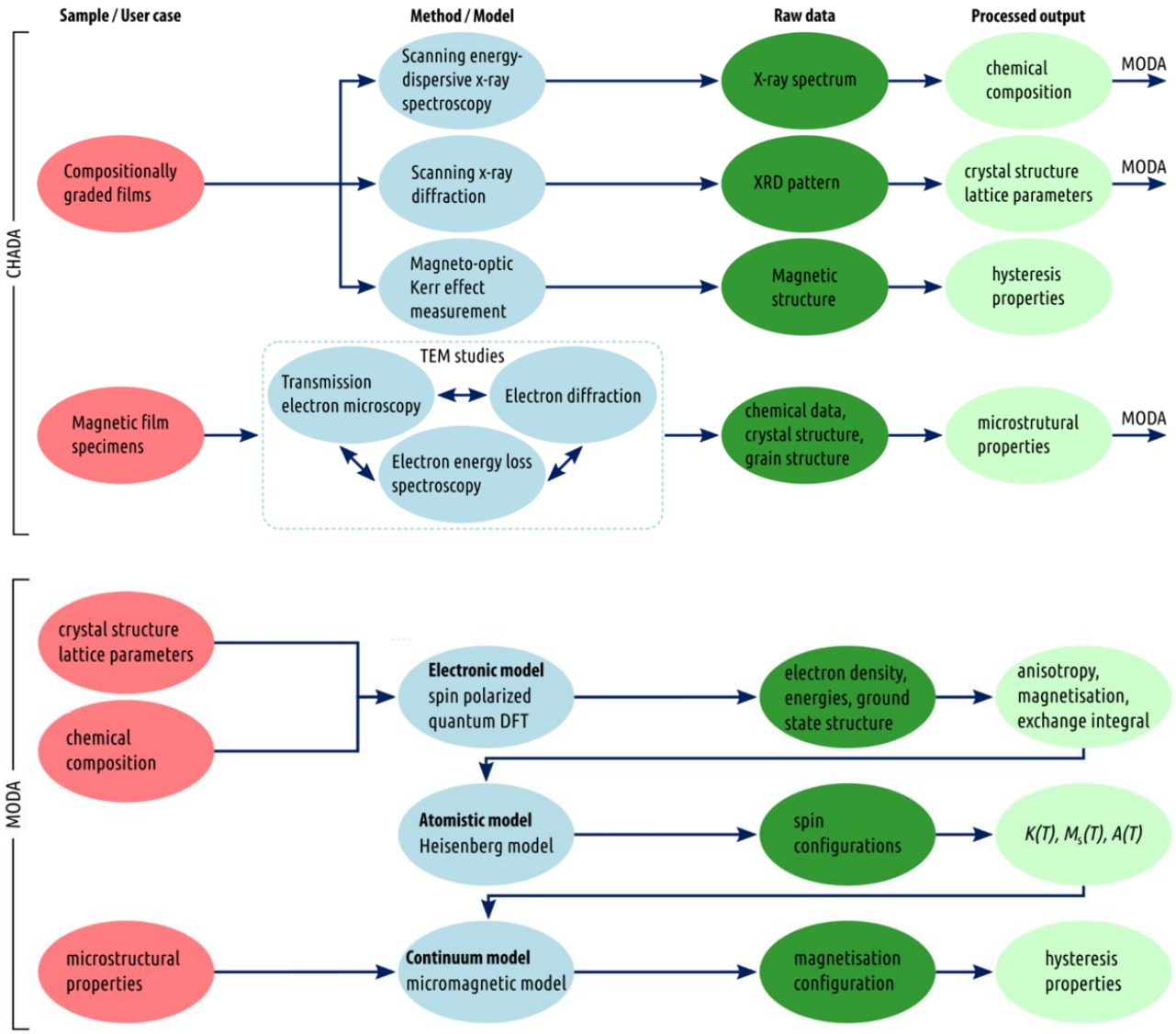

Figure 8: Linking of experimental data (CHADA) and modelling data (MODA) for the evaluation of the temperature dependent intrinsic magnetic properties and the hysteresis properties of magnetic materials.

3. Acknowledgement

Funded by the European Union (Grant agreement ID: 101135546). Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or the European Health and Digital Executive Agency (HADEA). Neither the European Union nor the granting authority can be held responsible for them.

Funded by the European Union

4. References

[1] European critical raw materials act, Fact sheet, March 2023.

DECODE: Cloud-connected Labs of Future for Energy Materials

Kourosh Malek[1,2], Michael Eikerling[1,2]

1. Introduction

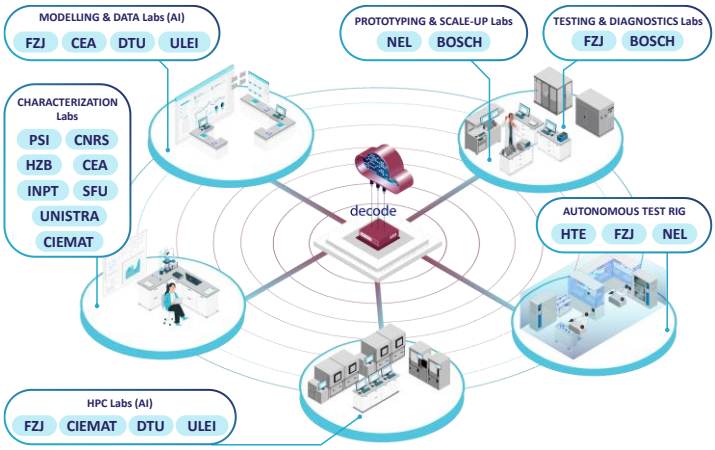

***Figure 9**: Representation of DECODE's Future Labs concept.*

The clean energy technology sector faces a major challenge with the pace of development trailing behind commercialization targets. The root cause hampering progress towards cleaner materials and technologies is that laboratories with complementary capabilities still largely operate in separation, with a lack of coordination among their efforts. The EU-funded DECODE project (**DE**-centralised **C**l**O**ud Labs for in**D**ustrialisation of **E**nergy Materials) aims to break down these barriers by creating a decentralised and adaptive cloud-connect labs concept. DECODE aims at transforming the development and innovation process for clean energy materials and technologies. The project envisions the creation of a decentralized platform that connects multiple labs to enhance the effectiveness and accelerate the progress of research and development in the field of clean energy technology. The core elements of the platform consist of the DECODE FABRIC, a matrix-like structure that facilitates collaboration, and a scoring system to assess integration readiness of methods and tools. An AI-enabled CPU orchestrates contributions from partner labs.

Initially focusing on hydrogen technologies, DECODE's vision may be expanded to other technologies including energy harvesting, storage, clean water and more. The platform strives for an unprecedented level of flexibility and adaptability, accommodating diverse strategies and technologies. In summary, DECODE accelerates clean energy innovation through interconnected labs, fostering a sustainable and cleaner future.

The overall objective of DECODE is to digitally connect multiple labs, boost the effectiveness, and accelerate the development and integration of materials for sustainable hydrogen technologies.

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Europe's transitioning to a sustainable and green future calls upon strategies for the accelerated development and scale-up of materials to respond to geopolitical threats to Europe's **technological sovereignty** and to the **supply chain security** of key raw materials.

The DECODE Consortium is a partnership of leading European research centres (RTOs) as well as industrial companies and academic partners representing various sectors of the industry such as electronic engineering, materials processing, algorithm development, software, and hardware design and development as well as integration and packaging technologies.

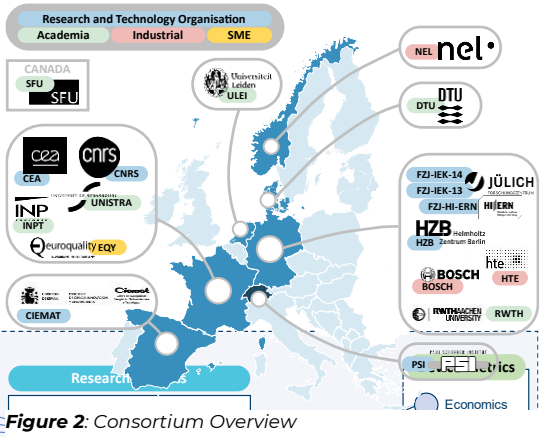

***Figure 2**: Consortium Overview*

2. General Methodology

The agnostic DECODE platform in comparison with the conventional approach is illustrated in Figure 5. At its core, DECODE strives to develop and deploy three innovative modules: 1) the **DECODE Foundry**, a semantic search engine for assembling methods and tools into practical workflows, 2) the **DECODE FABRIC**, a matrix structure that connects modelling and characterisation suites, and 3) the **DECODE CPU** for end-to-end orchestration of a given materials development to integration pipeline. The platform, designed for unprecedented flexibility and interoperability, harnesses AI-driven data management and ontological mapping to enable the seamless collaboration among partner labs. DECODE heralds a new era in collaborative and transferable clean energy research, with water electrolysis and hydrogen fuel cells as test cases.The DECODE platform will be built with a modular architecture, harnessing existing AI-cloud and data management infrastructure at Forschungszentrum JÜLICH - IEK-13 (Virtual Mind Labs).

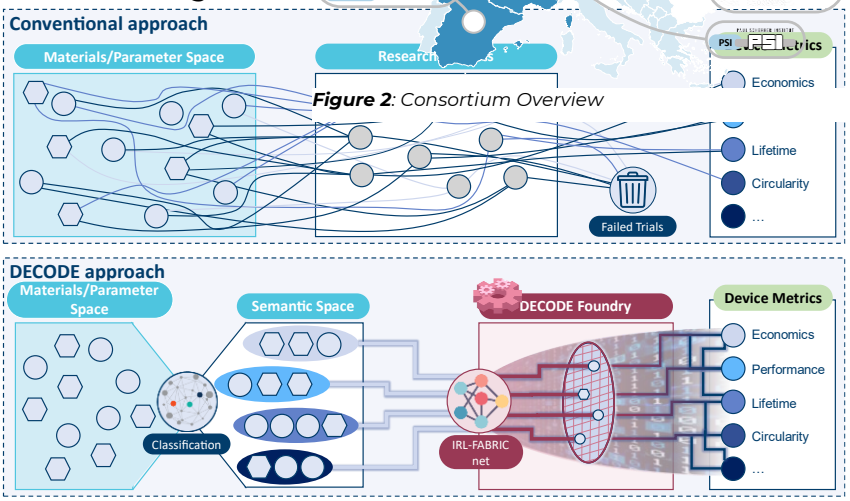

***Figure 3**: Conventional process vs. DECODE process. Modelling concepts (blue circles), characterisation tools (blue hexagons), methodologies (grey circles).*

3. Conclusion

The DECODE project[3] has been designed to achieve an integrated European materials platform, allowing a systemic use of tools and capabilities including materials modelling, characterisation, robotics, data documentation, ontologies, artificial intelligence, and

[3] This project has received funding from the European Union's Horizon Europe Research and Innovation Program under Grant Agreement No 101135537.

machine learning, which are orchestrated to accelerate the design, development and application of chemicals, materials and related processes and manufacturing.

Multiscale Characterisation and Simulation for Hydrogen Embrittlement Assessment: Development of an Open Knowledge Platform to Foster Capability Integration (HyWay)

Napat Vajragupta[1], Guntis Mosāns[2], Sicong Ren[3], Jānis Kampars[2], Tom Andersson[3], Anssi Laukkanen[3]

1. Introduction

Ensuring the safety of components used in the hydrogen infrastructure requires a comprehensive understanding of how hydrogen interacts with materials and how it alters or degrades mechanical properties. Once hydrogen atoms reach microstructure, interactions between hydrogen and advanced metallic materials start at the atomic level, affecting macroscopic mechanical properties. Hence, to acquire knowledge of these phenomena, academia and companies involved in constructing the hydrogen infrastructure need a multiscale methodology to assess hydrogen-material interactions. In this context, recent advancements in characterisation techniques can reveal hydrogen-material interactions from the atomic level up to the macroscopic scale. However, these characterisation tools still have limitations to be overcome by unifying multiple materials research disciplines:

1. The quality of characterisation results depends on the workforce's competence in tools operation. In this context, data-driven approaches and material modelling tools can support the multiscale characterisation campaigns, allowing a better interpretation of experimental data and providing more guidance on experiments.

2. Hydrogen-material interactions under actual service conditions are challenging to assess solely by experiments because of the time and cost required. To solve this research dilemma, we envision the multiscale and multiphysics material modelling platform as a solution to predict material behaviour under complex scenarios.

3. Typical problems when merging multiple materials research disciplines are data incompatibility and interoperability, demanding efficient Data and Knowledge Management Platform (DKMP) with ontology integration to establish relationships between domains, which follow Materials modelling - Terminology, classification, and metadata document.

The main objective of HyWay is to develop adaptive multiscale material modelling and characterisation suites for assessing interactions between hydrogen and advanced metallic materials and demonstrate their capabilities on hydrogen storage and transport components. Our ambition is to enable industries to be more efficient when developing and using new advanced materials, shorten the materials innovation cycle,

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[2] Riga Technical University
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seamlessly merge materials modelling and characterisation approaches along value chains, and create a robust material research ecosystem platform.

The realisation of multiscale materials modelling and characterisation suites for assessing interactions between hydrogen and advanced metallic materials for hydrogen storage and transport components relies on a seamless integrative approach involving immersive communication between physical and digitalised tools. To this end, the HyWay project consists of 3 key modules: Physical realm, Virtual world, and Data and knowledge management platform (DKMP).

2. HyWay Physical realm

Considering the complexities in the hydrogen-material interactions, it is imperative to use multiscale characterisation techniques and testing methods. We will materialise this using (a) multiple characterisation techniques, (b) mechanical testing at 3 different length scales, and (c) 3 different hydrogen charging methods. These experiments will be weaved together to understand the intricate structure-property correlations in advanced materials and to quantitatively evaluate the effect of hydrogen at the different length scales on the mechanical properties. These data will support development and validation of the multiscale and multiphysics materials modelling platform. To bridge the gap in the obtained experimental knowledge, we will incorporate the data-driven approaches to provide effective guidance on characterisation and improve the data interpretation.

3. HyWay Virtual world

Predicting the microstructure evolution and macroscopic properties changes of advanced materials under the complex boundary conditions along their entire life cycle requires a flexible and adaptive modelling scheme. We will develop a modularised multiscale and multiphysics material modelling platform for assessing hydrogen effects on advanced metallic materials' behaviour. Besides advancing in modelling, another emphasis will be on developing interchangeable modelling tools, allowing one to efficiently exchange data from each model depending on the end users' requirements. Once the platform is established, we will leave the modularised modelling platform open for further implementation by other researchers. The modularised multiscale and multiphysics materials modelling platform consists of 7 interdependent submodules: atomistic modelling toolset, hydrogen uptake models, hydrogen-induced phase transformation models, hydrogen transport models, continuum model of hydrogen effects on plasticity, hydrogen-aware fracture model, and macroscopic hydrogen-sensitive model. Besides an understanding of physical mechanisms obtained from the atomistic modelling, we will use it to derive material parameters for other simulation tools.

4. HyWay Data and knowledge management platform (DKMP)

Data generated from all materials characterisation techniques and multiscale and multiphysics material modelling tools to reveal hydrogen-material interactions under various conditions in HyWay will be massive and come from multiple sources, requiring a suitable materials ontology, which represents knowledge and information in a structured way using properties and relationships. We will advance the standardised

data management platform by integrating a materials ontology to understand hydrogen-material interactions under actual conditions exposed to the hydrogen storage and transport components. Another benefit of having an ontology-based DKMP is its ability to facilitate data interoperability between different disciplines. DKMP will be compatible with further integration as well.

SiToLub - Simulation Tools for the design of safe and sustainable Lubricants

Francesco Pagano[1], Franz Pirker[2], Xavier Borras[3], Salvador Moncho[4], Jonas Hoffmann[5], Jakob Kibala[6], Davide Don[7], Eugenia Valsami-Jones[8]

1. Introduction

The need to promote a low carbon economy while ensuring effective actions to overcome the obstacles that the lubricant companies are facing (e.g. ever-changing regulatory restrictions on the chemicals, more demanding technical requirement of the industry, etc.) has led to the need for using computational models to accelerate the time to market of novel lubricant formulations. So far, each modelling case has been focused on understanding properties under specific conditions. The SiToLub project, funded under the HORIZON-CL4-2023-RESILIENCE-01 topic, aims at creating an integrated multi-functional digital simulation environment, supported by artificial intelligence, to help the lubricant manufacturers to face these challenges and move towards Safe-and-Sustainable-by-design (SSbD) materials and products by pre-assessing lubricant formulations at the design phase. SiToLub will integrate tools to predict human and environmental toxicity, to simulate properties and the interactions within the application environment, to estimate life-time product performance and efficiency during use phase, and to foresee the sustainability aspects of the new formulation.

2. Objective and methodology

SiToLub project aims to develop a digital tool/platform based on integrated computational models with built-in artificial intelligence (AI) features for the Safe and Sustainable by Design formulation of new lubricants. The tools developed will provide assessment of the safety (toxicity to humans, ecotoxicity to environment and workers risk) and, at the same time, sustainability guidance to design ecofluids (coolants, greases, oils) in a clear and holistic way regarding the foreseeable physico-chemical properties and tribological performance.

The safety assessment will be realized by using molecular dynamic models developed by the partners.

The tribological models will allow the prediction of the energy consumption during use by providing friction force values and expected durability of the materials by using wear data about the materials in contact with different fluids. They will also provide

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[5] GreenDelta GmbH, Berlin, Germany
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information about the degradation of the fluids in use and the chemical reactions occurring. The models will be flexible enough to predict the behaviour of the materials for different working parameters applied for different applications (wind turbines, electric cars, industrial machining, etc.)

This ambitious and forward-thinking system will leverage on a series of tools, ranging from technical evaluation and prediction models (computational models supported by artificial intelligence), combined with established Life-Cycle Analysis (LCA) methodologies to consider the environmental, social and economic impact.

Interoperability must be ensured between experimental and modelling domains and between different knowledge domains to ensure an effective exchange of data and interaction. Harmonizing taxonomies, classifications, and definitions as well as documentation is essential for a seamless exchange of data and efficient liaison of different disciplines, their models, experimental techniques, and approaches. To systematize interoperability, a domain ontology will be created based on the top-level ontology EMMO [1], as well as other ontologies related to standardization of data documentation across different domains, as for example to materials and manufacturing.

To deal with data scarcity and insufficient data diversity, data augmentation and data synthesis methods will be applied to enable the simulation model to produce even more accurate results.

3. Outcome and exploitation

The final result of SiToLub will be an organic infrastructure composed by many interconnected elements, as represented in Figure 10.

The core of this infrastructure is the SiToLub platform that will store the data produced during and after the project and will harmonize them with the data coming from other existing databases, including the database of i-Tribomat and data directly produced by the SiToLub partners.

Another important section of SiToLub infrastructure is composed by the different computational models that will be developed during the project. As previously mentioned, 3 categories of models will be developed according to their purpose. The first category will be related to the assessment of toxicity and biodegradability of the components of the lubricants, to be sure that the formulation will be safe for the people and the environment. The second category of models is related to the prediction of the technical properties of the lubricants and their overall functionality. The last category of models will be used to assess the life cycle of the lubricants, and their impact on the society and on the economy.

Existing databases will be used to feed the modelling tools, but the reliability of the data used will be assessed by realizing experimental tests according to international standards or specifically developed protocols.

Anyway, the testing procedures for the assessment of safe and sustainable lubricants will be elaborated and will be an essential part of the SiToLub foundation.

Artificial intelligence methods will be used for producing synthetic data when needed and to select the best candidates as lubricant components.

To ensure sustainable industrial use of the project results, SiToLub project relies on the presence of the Open Innovation Test Bed i-Tribomat, that will be the core exploitation partner. The newly developed simulation methods, and the updated infrastructure previously described, will expand the services offered. Thus, European industry will have access, in addition to the materials characterization and simulation tools already developed, also to the newly built infrastructure for the SSbD formulation of lubricants.

Each of the simulation tools could be used as service for the evaluation of the properties and performance of the lubricants and their additives.

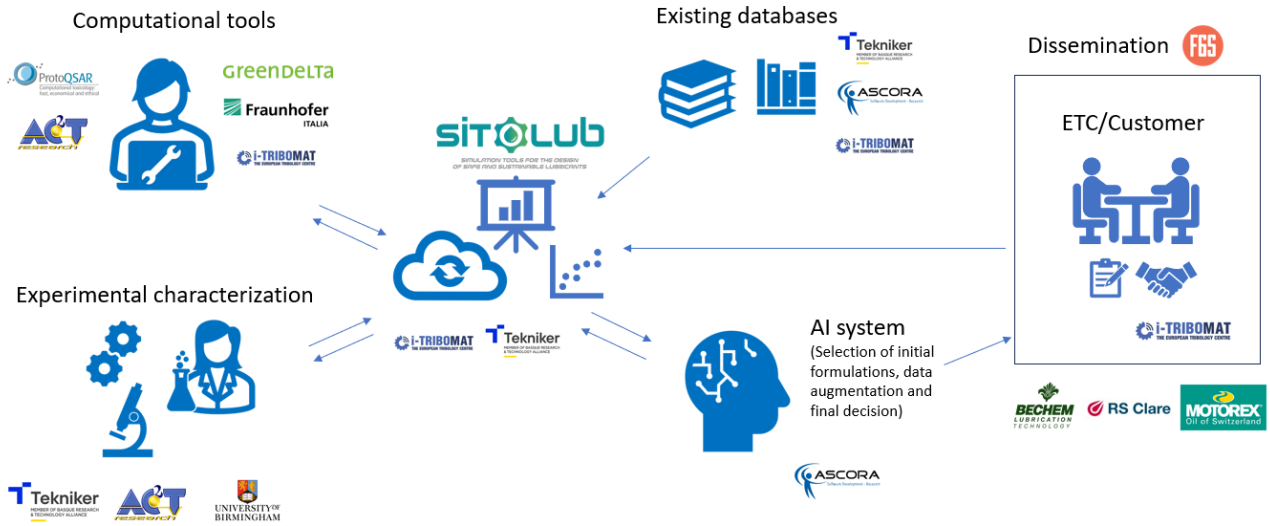

Figure 10. Exploitation structure of SiToLub

4. References

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CHEMATSUSTAIN: Implementing Innovative Methods for Safety and Sustainability Assessments of Chemicals and Materials particularly at Nano level in the European Union

Jelena Barbir[1], Estefania Carpio[1], Eleonora Foschi[2]

1. Abstract

In addition to contributing to the United Nations Sustainability Goals (UN SDG), the EU Green Deal includes the ambition of creating the first climate-neutral and circular economy continent by 2050. To do this, the policy goal of a zero-pollution economy for a toxic-free environment must be achieved. To this aim, the Chemicals Strategy for Sustainability (CSS) has been adopted, which aims to tackle the challenge of producing and using chemicals to address societal needs while respecting the planetary boundaries and safeguarding people and ecosystems, by dealing with pollution from all sources (Caldeira et al., 2022; European Commission, 2019; European Commission, 2020).

This CSS challenge gets operationalised through the development/implementation of two key R&I actions: 1) the Strategic Research and Innovation Plan (SRIP), and 2) the Safeand Sustainable by Design (SSbD) framework. Bearing in mind the pressing need to develop new methods or improve current ones, to support the improvement of safety and sustainability assessments of chemicals, the project "IMPLEMENTING INNOVATIVE METHODS FOR SAFETY AND SUSTAINABILITY ASSESSMENTS OF CHEMICALS AND MATERIALS PARTICULARLY AT NANO LEVEL IN THE EUROPEAN UNION (CheMatSustain)" will not only study the quantum effects from a fundamental point-of-view but also by identifying and measuring them through experimental techniques (high-resolution analysis, XPS and UPS), and determining the specific molecular recognition through their interaction with the environment, which is a quantum mechanical effect (invitro, microfluidic in-vitro, and in-vivo models and proteomics and transcriptomics and methods). The information obtained on these descriptors will then be integrated into the development of novel in silico models for the prediction (eco)toxicity properties of advanced materials. Finally, in-silico model prediction results will be combined to develop a new methodology for the complementary use of Risk Assessment and Life Cycle Assessment to improve criteria for the SSbD implementation framework. To date, significant progress has been made, as reported by the JRC Technical Report onSafe and Sustainable by Design chemicals and materials (Caldeira et al., 2022). However, further methodological advances are needed to support the full implementation of the SSbD framework, i.e., going beyond traditional green chemistry innovation approaches and integrating both safety-based and lifecycle-based considerations to ensure sustainability along the entire value chain. Today, nanoparticles

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can be found in an increasing number and broad range of consumer products, from cosmetics to kitchenware, electronics, renewable energy, and aerospace (Khan et al., 2022; Mech et al., 2020). Nanotechnology is expected to revolutionise our style of living, holding great promise for a bright and sustainable future (Khan et al., 2022; Mech et al., 2020). The EU has identified nanotechnology as one of the key technologies that will enable Europe's competitiveness and capacity to tackle the global problems of our time (European Commission, 2017). Considering the above, the overall objective of the project CheMatSustain is to identify, develop, test and deploy a set of tools to improve and harmonise screening and testing protocols, strategies, and hazard, risk and sustainability assessments of a sample of chemicals and (nano)materials in the European Union by developing robust, reliable and fast (test) methods and models, including high-throughput and *in silico* models, with the goal of improving their safety and sustainability.

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AI-driven multiscale methodology to develop Transparent Wood as sustainable functional material using SSbD

Päivi Kivikytö-Reponen[1], Stefania Fortino[1], Kari Kolari[1], Antti Puisto[1]

1. Introduction

Efficient design, production, and optimization of new safe and sustainable materials for various industrial sectors is a future grand challenge for our society. Wood-based composite materials offer a solution and have therefore been the focus of experimental research and development for years. Computational materials design has the capacity to speed-up the development of these materials. However, this requires reliable models currently unavailable.

The project *'AI-driven multiscale methodology to develop Transparent Wood as sustainable functional material'* (AI-TranspWood), funded by the European Commission within the call HORIZON-CL4-2023-RESILIENCE-01-23, aims to create an Artificial Intelligence (AI)-driven multiscale methodology within the Safe and Sustainable by Design (SSbD) framework for functional wood-based composites. The concept will be demonstrated for Transparent Wood (TW), a promising material with potential applications in several industrial fields, such as construction, automotive, electronics and furniture.

Utilizing AI tools and conducting advanced experiments, we aim to create multiscale models spanning from the atomistic level to continuum scales. These models will address the manufacturing and mechanical aspects of transparent wood (TW) and facilitate virtual screening of bio-sourced alternatives to the chemicals used in TW production.

2. Transparent wood

Transparent wood (TW) acquired attention since its discovery and morphological characterization in 1992 by S. Fink [1]. Its complex microstructure originates from that of pristine wood, and the resulting composite is heterogeneous across the scales, providing interesting features: unlike wood, it is a lightweight, transparent to visible light, and, by the subsequent treatments (i.e., functionalization, modification, and infiltration with suitable resins) it becomes the best candidate for replacing glass and some plastics in a variety of applications.

European market for TW composites is new, and a recent report [2] estimates that global Transparent Wood industry will generate $208.1 million by 2031 witnessing a Compound Annual Growth Rate (CAGR) of 9.0% from 2022 to 2031, due to TW emerging as a promising alternative to petroleum-based harmful plastics [3]. Being eco-friendly, lighter, stronger, and having lower carbon footprint compared to traditional building

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materials it is expected to become a popular choice for energy-efficient buildings and sustainable construction projects.

3. AI-driven multiscale methodology

Computational modelling of TW properties requires specific physics-based modelling approaches spanning across several scales and physical domains. Such approaches are restricted by the computational power available, and the profound knowledge required.

AI-Transpwood proposes a systematic approach containing 17 work packages (WPs, Fig. 1) for complementing physics-based modelling and providing tractable software tools with the help of AI and ML (Fig. 2). It involves physics-based models developed in WPs 1, 2, and 4, used to create AI-based surrogate models (WP7). These surrogate models are then improved by integrating physics submodels directly into AI methodology (WP8). Finally, advanced physics models, such as non-linear finite element approaches, are linked to AI. The entire reality described by physics models is then connected to AI technology handling aspects not accommodated by physics-based models, e.g., geometric variability and material uncertainties due to growth and production irregularities.

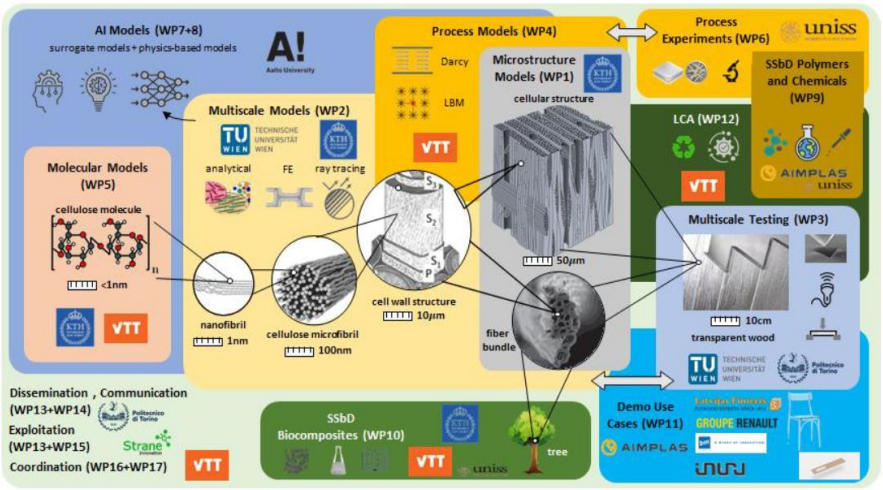

Figure 11: Structure of AI-TranspWood Project and associated WPs with leaders and main partners.

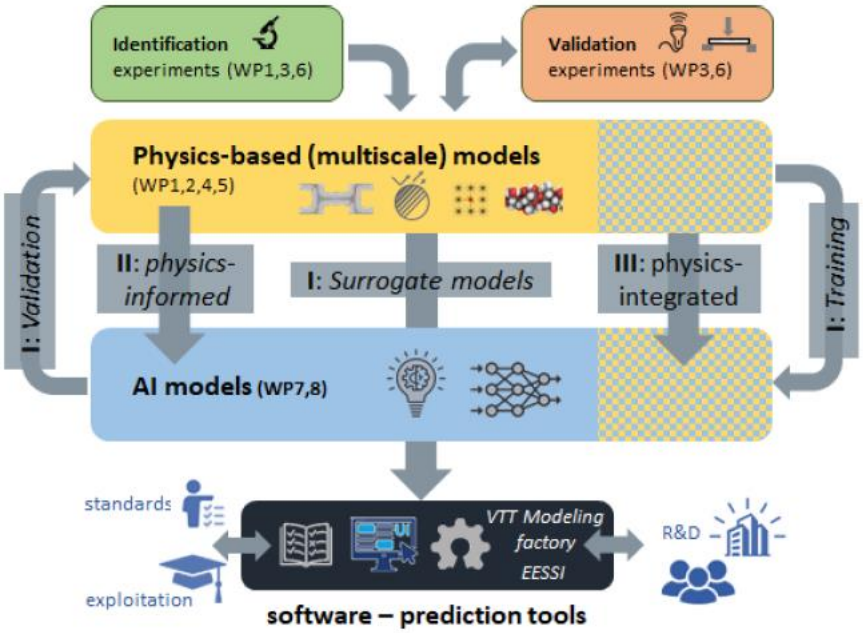

Figure 2: Conceptual three-stage process to link physics-based models to AI-methodology, and model classes which will then be implemented in predictive software.

4. Safe and Sustainable by Design concept

Safe and sustainable by design (SSbD) is a design approach where objectives such as minimizing hazardous chemicals use, reducing greenhouse gas emissions[2], and fostering materials reuse and recycling are built into product design. According to the call, "*the integration by computational modeling of the chemicals and materials functionality with the Safe and Sustainable by Design framework will have a key role in the green and digital transition of the European industry",* AI-TranspWood fully addresses this approach.

The AI-TranspWood project integrates efficiently advanced AI-driven computational models with the SSbD framework for wood-based composites and demonstrates the methodology for transparent wood (TW), with the vision to substitute substances of concerns such as plastic and glass in key applications. This will be possible thanks to the user-oriented design tools made available for industrial users.

In the project a formulation of safe and sustainable by design concept (SSbD) is defined for the purpose of screening polymers and chemicals selected for TW, and the final composites using data generated by models and eco-design or simplified LCA providing, identifying their safety and environmental and economic hot spots. The feedback from the screening study helps the material developers to improve the environmental performance at an early stage.

[2] https://ec.europa.eu/clima/eu-action/european-green-deal/2030-climate-target-plan_en

5. Models supporting design for lifecycle

After screening polymers, chemicals, wood and plant-based composites, SSbD formulation continues towards assessment of environmental impacts. This supports understanding of the sustainability of the whole service life of the selected materials and new transparent wood (TW) products to be developed. Finally, SSbD guidelines support the safe and sustainable design of use cases.

Environmental impacts are evaluated with data and knowledge gained during the project. The LCA and environmental footprint methodology will consider the whole value chain of the production system to quantify environmental impacts. Also, circularity and R-strategies of selected polymers and chemicals and biocomposites will be evaluated.

For supporting lifecycle of the products, the recycling of TW products will also be studied. Due to environmental and economic issues, mechanical recycling will be prioritized. However, due to the composition and nature of the polymers, chemical recycling will be required.

6. Conclusions

The aim of the project is to develop advanced TW through SSbD concept using AI-driven multiscale methodology. The communication between LCA and the material surrogate models published on open platforms will be created.

By developing AI-supported SSbD framework for TW, we contribute to the European Green Deal by providing innovative sustainable materials and cost-effective tools for European industries, paving the way towards green and sustainable transition. SSbD tools used by the chemicals and materials community with new transparent wood materials will increase the innovation capacity of SMEs and industry for future sustainable products.

7. References

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Acknowledgements to AI-TranspWood partners and funding by the European Commission, HORIZON-CL4-2023-RESILIENCE-01-23.

Battery manufacturing digital twin design in view of requirements for the digital product passport

Martin Thomas Horsch[1]

This contribution argues that the DigiPass CSA community should establish a subcommunity on digital product passports for battery materials and systems in collaboration with projects from the Battery2030+ CSA3 community, including BatCAT.

BatCAT is the project that will realize the BATTERY 2030+ manufacturability six-year programme within 42 months, addressing battery cell manufacturing innovation for Li-ion and Na-ion cells as well as redox-flow batteries, with a focus on vanadium-based technology. To achieve ambitious cost and performance targets, products and processes need to be optimized for energy density, longevity, and sustainability of batteries, leveraging the combined power of physics-based and data-driven modelling: “Fully digital manufacturing analogues will allow the understanding and optimization of process parameters and of their impact on the intermediate and final product. These virtual representations can be used to manipulate and therefore actuate in the physical world supporting [...] battery manufacturing facilities”[Amici 2022] BatCAT will develop such an integrated virtual development and optimization environment.

Redox-flow batteries are promising for energy storage in renewable energy and will help increase the buffer for temporal fluctuations in energy supply and demand. Lithium-ion battieres are ubiquitous and can contribute to the twin transition as a bridge technology, provided that a rigorous lifecycle analysis is done, based on knowledge integration, to balance beneficial and adverse effects.[Sadik 2023] Work on digital product passports has gained momentum in the context of the circular economy. At present, however, digital product passports are still an emerging field, without a universally agreed-upon standard. Developing a digital product passport system for batteries presents challenges and gaps in the current scientific and industrial landscapes. As the battery industry increasingly adopts digital product passport systems to manage the lifecycle of batteries and promote circular economy practices, it becomes imperative to address these gaps.

The current state of the art in industry is that repair and maintenance is often documented on paper, and companies lack knowledge of the origin and composition of their products. Digital twin technology permits advancing beyond this state of the art substantially, and in many ways. It is therefore a core aspect to developing the digital product passport for battery materials and systems.

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[1] Norwegian University of Life Sciences; martin.thomas.horsch@nmbu.no

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COST Action EuMINe - European Materials Informatics Network

Francesco Mercuri[1]

1. Introduction

COST (European Cooperation in Science and Technology)[1] actions play a pivotal role in fostering collaboration, innovation, and excellence across Europe's scientific landscape. With a focus on promoting pan-European networking, COST actions bring together researchers, policymakers, industry stakeholders, and other relevant actors to address pressing societal challenges, drive scientific advancement, and stimulate economic growth. By facilitating interdisciplinary collaboration and knowledge exchange, COST actions leverage Europe's rich diversity of expertise and resources to tackle complex issues spanning diverse fields such as health, environment, technology, and social sciences. Moreover, COST actions serve as catalysts for capacity building, training, and mobility, empowering researchers at all career stages to expand their networks, acquire new skills, and contribute to cutting-edge research initiatives. Through its decentralized, bottom-up approach, COST fosters inclusivity, diversity, and transparency, ensuring that all voices are heard and all regions of Europe are represented in shaping the future of science and innovation. As Europe's longest-running intergovernmental framework for cooperation in science and technology, COST continues to be a driving force for scientific excellence, collaboration, and impact, reinforcing Europe's position as a global leader in research and innovation.

The European Materials Informatics Network (EuMINe, COST Action CA22143)[2] has recently been launched in the framework of the COST programme 2023-2027.[3] EuMINe is a collaborative initiative aimed at revolutionizing the design, development and engineering of advanced materials through the integration of advanced modelling, data-driven and AI technologies. With the overarching goal of enhancing the competitiveness of the European research and development (R&D) landscape, EuMINe brings together a diverse community of experts, researchers, and industry stakeholders to address the multifaceted challenges and opportunities in materials development.

2. The EuMINe approach

The development of advanced materials plays a pivotal role in driving technological advancements across various sectors, including energy, healthcare, transportation, and environmental sustainability. However, the traditional empirical methods for materials discovery and design are often time-consuming, costly, and limited by the vastness of the materials space. In response to these challenges, EuMINe advocates for a paradigm shift towards a fully digital and data-centric approach, leveraging the power of computational modelling, artificial intelligence (AI), machine learning (ML), and high-performance computing (HPC) to accelerate the pace of materials innovation.

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EuMINe's activities are guided by several key objectives:

- Collaborative research coordination: EuMINe serves as a platform for fostering collaboration among researchers and institutions working on materials informatics. By promoting knowledge sharing, resource exchange, and interdisciplinary collaboration, EuMINe aims to accelerate the development and adoption of modelling and data-driven methods for materials discovery, characterization, and design.
- Standardization and methodology development: one of EuMINe's primary objectives is to develop shared standards, practices, and methodologies for the application of materials informatics and AI for advanced materials development. Through collaborative efforts, the network aims to harmonize best practices in data management, model validation, and predictive modelling, ensuring interoperability and reproducibility across diverse research domains.
- Infrastructure and tools development: EuMINe advocates for the development of robust infrastructure and tools to support the adoption of digital and data-driven approaches for advanced materials. This includes the use of high-performance computing resources, data repositories, and software platforms tailored to the needs of materials researchers and practitioners.
- Technology transfer and innovation: EuMINe facilitates technology transfer and innovation by fostering collaboration between academia and industry. By bridging the gap between fundamental research and real-world applications, EuMINe aims to accelerate the translation of research findings into commercial products, processes, and solutions.
- Capacity building and training: EuMINe prioritizes capacity building and training initiatives to empower researchers with the necessary skills and knowledge to leverage digitalisation for advanced materials. Through workshops, seminars, and educational resources, EuMINe seeks to cultivate a new generation of materials informatics experts and practitioners.

3. An open platform for materials informatics in Europe

The EuMINe COST Action realises an open and inclusive approach characteristic of COST actions, with over 150 participants hailing from 35 countries. Embracing the principles of collaborative networking, EuMINe provides a platform for researchers, practitioners, policymakers, and industry experts from across Europe to converge, exchange ideas, and collectively address the multifaceted challenges at the intersection of advanced materials development, digital transition and AI. By fostering a diverse and vibrant community of participants, EuMINe harnesses the collective expertise and perspectives of its members to drive forward innovation, advance knowledge, and boost the field of materials informatics. Through its open character and inclusive nature, EuMINe embodies the spirit of collaboration and cooperation that lies at the heart of COST actions, empowering individuals and institutions to collaborate across borders, disciplines, and sectors to address pressing societal needs and advance the frontiers of science and technology.

4. References

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Poster Presentations: Session 3

Ensuring regulatory Alignment in the R&I of Innovative Materials

Steffi Friedrichs[1], MACRAMÉ Consortium[2]

1. Introduction

The MACRAMÉ Project 'Advanced Characterisation Methodologies to assess and predict the Health and Environmental Risks of Advanced Materials' is fully aligned with the EU ambitions to secure the safety and sustainability of new chemicals, materials, products and processes in order to strive for zero pollution and toxic-free environments, as addressed in the EU's Chemical Strategy for Sustainability (2020), and in the European Green Deal (2019 & 2021); in doing so, the Project concentrates on methodologies that are applicable to nanomaterials, and widens them to '**Advanced Materials**' (AdMas) – a material category that includes but surpasses that of 'nanomaterials' (EU, 'Definition of a Nanomaterial') - in commercialised products and that are aligned with the future-oriented innovation, safety and sustainability considerations of the OECD (OECD (2020)), the EU (EU (2022)), and several of its Member States (e.g. Germany (2021)). This will be achieved through development and demonstration of novel methodologies, and by advancing their harmonisation & standardisation on **three MACRAMÉ Material Families** of **inhalable carbon-based AdMas** of various morphologies and dimensions (Tiwari *et al.* (2012)), beyond spherical particles: **(a) graphene-related material** (GRM), **(b) carbon nanofibres** (CNFs), e.g. carbon nanotubes (CNTs), and **(c) Poly Lactic-co-Glycolic Acid (nano)particles** (PLGA). The focus on carbon-based AdMas addresses unsolved detection and characterisation issues, especially in complex media. In doing so, MACRAMÉ builds on >15 years of research and innovation (R&I) and knowledge pooling in nanosafety, formed through numerous European and international collaborations. MACRAMÉ will add value to the results of collaborations, such as the Malta-Initiative, and the Graphene Flagship Validation Service and Standardisation Committee, to proactively support EU industries in becoming world-leaders in clean technologies and products and achieving the Green Deal's ambitious timeline.

2. Startegic R&I to support Harmonisation, Standardisation & Safe and Sustainable by Design

The **MACRAMÉ R&I Approach** (Figure 12) aims to widen the development of harmonised test guidelines (TGs) and guidance documents (GDs) (OECD) and standards (CEN, ISO) to **market-relevant AdMas in their complex product matrices**. This will be achieved by defining the R&I Strategy through life-cycle assessment for **five market-relevant industrial MACRAMÉ Use-Cases.** These **define the selection** of the **MACRAMÉ R&I Activities** and development of **MACRAMÉ Methods**, and the benchmarks chosen for monitoring the progress R&I. MACRAMÉ R&I Activities include a range of novel sample preparation techniques and ambitious quantitative detection and imaging methodologies that support reliable and reproducible determination of AdMas in different complex matrices (**AdMa@CMs**) and using **inhalation as their main exposure**

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[2] cf.: https://macrame-project.eu/the-macrame-consortium/

route. By applying, combining and evaluating both established and novel inhalation toxicity tests a tiered approach to toxicity testing will be developed that will provide data on state-of-the-art characterised control materials for the **MACRAMÉ Control Material Library**. The library will serve future AdMa toxicological research. The ultimate **MACRAMÉ Outcomes** are proposals for harmonisation and (pre-)standardisation projects to be provided to and further elaborated with the relevant bodies, (i.e. OECD, VAMAS/CEN/ISO). The proposals will be founded on **robust summary datasets**, **scientific documents** and **recommendations for hazard- and risk-assessment methodologies for AdMas in complex product matrices** (AdMa@CMs). All data and information, obtained from external sources and generated during the Project, will be handled and stored in the **MACRAMÉ Information Hub** - the Project's central information processor, whose interoperability is based on a **Data Stewardship** concept, designed according to IndustryCommons principles.

The resulting efficiency and effectiveness of MACRAMÉ Methods will be demonstrated through their application in Use-Case evaluations, using LCA-, LCC- and 'Safe & Sustainable by Design' (SSbD)-based (EWARN (2022)), highlighting benefits like reduced costs of regulatory compliance, by following a **MACRAMÉ Safety & Sustainability Matrix**. This matrix will be a modular building block for MACRAMÉ's information-transferring interfaces for different scientific and regulatory communities, and thus provide a stepping-stone for Europe's route towards a ***'one substance – one assessment'*** approach (European Green Deal (2019)) and promote an open strategic autonomy (ETUI (2021)) through key enabling and emerging technologies, including digital ones.

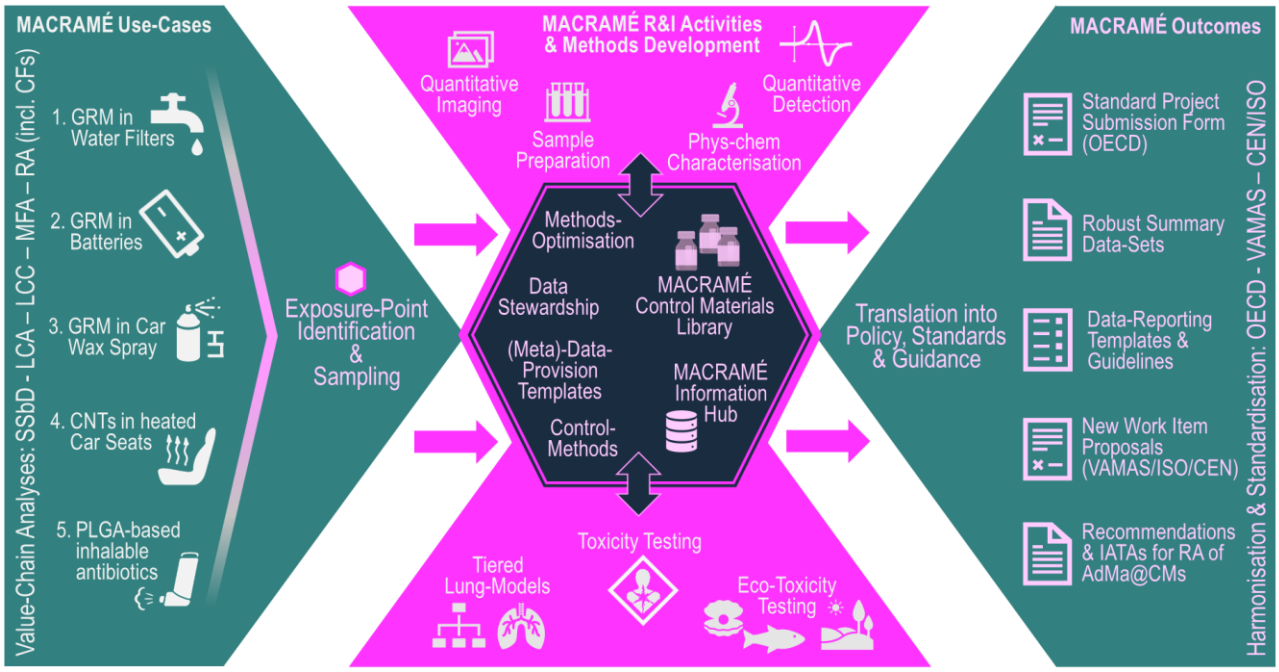

Figure 12: Illustration of the MACRAMÉ R&I Approach (AdMa@CMs: Advanced Materials in complex matrices; CF: Characterisation Factor; GRM: graphene-related material; IATA: integrated approaches to testing and assessment; LCA: Life-Cycle Assessment; LCC: Life-Cycle-Costing; MFA: Material-Flow Analysis; RA: Risk-Assessment; SSbD: Safe-&-Sustainable-by-Design).

3. Ensuring regulatory Relevance in the MACRAMÉ Project

To ensure the maximum impact and engagement with industrial actors, policy-informing and –making, as well as standardising bodies, two enhance the chances of acceptance and advancement of the developed methods toward standardisation and harmonisation.

The 1st MACRAMÉ Regulatory Risk Assessors Summit, held on the 27th – 28th November 2023 (as an in-person event), aimed to establish the concept of conducting environmental, health and safety assessments of AdMas along the entire life cycle of a product. In doing so, the Summit borrows from and applies elements from both **risk-** and **life cycle assessment** disciplines and introduces the concept of sustainability and its implementation in the **Safe and Sustainable by Design framework**, to elaborate needs, challenges and approaches for regulatory risk assessors. The first day of the Summit laid the foundation by providing insights into the policy frameworks of the European Green Deal, the SSbD framework, and LCA. Short talks and a panel discussion by scientists, regulators, large industry and SMEs, and consumers focussed on how the different stakeholder groups perceive and approach sustainability in challenges they face in risk assessment and how LCA-based approaches may help in addressing these challenges. The second day featured three breakout sessions led by experts for (a) occupational safety, (b) consumer safety, and (c) environmental safety, respectively, in order to further elaborate on needs and challenges. The outcomes of the breakout discussions form the basis for recommendations on future needs for AdMas in risk assessment within a Life Cycle context, including standards and test guidelines; they furthermore provide additional guidance to the mid-term review and (re-)confirmation of the Project's R&I Strategy.

4. Acknowledgements

The MACRAMÉ project has received funding from the European Union's Horizon Europe Research and Innovation programme under grant agreement No. 101092686. Associated Partners (i.e. (a) Swiss Partners and (b) UK Partners) have received national funding from (a) the Swiss State Secretariat for Education, Research and Innovation (SERI), and (b) Innovate UK.

CHIASMA - Accessible Innovative Methods for the Safety & Sustainability Assessment of Chemicals & Materials

Tommaso Serchi[1], Emma Arnesdotter[1], Pamina Weber[1], Steffi Friedrichs[2], CHIASMA Consortium[3]

1. Introduction

The CHIASMA Project aims to devise and demonstrate a comprehensive set of **New Approach Methodologies (NAMs)** for chemicals and advanced materials, and integrate these into a user friendly, reliable and robust framework to perform human and environmental safety evaluation in a regulatory context. The **CHIASMA SSbD (Safe & Sustainable by Design) Assessment** will be based on an iterative approach that leverages on different consecutive assessment steps based on **chemocentric models**, **biocentric tools, and experimental NAMs**.

The CHIASMA NAMs, alone or combined into IATAs, will be developed to answer specific regulatory needs, focusing on regulatory requirements for human and environmental safety and assessment, aiming at applying it to the EU's SSbD approach in terms of defining safety and sustainability along the complete life cycle of a substance/material. A harmonised composition of the project consortium encompassing academic and research centres as well industry and regulators will ensure CHIASMA's value at continental level and beyond. The Project will ensure development and implementation of innovative NAMs to support EU strategies, such as the EU Chemicals Strategy for Sustainability (CSS), the JRC Safe and Sustainable by Design (SSbD) framework, and the AMI3030 initiative (to name but a few).

CHIASMA will promote EU leadership in the sector and provide a significant advance in the research field. The CHIASMA's link to industry and to EU and global regulators and policy makers (e.g. OECD, EURL ECVAM, ECHA, EFSA, US-EPA, and US-FDA) will ensure the relevancy and applicability of the developed approaches, which will be tested on three test cases, namely PFAS, (nano-)pesticides, and 2D chemicals/materials for energy applications, demonstrating regulatory relevance and trans-domain applicability of the CHIASMA-framework.

2. The CHIASMA Project

The CHIASMA Project is fully aligned with the EU strategies for the development of the SSbD Framework to ensure safety and sustainability of enabling and emerging technologies – including those based on chemicals and materials, as addressed in the EU's CSS, in the European Green Deal and in the Advanced Materials 2030 Initiative. CHIASMA will focus on developing NAMs and improved **Life Cycle Impact Assessment** (LCIA) approaches and strategies, to ultimately integrate these into the **CHIASMA**

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[2] AcumenIST SRL
[3] cf. www.CHIASMA-Project.eu

Framework for the combined assessment of SSbD to support REACH (regulation for the Registration, Evaluation, Authorisation and Restriction of Chemicals), CLP (regulation for Classification, Labelling and Packaging of chemicals) and other relevant regulations, such as the (proposed) Ecodesign for Sustainable Products Regulation and the EU Ecolabel regulation.

The resulting integrated **CHIASMA SSbD Assessment** (for safety- and environmental-assessment), will be successively built on the coherent development, refinement and demonstration of NAMS based on both ***in silico*** and '**experimental**' methods (*i.e.,* CHIASMA's collective term for ***in vitro* methods, human *ex vivo* methods and non-mammal *in vivo* methods**), in order to enable risk assessors, SMEs, large enterprises and regulators to address REACH and CLP relevant endpoints using human-centric and 3R-compliant approaches. The developed NAMs, refined and demonstrated by CHIASMA will be deployed as 'Swiss army knife' to generate data (e.g., newly generated or as the result or re-processing of existing data), and including *in silico, in vitro* and *in chemico* approaches that will be used alone or in combined approaches, such as Integrated Approaches to Testing and Assessment (IATAs), to generate specific regulatory relevant results for the EU SSbD Framework.

The CHIASMA SSbD Assessment and the *in silico* and experimental NAMs will be 'in-project' validated against three groups of socially and environmentally relevant chemicals and materials groups:

a) Demo-Case 1: Polyfluoroalkyl Substances (PFAS),
b) Demo-Case 2: (nano)-pesticides, and
c) Demo-Case 3: 2D materials for energy applications.

The focus on these three groups is justified by their high health impact, environmental persistence, and large industrial use, which lead to high societal concern. CHIASMA builds on many years of research and innovation (R&I) and knowledge pooling in chemical safety and nanosafety, development and implementation of computational models and of advanced biological models for prediction of safety and environmental impact, generation of conceptual frameworks for assessment formed through European and international collaborations.

CHIASMA will contribute to the global efforts towards the green and digital transition, ensuring **more robust and more ethical regulatory-ready methods** to enable stakeholders to achieve the ambitious European goals for a sustainable and toxic free society. CHIASMA will boost the efforts of the scientific community and authorities to **generate, validate and implement new alternative methods and strategies for the animal-free assessment of chemicals and materials**.

3. The CHIASMA R&I Approach

The **CHIASMA R&I approach to testing and assessment** (see Figure 13) aims to provide regulators with an integrated framework (the CHIASMA SSbD Assessment) allowing human and environmental safety and environmental impact assessment using an iterative multi-step approach based on next generation safety assessment (NGSA) approaches. The CHIASMA SSbD Assessment combines the elements, corresponding to the numbers in Figure 13:

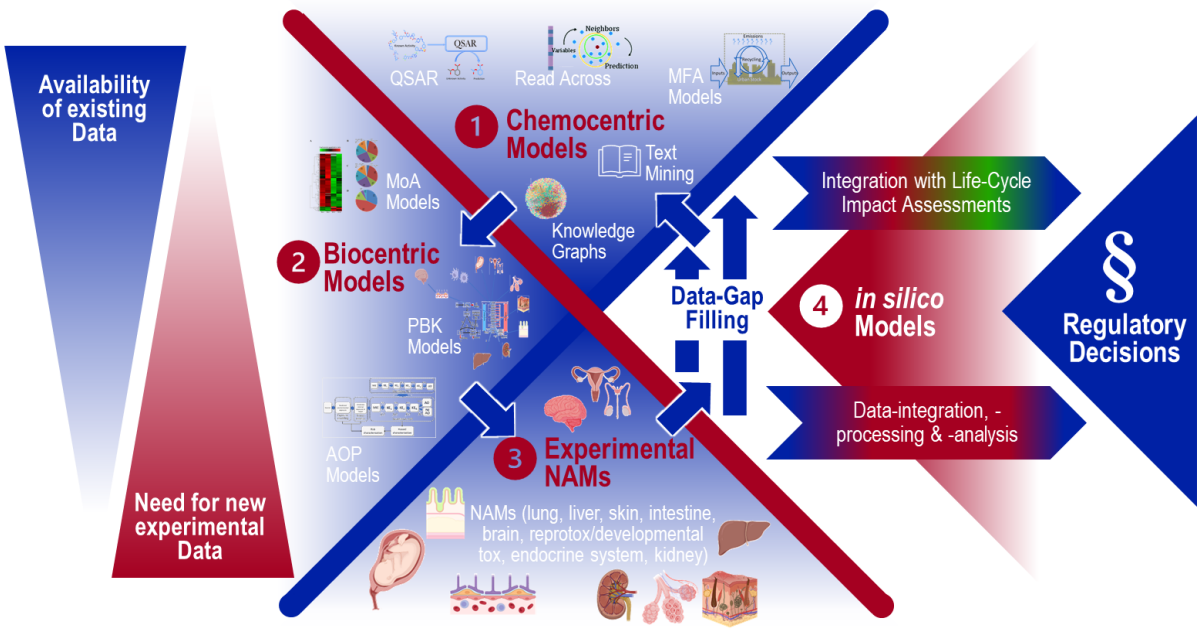

Figure 13: Illustration of the CHIASMA R&I approach to testing and assessment of materials using an iterative approach based on the integration of (1) chemocentric, (2) biocentric and (3) new experimental models into a conceptual framework for data-integration and -processing.

1. **Chemocentric models**, powered by **state-of-art artificial intelligence**, including:
   - Chemocentric models for the prediction of behaviour and properties of chemical systems.
   - Quantitative Structure-Activity Relationship (QSAR) models relating chemical features to biological effects.
   - Material Flow Analysis models (MFA) to predict chemical/material releases along the products' life cycle.
   - Text mining tools to process, analyse, and extract valuable information from large amounts of text data.
   - Knowledge Graph to capture, structure and analyse existing data, inferring new links and conclusions.
   - Read Across to predict properties for the target substance(s) based on properties of analogous substances.
2. **Biocentric models**, consisting of:
   - Physiologically-Based Kinetic models (PBK) to predict behaviour and distribution of chemicals in the body.
   - Adverse Outcome Pathways models (AOPs) to provide a systematic and comprehensive understanding of key events (KEs) and molecular initiating events (MIEs) that lead to an adverse outcome following exposure.
   - Mechanism of Action (MOA) models that describe the molecular biology processes and interactions following exposure to identify the specific targets, pathways, and interactions that are involved.
3. **Optimised experimental NAMs**, representative of the following human biological systems:

- Human organs and systems (brain, reproductive/developmental and endocrine systems, kidney, and liver).

- Human internal biological barriers (blood-brain-barrier (BBB) and blood-placental-barrier (BPB).
- Human external barriers (lung alveolar barrier, skin and small intestine).

4. **Data integration, processing and analysis modules** that will also include innovative Life Cycle Impact Assessment (LCIA) methods for better integration of toxicity in human and environmental assessment.

INSIGHT – Integrated Models for the Development and Assessment of High Impact Chemicals and Materials

Dario Greco[1], Angela Serra[1], Laura Saarimäki[1], Steffi Friedrichs[2], INSIGHT-Consortium[3]

1. Introduction

The INSIGHT project will provide a **novel, integrated framework for mechanistic impact assessment of chemicals and materials**. This multi-layer framework consists of a data graph, a model graph and an impact outcome pathway (IOP) graph that predict the health, environmental, social and economic impacts of chemicals and materials (Fig.1). The three graphs will be systematically interlinked together and used for integrated impact assessment of chemicals and materials for next generation integrated SSbD. Although individual models and data sets for impact assessment exist, they have never been integrated in a network structure. Thus the individual graphs and their integration represent a novel way to approach impact assessment in a mechanistic and holistic way. INSIGHT will save industry money and time in developing and producing chemicals/materials and products derived from them. It will help regulators and policy makers, make informed decision-making that improve safety and sustainability. INSIGHT is fully aligned with the EU principles of safety and sustainability of enabling and emerging technologies of chemicals and materials, as addressed in the EU's Chemical Strategy for Sustainability (2020), in the European Green Deal (2021) and in the Advanced Materials 2030 Initiative (AMI2030). INSIGHT supports the European Green Deal, through which Europe aspires to become the first climate neutral continent by the year 2050. Results from INSIGHT will support policy development in the areas of neutrality, biodiversity protection, public health, and circular economy. INSIGHT is also aligned with the EU's Chemical Strategy for Sustainability (CSS) and will aid the development of a dynamic economy respecting planet Earth as a whole, avoiding harm to humans and the environment. Finally, INSIGHT is funded upon and supports extensively the computational framework being developed within multiple actions including the PARC project, an EU-wide programme that supports chemical risk assessment and risk management.

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[2] AcumenIST SRL
[3] cf. www.INSIGHT-Project.org

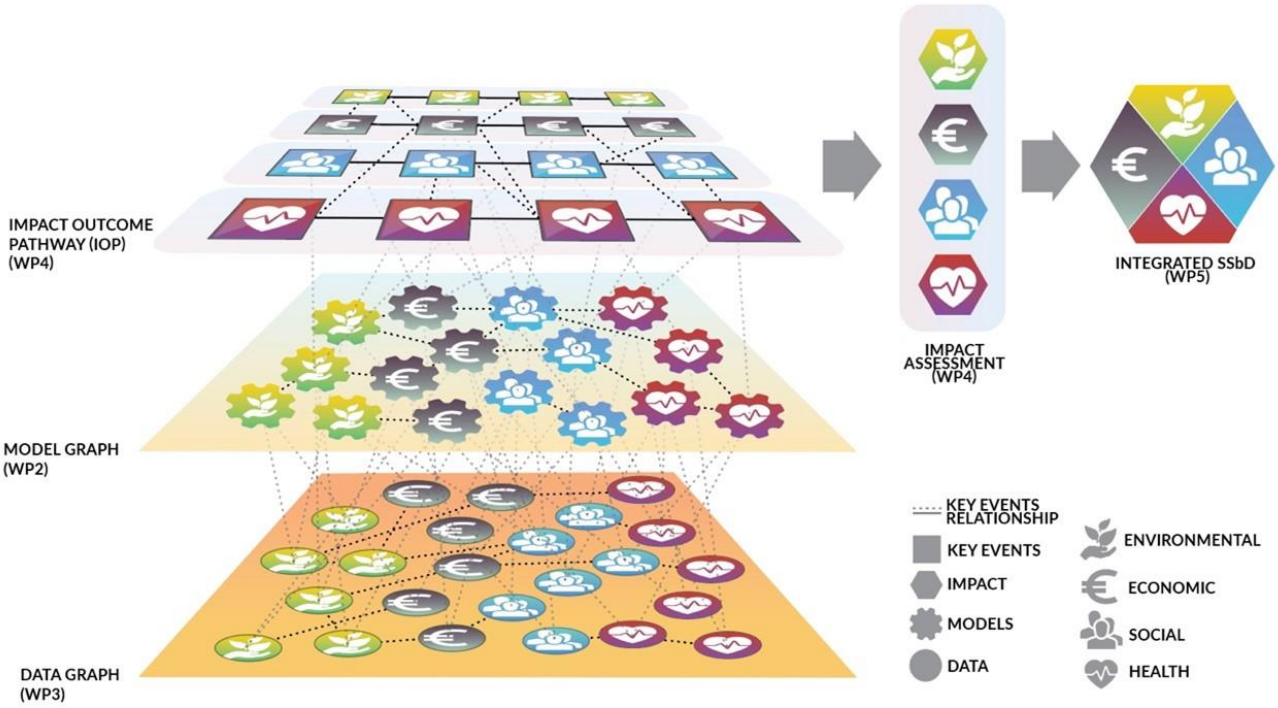

Figure 14: Illustration of the INSIGHT Framework for integrated impact assessment and SSbD.

2. INSIGHT's R&I Objectives

A new era just initiated, in which artificial intelligence and machine learning are creating paradigm shifts in many fields of human activity. Consequently, new functional paradigms of human-AI collaboration are urgently needed. In this scenario, chemical and material development is no exception. Specific challenges including lack of coordination between stakeholders (industry, regulators and academia), limited access to relevant data and lack of method standardisation have thus far hampered the emergence of a comprehensive approach to SSbD. Despite the existence of several frameworks for assessing chemicals and materials throughout their lifecycle, this field remains fragmented, with novel computational approaches disjointed and difficult to access and use. Similarly, FAIR data is necessary for AI-enabled tools, but so far, no clear action has been taken to integrate them from multiple available sources. INSIGHT is designed to drive the innovation towards digitally enabled circular, climate-neutral and sustainable economy by democratising the use of cutting-edge AI-enabled methods to SSbD. Chemical safety is based upon the concept of Integrated Approaches to Testing and Assessment (IATA), where multiple sources of information are used. INSIGHT will expand the IATA concept by developing the next generation Safe and Sustainable by Design (SSbD) procedure in which social, economic, health and environmental impacts are evaluated in a mechanistic and integrated fashion.

Hence, the INSIGHT project aims to:

1. Develop an integrated framework for mechanistic impact assessment based on the novel concept of IOP;
2. Provide curated and user-friendly FAIR data and computational models and workflows that support the development of the next generation SSbD chemicals and materials;

3. Provide open, accessible and interactive guidelines, enabling end users and stakeholders to access and operate the framework.

INSIGHT aims to foster a paradigm shift in the assessment of sustainability and safety of chemicals and materials, from the current fragmented situation towards a holistic and integrated approach. INSIGHT will use the SSbD principles and Life Cycle thinking approach to consider the intrinsic properties of chemicals and materials, production phase, end-user utilisation phase, and functionalities of the product for a comprehensive social, economic, health and environmental impact assessment. Health impacts will be assessed through hazard and risk models, while environmental impacts will be assessed through Life Cycle Impact Assessment (LCIA), following the Product Environmental Footprint methodology. Socio-economic impacts will also be addressed using social-LCA framework and Life Cycle Costing principles.

3. INSIGHT's Policy Alignment

INSIGHT is fully aligned with the EU principles of safety and sustainability of enabling and emerging technologies of chemicals and materials, as addressed in the EU's Chemical Strategy for Sustainability (2020), in the European Green Deal (2021) and in the Advanced Materials 2030 Initiative (AMI2030). INSIGHT supports the European Green Deal, through which Europe aspires to become the first climate neutral continent by the year 2050. Results from INSIGHT will support policy development in the areas of neutrality, biodiversity protection, public health, and circular economy. INSIGHT is also aligned with the EU's Chemical Strategy for Sustainability (CSS) and will aid the development of a dynamic economy respecting planet Earth as a whole, avoiding harm to humans and the environment.

4. INSIGHT's Decision-Support System & GUI

INSIGHT will develop an integrated decision-support system in the form of interactive decision maps. These maps will be multi-level workflows designed for guided decision-making by industrial and regulatory stakeholders and will be adapted to multiple types of SSbD use cases.

The decision maps will also guide the development of the INSIGHT framework GUI (graphical user interface).

Figure 15: Illustration of the decision maps and the INSIGHT Framework GUI.

The GUI will be customisable to suit different user groups' needs and preferences. A Software as a Service (SaaS) option will also be available, hosted on a scalable and secure cloud infrastructure, making it easier for end-users to collaborate and share data with partners and stakeholders, and providing an additional level of convenience and accessibility.

PINK – computational approaches for industry-ready Safe-and-Sustainable-by-Design

Thomas E. Exner[1], Joh Dokler[1], Steffi Friedrichs[2], Francesca L. Bleken[3], Anna L. Costa[4], Francesco Mercuri[5], Haralambos Sarimveis[6], Antreas Afantitis[7], Antonino Marvuglia[8], Tommaso Serchi[9], Dario Geco[10], Penny Nymark[11], Martin Himly[12], Karin Wiench[13], Philippe Jacques[14], Iseult Lynch[15], Georgios Gkoutos[16], and Roland Hischier[17]

1. Introduction

The PINK project [1] (Provision of Integrated Computational Approaches for Addressing New Markets Goals for the Introduction of Safe-and-Sustainable-by-Design Chemicals and Materials) is funded under the call HORIZON-CL4-2023-RESILIENCE-01-23 - Computational models for the development of safe and sustainable by design chemicals and materials and coordinated by Slovenia-based SME Seven Past Nine d.o.o. It started in January 2024 with a team of 12 beneficiaries, 2 affiliated entities and 2 associated partners and will run for four years.

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[17] Advancing Life Cycle Assessment, Swiss Federal Laboratories for Materials Science and Technology, St. Gallen, Switzerland

2. PINK's objectives

Safe-and-Sustainable-by-Design (SSbD) advanced materials and chemicals (AdMas&Chems) are a central requirement for reaching the ambitious goal of making Europe the first digitally-enabled circular, climate-neutral and sustainable economy. Such new AdMas&Chems need to provide the high functionality required for their advanced applications, whilst simultaneously exhibiting improved safety and sustainability performances that take into account the complete value chain and life cycle, as outlined in the SSbD framework proposed by the EU Joint Research Centre and adopted in the Commission Recommendation of 8 Dec. 2022. To facilitate adoption by industry and, by doing so, foster the twin green and digital transition of Europe's economy, PINK's overarching aim is to produce innovative modelling software and integrated workflows for the development of AdMas&Chems, which are combined into an industry-ready open innovation platform, the PINK In Silico Hub (PINKISH).

3. PINK's tiered approach

PINK takes a holistic approach addressing the needs of industry by solving a multi-objective optimisation problem to improve and balance the four requirement categories functionality, cost-efficiency, safety and sustainability (Figure 1). All five steps of the SSbD Framework (hazard assessment, human health and safety aspects in the production and processing phase, human health and environmental aspects in the final application phase, environmental sustainability assessment, and socio-economic sustainability assessment) are integrated into selection considerations at each stage of the AdMas&Chems development, starting with a limited set of evaluation criteria and rough estimates (low-tier methods) and moving to higher-tier methods in later stages. In this way, confidence in the predictions is continuously improved over multiple design cycles by producing new knowledge on a constantly reduced set of better performing candidates.

PINK combines computational models and a decision support system (DSS) that exploit the combined power of first-principles simulation and pre-existing data, which - in itself - is further improved by advanced artificial intelligence (AI) technology. This requires the integration of tools from different and hitherto independently developed areas (e.g. materials modelling, (nano)safety, life cycle assessment). PINK provides this integration in the form of PINKISH based on an advanced semantic and technical Interoperability Framework, giving access to all information and knowledge, and executing SSbD workflows customisable to (a) the application area of the AdMas&Chems, (b) their safety and sustainability concerns of the existing materials, and (c) the status of the relevant development project (from early design ideas to registration and market entry). Industry readiness of the solution will be guaranteed by improving usability, practicability, user experience, and 'data provenance' documentation and security and by integrating these as important aspects into the development of new modelling software and decision support services. The sequence of implementation of the tools will be customised to real-life needs, to improve existing and new AdMas&Chems by industry partners in the PINK Developmental Case Studies and Industrial Demonstrators.

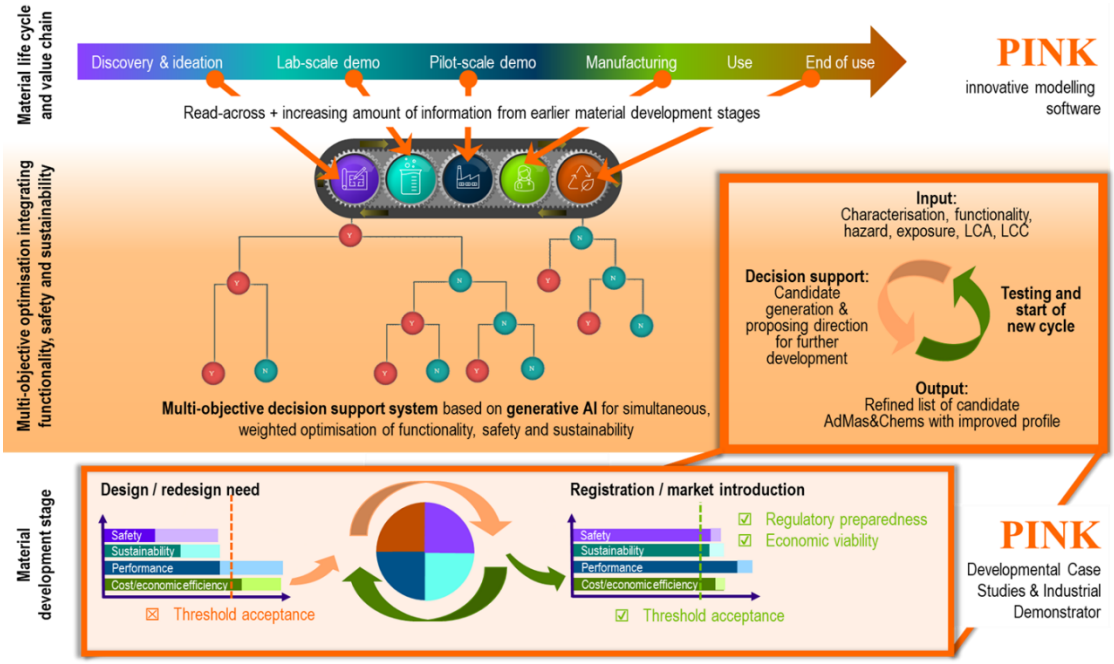

Figure 16: Schematic presentation of the PINK R&I Approach of integrating the SSbD Framework into the development cycle of AdMas&Chems. This will be achieved by solving the multi-objective optimisation problem (middle part) to improve and balance the four requirement categories (i.e. functionality, cost-efficiency, safety and sustainability, lower part) at each stage of the development. Existing data will be integrated and data gaps be filled using innovative modelling and simulation approaches from the complete life cycle and value chain (upper part).

4. Conclusions

PINK's central objectives can be summaries as:

- develop a toolbox of data resources, models and workflows (PINK Services), benefitting from the interoperability and synergy of integrated approaches and provide them as openly accessible software tools and web services;
- build a framework and toolset for technical and semantic interoperability (Interoperability Framework and Infrastructure), based on high FAIRness (findable, accessible, interoperable and reusable) standards essential for information transfer within PINK and enabling re-use by other SSbD workflows or platforms;
- integrate all data and modelling services into the PINKISH platform to facilitate data visualisation, analysis, and the implementation of a comprehensive AI-enabled SSbD decision support workflow; and
- showcase how the computational and digital approaches can boost the innovative capacity of industry and especially SMEs in Developmental Case Studies and Industrial Demonstrators providing real-world stress testing of the provided solutions.

5. References

[1] https://pink-project.eu

6. Acknowledgement

PINK (grant agreement No. 101137809) have received funding from the European Union's Horizon Europe Research and Innovation programme.

A look inside the DILAPRO project: Digital Twins of Laser Processing for Multi-Capability Manufacturing of Complex Components and Certification

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The DILAPRO project aligns with the focus on advancing smart production technologies for manufacturing complex products. It emphasizes two key aspects: developing multiscale physics-based models and machine learning techniques to enhance manufacturing predictions and creating Laser-materials interaction Digital Twins to assess materials quality from microstructure perspectives. The overarching goal is to expedite the manufacturing of complex products, ensuring they meet industrial standards in design, quality, cost, and sustainability, particularly in laser-based technologies like additive manufacturing.

DILAPRO aims to enhance additive manufacturing and laser production of complex products by developing Digital Twin software to assess materials properties, creating tools for digital certification, and demonstrating effectiveness in various sectors, particularly energy. The project's objectives are divided into specific goals for DILAFACT and DILACERT software and overall project objectives.

DILAFACT, the first software component of the DILAPRO project, introduces a sustainable and scalable platform termed "Digital Laser Factory". It facilitates laser process planning by digitally twinning laser-material interactions, encompassing additive, subtractive, and thermal processes. By leveraging this platform, manufacturers can meticulously plan and refine their production processes, even for new or short-run parts, based on various factors such as available technology, material properties (especially microstructures), economic conditions, and environmental considerations. This approach enables European manufacturers to embed sustainability at the core of

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their production operations, leading to a projected reduction of raw material consumption by 64% and related energy consumption by 5-27%.

The second software component, DILACERT (Digital Laser Certification), addresses a significant challenge in the deployment of evolving laser and additive manufacturing technologies: certification and standardization processes. Current certification models entail lengthy data processing and evaluation stages, imposing significant barriers to the speed and labour requirements of producing complex parts through these methods. DILACERT streamlines much of these procedures, enabling end-users to swiftly process and format production data either through inputs from DILAFACT or in-line monitoring systems. Furthermore, it lays the groundwork for the future development of remote, (semi-)automated "digital certification" processes for produced parts, marking a substantial paradigm shift in complex part production.

The project develops a common methodology for physical simulation, predicting microstructure and material properties, and contributes to developing standards and policies for future manufacturing. By simulating laser manufacturing processes, implementing online monitoring, and applying existing standards, DILAPRO aims to pre-certify laser-produced complex parts, demonstrating economic and environmental benefits and fostering community acceptance and uptake of its technologies.

Multidimensional Integrated Quantitative Approach To Assess Safety And Sustainability Of Nanomaterials In Real Case Life Cycle Scenarios Using Nanospecific Impact Categories

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1. Introduction

The INTEGRANO project addresses shortcomings and gaps in current safe and sustainability assessment approaches of Nano Materials (NMs) and Nano-enabled products (NEPs). Following the Framework for Safe and sustainable by design chemicals and materials[1], the project proposes a general assessment approach based on quantitative evidence to be applied in practice for specific Nano Materials (NMs) design cases.[2] The project will develop novel NMs impact categories (ICs) for nanotoxicity and eco-nano-toxicity assessment for the integrated application of standardised assessment methodologies. The synthesis, incorporation, use phase and end-of-life NMs life cycle stages (LCS) will be addressed for targeted case studies by leveraging the results and the results of case studies and methodology developed in the ASINA project[3-8], The collected/generated data will be used to meet the project's objectives to formulate design hypotheses and make design decisions by applying a data-driven approach and methodology, providing stakeholders with a digital supported decision process to tackle the Safe and Sustainable by Design (SSbD) challenge in the NMs context[9-11].

2. INTEGRANO – A general SSbD assessment approach based on quantitative evidence

INTEGRANO implements a defined protocol for the SSbD analysis of NMs and NEPs, relying on quantitative assessment supported by generation of a specific and harmonised dataset produced across a range of experimental and modelling activities (Figure 1) referred to a defined design of experiment matrix. The collection, storage and sharing of data within the INTEGRANO project will be mediated through the bespoke INTEGRANO Data Management Platform and associated INTEGRANO database. The Data Management Platform provides a structured interface to ensure that data collection across the life cycle stages is complete with respect to what is required to achieve the goals of the project and ensures that for each case study a harmonised dataset is produced which adheres to F.A.I.R. data principles. INTEGRANO proposes

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quantitative case-specific, and human-centric methodology, which is supported by the artificial intelligence algorithm also implemented within the ASINA project, enabling the selection of SSbD solutions by simultaneously addressing multiple and composite KPIs related to the safety, environmental, economic and functional dimensions. The methodology associates the generated harmonised data set to a specified DoE matrix. The advantage is found in the inherent minimum number of necessary and sufficient specific tox and eco-tox F.A.I.R. primary, functional and physicochemical data required, which implies minimising the experimental burden, while reducing the time and cost for developing each NM design case study. The SSbD cases represented in the decision spaces are associated to the corresponding performance level reported in the performance space and to the corresponding physicochemical SSbD cases data, thus enabling correlation between NMs physicochemical features and their related functional performance, safety and sustainability level. This opens up routes to further scientific investigations and grouping theory developments.

Overall, the SSbD workflow and related data generation and processing is organised in four stages:

i. Goal and scope definition.
ii. Data generation and Inventory by experimental and modelling work, data curation and F.A.I.R.ness compliance assessment.
iii. SSbD impact assessment: digital computation of the set of SSbD solutions with INTEGRANO Decision Support Tool.
iv. Interpretation of results, possible protocol reiteration, or final decision on the SSbD selected case operated by the NM (NEP) designer (decision maker).

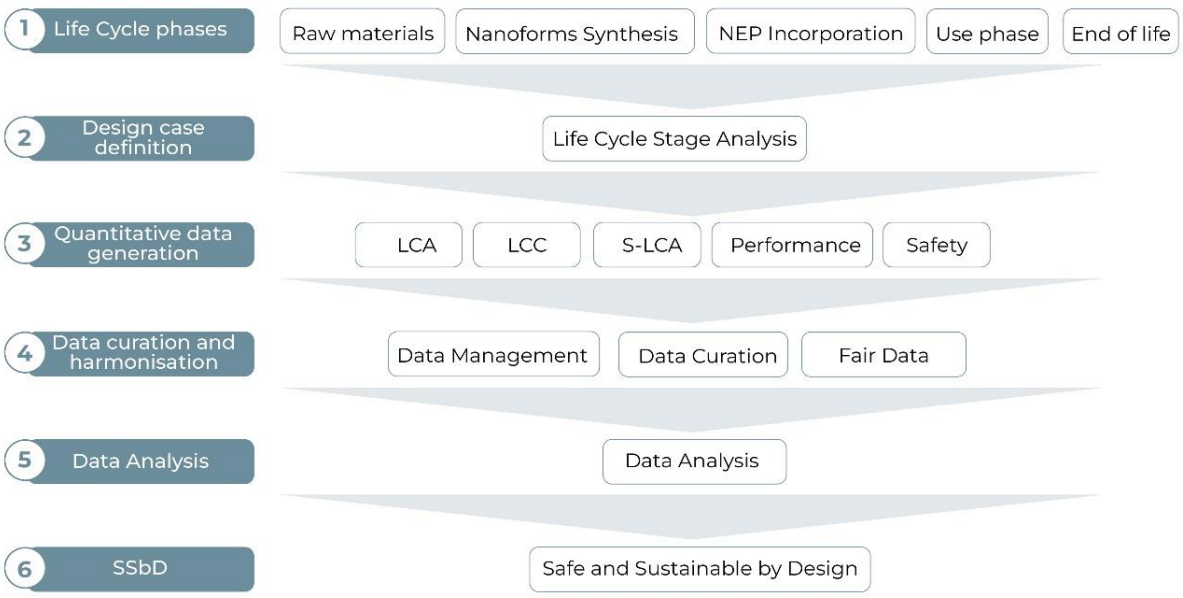

Figure 17 General view of data generation from each Life Cycle Phase towards the generation of the Safe and Sustainable by Design solutions by the INTEGRANO Decision Support Tool.

3. Conclusions

The methodology presented is a case-specific evidence based quantitative approach to SSbD within nanomaterials manufacturing, and which can be extensively applied more generally across materials and chemicals development. The approach requires a minimum amount of experimental data; thus, it is particularly suitable for research and

development activities, also leading to enhanced feasibility for implementation in industrial production design cases where minimal prior data is available. By leveraging the artificial intelligence algorithm implemented in the MultiOpimal™ decision support system the proposed methodology allows for informed human-centric decision making in the development of nanomaterials and nano-enabled products. This translates into research and technological development cost and time reductions, with >95% reduction in time-to-market, opening new frontiers in science and material engineering as well as in synthesis of new chemicals based on a quantitative and predictive approach.

4. Acknowledgements

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SSbD4CheM: Safe and Sustainable by Design framework for the next generation of Chemicals and Materials

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1. Introduction

The Horizon Europe project SSbD4CheM brings together stakeholders from industry, government, academia, and civil society to develop and promote best practices for safe and sustainable product and process design, through demonstration in three case studies. SSbD4CheM aims to meet the EU's strategic objectives for digital, enabling, and emerging technologies, sectors, and value chains. This is achieved through the development of a comprehensive Safe and Sustainable by Design (SSbD) framework, which utilizes new science-based approaches to identify and address potential hazards and risks, along with innovative technologies to support the design of safer and more sustainable products and processes. (Figure 1). SSbD4CheM objectives include:

1) Establishment of a SSbD framework that facilitates development of the next generation of chemicals and materials applicable to renewable composites in automotive value chain, PFAS-free coatings for textile and cellulose nanofibers as additive in cosmetics to replace plastic microbeads,
2) Development of efficient hazard screening tools for alternative assessment of next generation chemicals/materials/products combining *in silico* tools and multicriteria analysis,
3) Advanced explorative ex-ante Life Cycle Assessment (LCA) method supported by molecular and data-driven modelling to fill data gaps for (novel) materials and chemicals,
4) Integration of chemical/(nano-)material characterization methods to assess products' environmental safety and quantify emissions to support occupational and consumer safety limits, and contribute to exposure and risk assessment,
5) Development of alternative, in vitro models, as part of New Approach Methodologies (NAMs) for adequate exposure scenarios,
6) Harmonization and validation of analytical and toxicological methods for proposition to regulatory and standardization bodies to contribute to the

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development of new standards and facilitate market acceptance of SSbD4CheM project results, and

7) Enhance overall SSbD4CheM impact through stakeholder engagement, training, dissemination, and exploitation and drive industrial innovation.

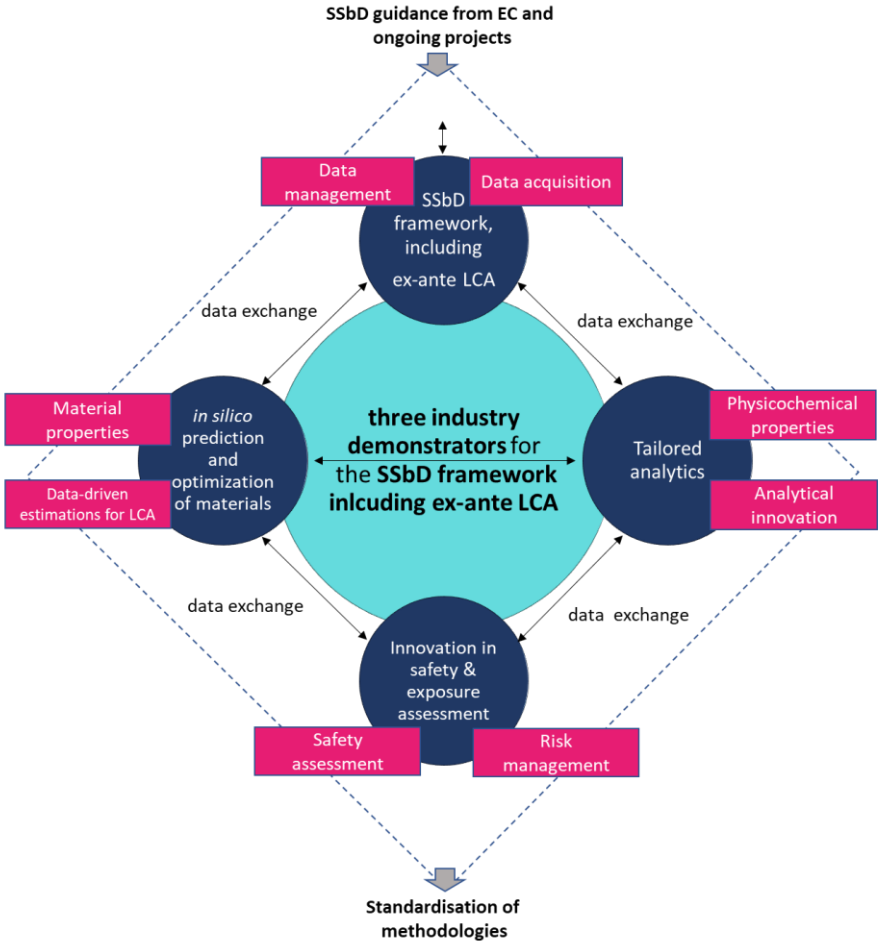

Figure 1: A comprehensive SSbD4CheM toolbox equipped with resources and tools for developing safe and sustainable products and processes.

2. Project Objectives

The strategic goal of SSbD4CheM is to introduce screening and testing methods for safe and sustainable material development in three relevant demonstrators being textile, automotive and cosmetics industry. The demonstrators will be the starting point for further implementation and standardisation of the new methods. The materials/chemicals of the demonstrators include per- and polyfluoroalkyl substances (PFAS) free textile coatings and natural fibres in different composite materials. Screening and testing methods focus on I) physicochemical characterisation with volatile organic compounds, non-uniform particles, and composition of the material, as well as II) risk assessment with exposure and hazard assessment and III) *in silico* prediction tools to reduce experimental delay. For each of the demonstrators an SSbD assessment is performed which will be fed with existing data and newly determined data based on the demonstrators.

3. Case Study 1: Textile

The textile use case's main objective is the experimental development based on the incorporation of bio-based self-cleaning/water repellent and antimicrobial treatments for apparel textiles for the textile market developed by plasma polymerisation and deposition of the coating using the Atmospheric Pressure Plasma (APP). The purpose is to facilitate cleaning and durability of the textile (Polylactic acid yarns, Recycle Polyethylene (PET), virgin PET and their knitted fabrics). These self-cleaning materials will improve the final performance of the apparel textile (Figure 2).

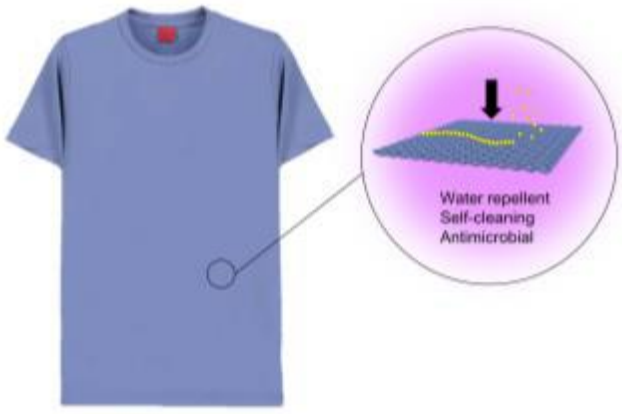

Figure 2: Modification of materials' surfaces for the production of self-cleaning textiles during the SSbD4CheM project.

4. Case Study 2: Automotive

SSbD4CheM project focuses on the renewable composites' formulation development considering recycled polypropylene and polypropylene made from renewable resources as a matrix in combination with micro-fibrillated cellulose and wood fibres as a green alternative for lightweight materials to reduce dependency on oil-based materials and increase materials circularity (Figure 3). Since interior trims are very close and interact with passengers in a relatively close environment, it is important to guarantee they are not an issue in terms of human safety and health. Thus, novel composite materials based on either renewable and/or recycled plastic reinforced by cellulose and wood-based filler will be investigated covering emissions and hazard assessments to enable safe use of such materials from the early R&D phase without any effect on passengers (prototyping).

Figure 3: Automotive interior parts to be modified by renewable composites produced during the SSbD4CheM project.

5. Case Study 3: Cosmetics

Nanocellulose, concretely cellulose nanofibrils (CNF) and cellulose nanocrystals (CNC), a natural material derived from cellulose fibres, has been gaining attention as a potential ingredient in cosmetics to replace plastic microbeads (Figure4). Nanocellulose has unique properties that make it attractive material for cosmetic formulations, including its high surface area-to-volume ratio, ability to absorb and retain moisture, and compatibility with a wide range of other ingredients. One potential benefit of using nanocellulose in cosmetics is its sustainability and biodegradability. As a natural, renewable material, it offers an alternative to synthetic ingredients such as physical peeling, scrub agents, dispersion stabilisers or texture modifiers that may be less environmentally friendly (e.g., plastic microbeads and nylon 6 or 12). However, it is important to note that the production of nanocellulose itself can have environmental impacts, so it's important to consider the entire lifecycle of the material.

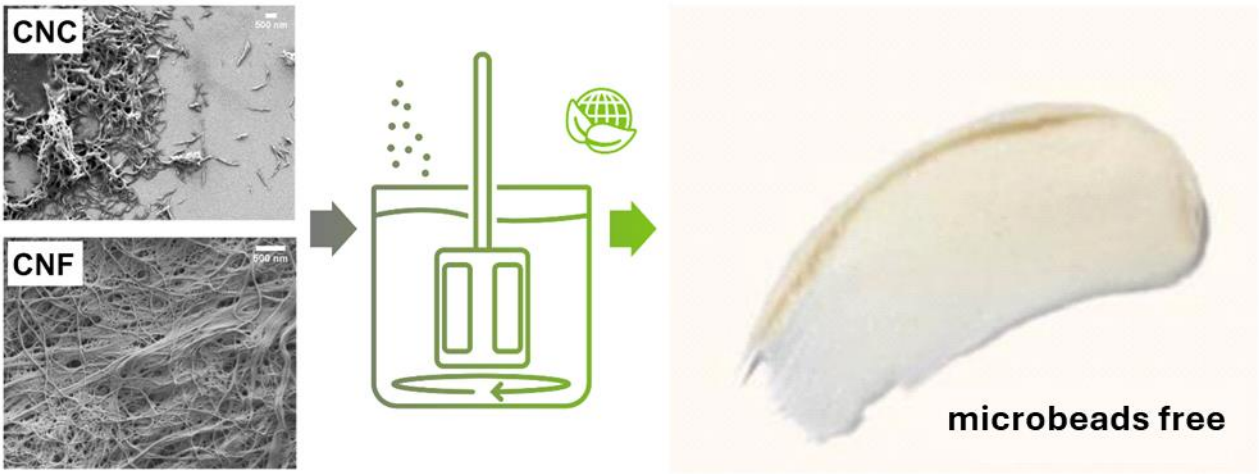

Figure 4: Preparation of cosmetic products using nanocellulose additives (SEM micrographs of CNC and CNF as adopted from [2]) during the SSbD4CheM project.

6. Conclusions

The materials developed within the three different SSbD4CheM case studies will be investigated utilizing computational (e.g., molecular simulations, machine learning, etc.) and advanced analytical techniques (e.g., time-of-flight mass spectrometry, cryo-focused ion beam-ion mass spectrometry advanced imaging, multi-angle light scattering, Scanning electron microscopy with energy dispersive X-ray spectroscopy, Gas Chromatography, Mass Spectrometry). The Safety evaluation methods for human epidermal and dermal topical exposure will be conducted using human skin ex vivo and in vitro models as well as computationally through molecular dynamics simulations. Finally, to guide research and development strategies from the beginning of the material development and ensure environmental competitiveness ex-ante LCA will be performed.

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An SSbD integrated impact assessment framework for advanced materials developed by SUNRISE

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1. Introduction

The European Green Deal policy aims outlined in the Chemicals Strategy for Sustainability and the Zero Pollution Action Plan emphasize the need for a transition towards a Safe and Sustainable by Design (SSbD) approach to chemicals and materials (EC, 2019; EC, 2020). This initiative seeks to transform the EU into a modern, resource-efficient, and competitive economy by turning environmental, health, safety, and sustainability challenges into opportunities in various policy areas, including chemicals. To support this transformation, the European Commission (EC) has recommended the establishment of a European assessment framework for SSbD of chemicals and materials, based on a holistic approach developed by the EC's Joint Research Centre (EC, 2022; C. Caldeira et al., 2022). To support the practical implementation of the EC-JRC framework by stakeholders, especially industry, the Horizon Europe SUNRISE project received funding to develop integrated approaches for health, environmental, social, and economic impact assessment of products enabled by advanced materials (AdMa).

2. Methods

The SUNRISE project combines the bottom-up development of methods for assessment of health, environmental, social and economic impacts with their top-down integration in an overarching Integrated Impact Assessment Framework (IIAF). This framework is designed to support SSbD decision-making along supply chains and lifecycle stages of AdMa and their products. The process of developing and testing the IIAF in cocreation with the stakeholders within a trusted real-world environment will improve our understanding of potential safety and sustainability trade-offs. This new knowledge will

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[10] EMERGE Ltd, Sofia, Bulgaria

be transferred to regulators and policy makers at EU and national level to support them in the implementation of SSbD-related policies for chemicals and materials.

3. Results

The IIAF, fully aligned to the EC-JRC SSbD framework, is a 4-tiered approach with each tier corresponding to an integrated methodology (supported by a toolbox) for health, environmental, social and economic impact assessment targeting different groups of users at different stages of the innovation process and requiring a different level of data and expertise. Tier 0 is a fast-screening method based on a questionnaire composed of 18 key questions designed for situations when an innovator needs to prioritise from a high number of possible design alternatives, which is a typical scenario for large industrial companies. Tier 1 is further qualitative screening at the early R&D stages of the innovation process that aims to identify hotspots of possible safety and sustainability concerns along the lifecycle. Tier 2 is a semi-quantitative assessment based on a weight-of-evidence approach applied in the product optimisation phase when a mix of qualitative and quantitative data are already available. Finally, Tier 3 involves a comprehensive quantitative safety (regulatory risk assessment) and sustainability (LCA (Life Cycle Assessment), LCC (Life Cycle Costing), and S-LCA (Social Life Cycle Assessment)) analysis for materials/products to be released on the market. To support generation of robust input data for the integrated methodologies we will develop and apply Integrated Approaches to Testing and Assessment (IATA), New Approach Methods (NAMs) as well as screening level and more advanced sustainability assessment tools based on LCA, s-LCA, LCC, Cost-benefit Analysis (CBA), and circularity analysis on a global scale.

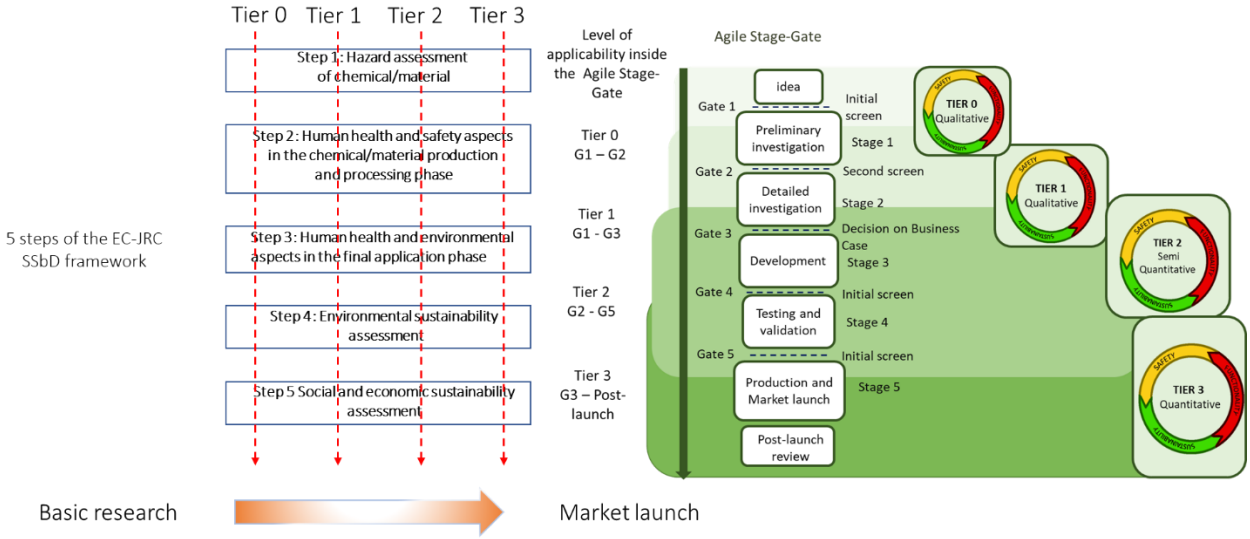

Figure 18: SUNRISE 4-tiered Integrated Impact Assessment Framework.

4. Conclusion

Implementation of the IIAF will ensure better regulatory compliance for AdMa based products and can have an impact on shortening the time of new materials/products to reach the market, thereby supporting the Green Deal policy objectives for the transformation of the EU into a modern, resource-efficient and competitive economy.

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Development of PFAS-free coatings in a safe and sustainable by design (SSbD) approach- the PROPLANET project

Eleonora Longhin[1], Dimitra Danai Varsou [2], Erin McFadden[1], Tatiana Honza[1], Tanima Sengupta[1], Sivakumar Murugadoss[1], Solveig Brochmann[1], Antreas Afantitis[2], Maria Dusinska[1], Elise Rundén-Pran[1]

Poly- and perfluoroalkyl substances (PFAS) are widely used in diverse production sectors, including constructions, food packaging and textiles, for their water- and oil-repellence properties, high thermal stability, and durability. Despite these advantageous properties, PFAS have been heavily debated due to their high persistency in the environment and potential adverse health outcomes. Some PFAS species are subject to restrictions, and the European Chemicals Agency (ECHA) issued a full ban proposal in February 2023.

In this context, the EC Horizon Europe project PROPLANET aims to develop novel PFAS-free coating materials, to overcome the barriers for environmental and human safety, chemical improvements, and circular value chains. The main goal of PROPLANET is to design and optimise three innovative coatings for the industrial sectors textile, food-packaging, and glass, by applying Safety and Sustainability by design (SSbD) principles.

The PROPLANET approach for the safety of the new coatings is based on risk assessment and management requirements, and builds on previous experience and knowledge on hazard assessment, methods standardization, computational models and safe-by-design tools developed within H2020 projects such as RiskGONE, NanoSolveIT and SABYDOMA. A stage-gate approach for safety evaluation along the development process should ensure safer products by a cost- and time efficient manner. Starting from the early development phase of the materials, existing information and data on the toxicological properties of the individual chemicals have been collected, and data gaps identified. New approach methodologies (NAMs), both *in vitro* and *in silico* methods, have been reviewed and selected for gap filling studies, using a tiered approach consistent with the development and life-stage of the materials. In this respect, the development of Quantitative Structure-Activity Relationship (QSAR) models can contribute to the identification of safer PFAS-alternative substances. In this work, the Ames test for Mutagenicity endpoint was investigated using *in silico* in-house QSAR models.

In addition, the formulations developed (the chemical mixtures) are tested using *in vitro* methods for human hazard assessment. A tiered approach is applied in the project, where the traditional cellular models (or 2D models) and screening assays are used for hazard assessment in the earlier development phases of the project, and advanced (3D) models and assays will be used to test the final products. The testing strategy addresses main toxicological endpoints according to regulatory requirements and takes into

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consideration Adverse Outcome Pathways (AOPs) addressing key events linked to the potential toxicity of the new materials.

To conclude, the coatings are evaluated based on their technical performance while ensuring the safety and sustainability throughout their life cycle. This work also supports the international effort towards the acceptance of NAMs for regulatory use in view of next generation risk assessment (NGRA).

The interlinked SUNSHINE Trusted Environment and Foresight Framework as a tool for detecting emerging trends in AdMa Innovation

James Baker[1], Cyrille Durand[1], Devendra Joshi[1]

Major industrial sectors such as energy, cosmetics, electronics, construction, food and healthcare are investing in research and technological development of advanced materials (AdMa) such as multi-component nanomaterials (MCNMs). These innovative materials can offer significant technological benefits over existing materials, since the integration of different components in a unique system can lead to improved functionalities, better performance coupled to energy and material savings which contribute to the overarching aims of the European Commission, in the form of the Green Deal, digital circular economy and climate change targets. Nevertheless MCNMs pose significant challenges in terms of regulatory compliance and environmental, health and safety (EHS) concerns, many of which are addressed by the European Research project Sunshine[2], funded under the H2020 programme.

Innovations tend to develop rapidly and in a myriad of directions such that regulators often have difficulties to follow and assess the implications of these innovations, and therefore are not always able to provide timely and adequate regulatory cover. Regulatory Preparedness, ensuring regulations are fit for purpose and ready for implementation, requires that regulators are made aware of upcoming trends and developments by industry. The **Sunshine** project aims to streamline and facilitate that process by developing and testing a Foresight Framework integrated into a Trusted Environment, which will host regulators, innovators, industry and key experts.

The essential first step is to create a forum where actors can freely share, comment, discuss and evaluate sensitive information, in other words a Trusted Environment (TE). The Foresight Framework cannot operate unless it is securely embedded in a TE. Establishing the TE depends on establishing the operational rules which can be accepted by all actors, and which are enshrined contractually in the rules of the TE, and a selection of these rules are shown in Figure 1.

A TE provides some clear opportunities for Industry and Regulators in particular, including:

- Creating a safe space for open discussion
- Raising common issues that could prevent a level playing field in the market
- Gaining visibility at supply chain level to anticipate future investments
- Early and voluntary industry involvement in the setting of new regulation
- Provides aligned communication & dialogue with civil society/NGOs
- Accelerates the resolution of cross-cutting issues that could slow the market expansion

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[2] The SUNSHINE project is funded under the European Union's Horizon 2020 Research and Innovation programme, Grant Agreement 952924

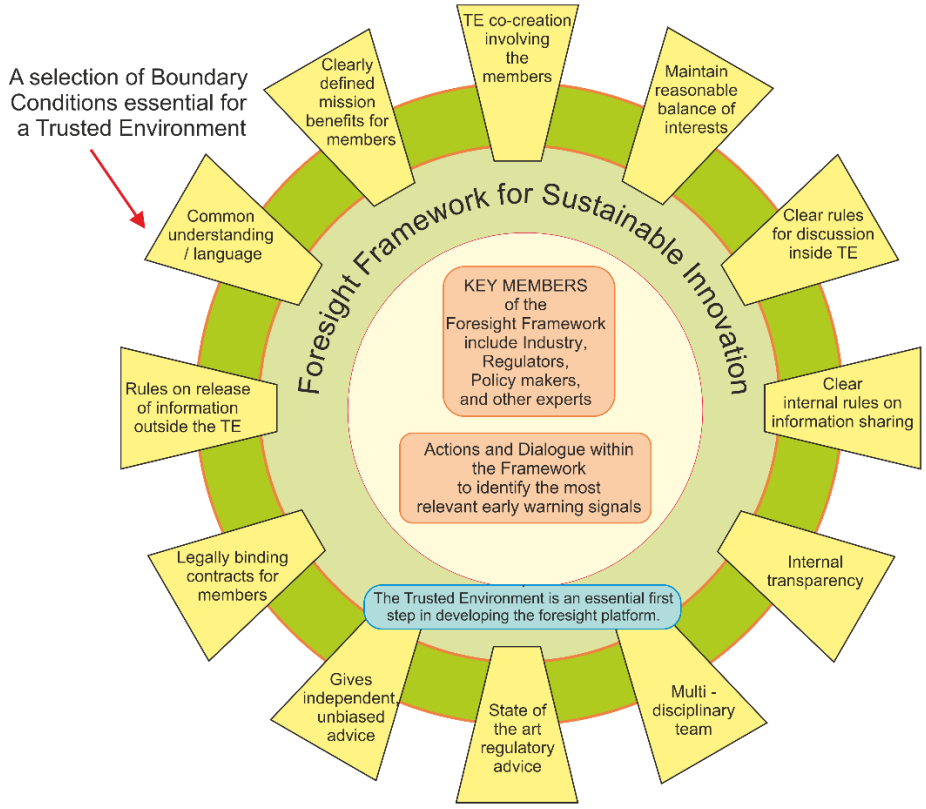

*Figure 19: The linked **Sunshine** Trusted Environment and Foresight Framework currently under development by TEMAS Solutions and RIVM together with partners JRC and Yordas.*

Trust between the members of the TE, and therefore the Foresight Framework is key, and therefore strict adherence to the rules of the **Sunshine** TE is essential. Potential barriers to be avoided include:

- Unclear/no rules on disclosure and management of sensitive information
- Lack of commonly agreed scope and goal
- Lack of mutual interests/benefits
- Perception of a non-inclusive working process
- Opaque decision-making process
- Unbalanced representation of stakeholders' interests along the supply chain

The Foresight Framework, developed and piloted in the **Sunshine** project, comprises a number of steps by which various sources and databases are mined in order to identify weak signals or signs of upcoming industrial innovation and development (see Figure 2). A selection of available sources of relevant information, mostly literature, will be mined by suitable software and a selection made of the indicators of upcoming trends and developments in AdMa which can be of potential interest to regulators. Refined processing will produce at regular intervals throughout a year a set of information which must be scrutinised and evaluated by the experts within the Trusted Environment. This selection of information will be the main output of the Foresight Framework, and will be integrated into the **Sunshine** e-infrastructure, and will support the development of Regulatory Preparedness in the **Sunshine** project.

The creation of a Foresight Framework included in a Trusted Environment will benefit both SSbD and Regulatory Preparedness because when knowledge is openly shared between industry stakeholders and Regulators from the early stages of innovation, the time for Advanced Materials such as MCNMs-based materials and products to reach the market can be substantially reduced, while ensuring high levels of human and environmental safety. A preliminary survey of industry working in the field of nano or advanced materials have expressed interest to be part of a Foresight Framework.

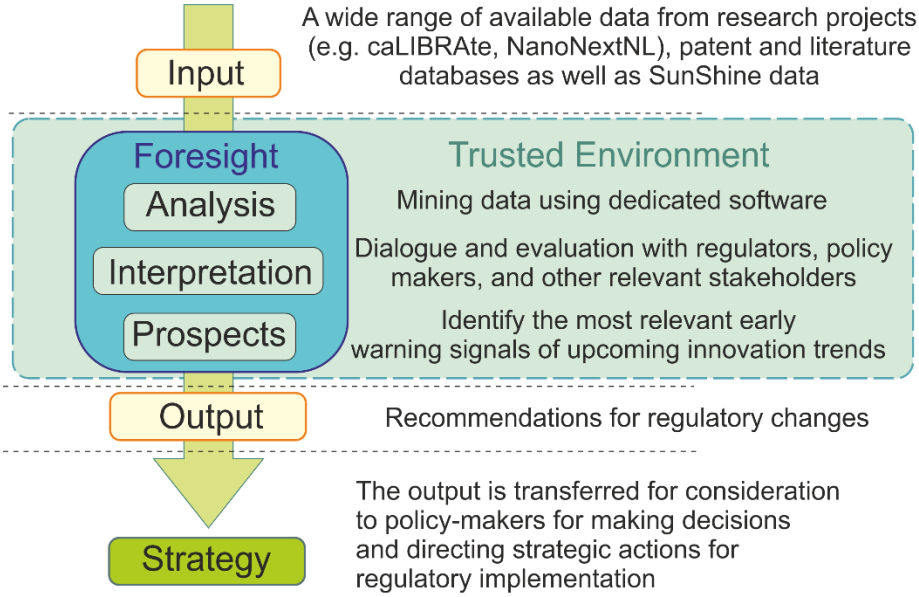

*Figure 2: A simplified overview of the steps in the **Sunshine** Foresight Framework*

Improving the anticipatory capabilities of regulators and (regulatory) risk assessors and to facilitate, where needed, timely adaptation of (safety) legislation, guidance guidelines and standards. Timely clarity on how regulators deal with novel materials such as MCNMs reduces uncertainty for industry about the information needed to comply with a regulation and how testing should be performed.

The implementation of the **Sunshine** Foresight Framework will support Regulatory Preparedness leading to a shorter time to market of MCNMs or MCNMs-enabled products.

Tackling Innovation Challenges in an Industry 5.0 context with an Ontology-based Open Translation Environment

Gerhard Goldbeck[1], Otello M Roscioni[1], Michael Noeske[2], Jesper Friis[3]

1. Introduction

In order to reach the goal of a more sustainable, human-centric and resilient European Industry, as discussed in a report by the European Commission on Industry 5.0 [1], innovation systems and processes are required that firmly put the human in the loop.

The OntoTrans project [2] has been contributing to these objectives [3] by (a) further developing and testing the so-called "Translator" approach [4, 5, 6] to industrial innovation, (b) expressing human knowledge and joint understanding of innovation challenges in a standardised, well-grounded, machine-readable ontology, and (c) building and implementing a set of tools that help to democratise the use of diverse information sources (including materials modelling), empowering users to make informed decisions.

2. Translation for human-centred innovation

Translation in the context of innovation and Industry 5.0 is a process that involves teams that guide the interaction and knowledge exchange between actors in customer-focused industrial R&D. The teams typically involve experts from different fields including the materials//manufacturing domain experts, but also computer science and semantic technologies that build and customise digital tools to support gathering and exchanging relevant knowledge. Together they follow the six steps of translation [4]. OntoTrans revealed that solving an overarching innovation challenge may embrace assessing a series of characteristically related innovation cases sharing relevant concepts and datasets which in manufacturing represent distinct combinations of materials and processes. The project has confirmed the pertinence of the underlying translation approach and supports it with a range of digital tools and technologies, which together are called the Open Translation Environment (OTE).

3. Semantic knowledge management

Semantics provides the ability to carry out unified analysis of data from different data sources, enables augmented analysis, recommendations and AI orchestration. These developments are driven by the need and opportunity of democratising data access and enabling 'self-service' analytics.

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Despite the success of semantic knowledge management in a range of business and technology fields, materials semantics remains somewhat scattered [7] and with little industrial uptake.

To address this issue, a number of EU projects have been developing an ontology framework that incorporates fundamental principles and concepts from the natural sciences, in particular physics, chemistry and materials science: the EMMO (Elementary Multiperspective Material Ontology) [8]. It is unique in providing users with a combination of rigorous, science based axiomatisation and flexibility of expression. On that basis, the OntoTrans project has built a semantic knowledge system based that enables users to represent innovation challenges and connect them to a range of data sources including data from modelling and simulation. It facilitates the creation of FAIR data.

In particular, the OTE framework employs semantic mapping techniques to convert raw data from various formats into machine-readable RDF instances [9]. Through pipelines connecting data resources to parsers and semantic mapping schemas, the OTE facilitates the creation of structured, semantically enriched information. This process ensures that data is documented in a standardized ontological form, laying the foundation for FAIR datasets.

Central to the OTE framework is the creation of a knowledge base supported by domain ontologies and populated with RDF instances organising data and metadata in a structured way. Thus, the OTE enables users to capture and organize relevant information systematically, fostering collaboration between various stakeholders in Industry 5.0.

4. OTE tools: connecting data sources and data exploration

Since OntoTrans needs to work with a wide range of data sources as well as connect to models that can generate data on demand, OntoTrans has developed the OTEAPI [10] package, which can be described as an actionable data documentation system for semantic interoperability. The OTEAPI plugin architecture facilitates the implementation of various data interfaces in one place. The creation (i.e., configuration) of OTEAPI pipelines provide a simple interface for data providers to document their data (Figure 1).

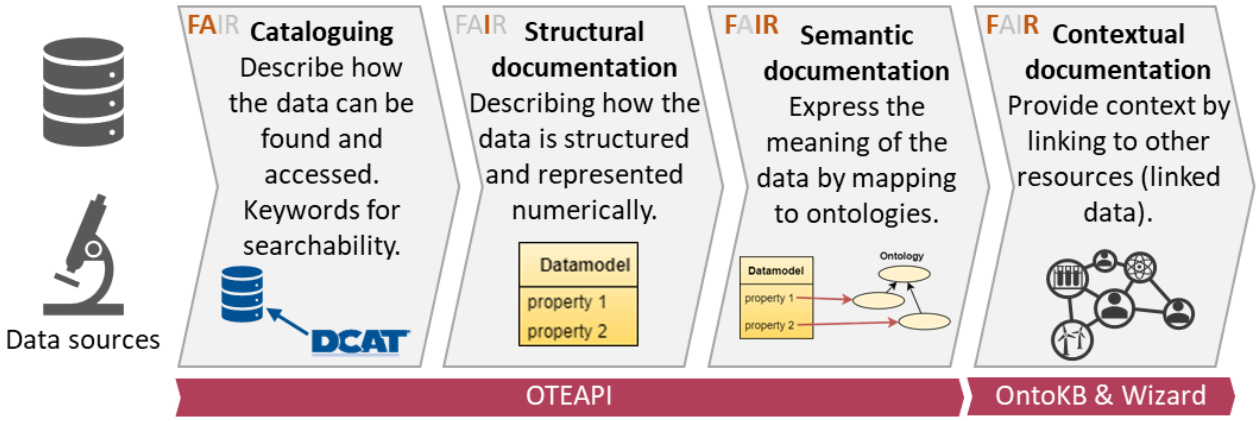

Figure 1. The four levels of data documentation. The aspects of FAIRness that each level contribute to is also indicated.

The OTE incorporates an Exploratory Search System (ESS) [11] designed to enhance information-seeking tasks through semantic-enriched data exploration. By leveraging the underlying semantic structure, users can interactively search and navigate through the knowledge base, facilitating the retrieval and discovery of relevant information.

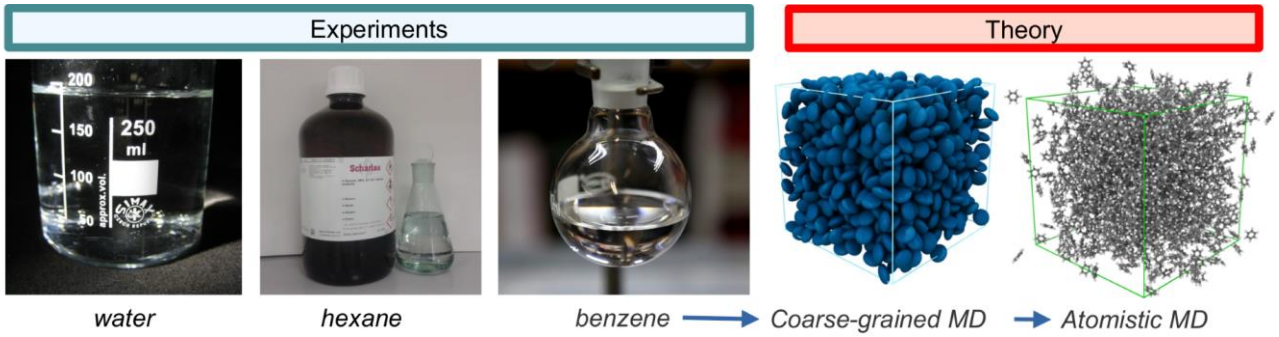

Figure 2: OTE enables FAIR data starting from common data formats such as a spreadsheet and plain-text log files. The use case used to demonstrate the OTE includes a dataset of experimental properties for three solvents, and the thermodynamic output simulations.

5. Conclusions

The Open Translation Environment is a set of open-source software for the creation of FAIR data in materials science. By integrating semantic technologies into the data documentation and knowledge creation process, the OTE framework enables users to represent, access, and utilize information in a standardized and interoperable manner. he OTE facilitates a translation approach to advance materials innovation in an Industry 5.0 context.

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7. Acknowledgments

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Bridging the Gaps in Nanosafety for Animal-Free Prediction of Adverse Outcomes

Vladimir Lobaskin [1], J. Štrancar[2], I. Urbančič[2], T. Stoeger[3], U. Vogel[4]

1. Introduction

On a daily basis, people are exposed to a multitude of health-hazardous airborne particulate matter with notable deposition in the fragile alveolar region of the lungs. Hence, there is a great need for identification and prediction of material-associated diseases, currently hindered due to the lack of in-depth understanding of causal relationships, in particular between acute exposures and chronic symptoms.

The current animal-based testing of novel materials' short- and long-term health effects is slow, expensive, and has limited capacity, which stifles the development of advanced materials and hinders efficient regulation of the market. To enable cost-efficient high throughput screening required for industry and regulation, one should shift the focus of nanosafety testing from late endpoints to early key events (KEs) leading to adverse outcomes (AOs). As such tests can only be based on mechanistic understanding, we need to close the knowledge gaps and match KEs *in vitro* and *in vivo*.

2. Methodology

Within the H2020 SmartNanoTox project, we had applied diverse advanced microscopies and omics to *in vitro* and *in vivo* systems, together with *in silico* molecular and coarse-grained modelling and determined herein that the long-lasting response to a single exposure can originate from the interplay between the newly discovered nanomaterial quarantining and nanomaterial cycling between different lung cell types [1]. This new insight allowed prediction of the spectrum of lung inflammatory responses associated with materials of interest using only *in vitro* measurements and *in silico* modelling, potentially relating outcomes to material properties for a large number of materials, and thus boosting safe-by-design-based material development.

Following the initial discoveries, in the Horizon Europe nanoPASS project we had developed the automated translation of the automated *in vitro* observations into *in silico* model, that enables automatic discovery of the early mode-of-action and further on automated disease evolution prediction. Because of its profound implications for animal-free predictive toxicology, this work paves the way to a more efficient and hazard-free introduction of numerous new advanced materials into our lives.

Our key bridging methods are intravital in vivo microscopy, quantitative time-lapse *in vitro* microscopies, and automated identification of the modes of action (i.e. KE relationships) with proprietary *in silico* algorithms, supported by datamining of the

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worlds' largest *in vivo* database and single-cell omics data, and computational modelling of structure-function relationships.

3. Results

In the nanoPASS project, we aim to 1) develop new *in vitro* systems that can replicate early KEs leading to AOs related to inhalation of NMs, 2) identify methods to track the dynamics of these KEs, 3) develop quantitative *in silico* models to predict AOs, and 4) calibrate the *in vitro*/*in silico* AO predictions against *in vivo* data for 40+ well-characterised benchmark materials. We will also validate the AO predictions on several families of industrial materials, sampled from different stages of their life cycle, and then propose reliable testing protocols and guidelines. With the consortium of 6 complementary research laboratories, SME as technology developer and provider, material producing company as potential end-user, and an industrial association to facilitate dissemination, nanoPASS covers the whole value chain of the new animal-free safety testing technology, and thus paves the way towards safe adoption of new nanotechnologies.

4. Acknowledgements

We acknowledge funding from the EU Horizon2020 framework under grant agreements No. 686098 (SmartNanoTox project), Horizon Europe under grant agreement No. 101092741 (nanoPASS project).

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Ontology-based Decentralized Sharing of Industry Data in the European Circular Economy

Mikael Lindecrantz[1], Eva Blomqvist[2]

1. Introduction

Circular economy aims at reducing value loss and avoiding waste, by circulating material or product parts before they become waste. Today, lack of support for sharing data in a secure, quality assured, and automated way is one of the main obstacles that industry actors point to when attempting to create new circular value networks. Together with using different terminologies and not having explicit definitions of the concepts that appear in data, this makes it very difficult to create new ecosystems of actors in Europe today. Semantic interoperability of data is one of the biggest barriers towards data sharing in the Circular Economy.

A solution to these challenges needs to leverage open standards for semantic data interoperability in establishing a shared vocabulary (ontology network) for data documentation, as well as create a decentralized digital platform that enables collaboration in a secure and confidentiality-preserving manner. This vocabulary can then be used to construct digital twins of circular value networks to further enable open collaboration. Once defined, the blueprints of these digital twins will be reusable as templates and can be reused with a different set of actors or used within a different industry domain. Established Semantic Web technologies and standards provide the technical foundations for information flows that will transform European Industry towards a CE, by means of digitalization and data sharing.

This vision includes several open research problems, including the development of ontologies that need to model a wide range of different materials and products, not only providing vertical interoperability but also horizontal interoperability, for cross-industry value networks. As well as transdisciplinary research on methods to find, analyse and assess new circular value chain configurations, and form their decentralized digital twins. The solutions will allow for automation of planning, management, and execution of circular value networks, at a European scale, and beyond. Thereby supporting the acceleration of the digital and green transitions, automating the discovery and formation of new collaborations in the circular economy.

2. The Onto-DESIDE vision

To address the above challenges, an EU-funded project, Onto-DESIDE, was started in 2022. Onto-DESIDE develops a standards-based web technology platform for allowing data sharing about materials, products and processes at a global scale. Since access to verifiable information is central, well-established open standards for secure and confidentiality-preserving information sharing are core components. Ownership and

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storage of data should remain with the data producer; hence a decentralized approach is necessary. Metadata and structures for transforming data into information (semantic descriptions, i.e. ontologies) are open, and comply with FAIR principles, to enable the highest possible degree of semantic interoperability and automation in data sharing. For sensitive data, methods allowing for proof of existence of the data can be used, where proofs can be shared while actual data is kept private.

Another aspect is to address the use of these technologies in a business context, and study the circular economy as a complex system to develop integrated tools and methods for further enhancing CE. Although the importance of various 'flows' - namely: resource flows, information flows, value flows, and energy flows - has been widely acknowledged within the transformation to CE, so far, they have not been integrated or linked into a single framework or approach. Without such integration or linking it is currently not possible to make robust designs of circular value networks, and to conduct value network coordination towards implementation and operation within industry. Moreover, this should result in robust value networks that are profitable, equitable, and invite long-term collaborations and partnerships. Therefore, apart from the solutions needing to be technically feasible, there is also a need to explore how such value networks can be designed and developed, using the ontologies for data documentation and data sharing, but considering the interplay of resource, information, value and energy flows, i.e. considering how the value network will behave as a system.

3. Onto-DESIDE core outcomes

Within the Onto-DESIDE project, four core components are envisioned:

- **A network of ontologies** for data documentation, that allows for semantic interoperability and supports flexible, automated, decentralized data sharing between industry actors.
- **An open circularity platform**, i.e. a secure and confidentiality-preserving decentralized data sharing platform allowing the creation of digital twins of circular value flows, by enabling FAIR sharing of data between industry actors, facilitating the initiation of new collaborations in the circular economy.
- **Methods** to find, analyse, and assess new circular value chain configurations opened up by considering resource, information, value, and energy flows as an integral part of transitioning to a circular metabolism within industrial systems through co-design and co-creation.
- **Validation** - demonstrating and quantifying the potential for increased retainment of value when applying the above outcomes in cross-border and cross-industry sector circular value networks in Europe.

The overall project research methodology divides work into three iterations. In the first project iteration a first version of a Circular Economy Ontology Network was developed, short CEON[3]. This was then used as the backbone for semantic data interoperability, sharing, and querying in a data sharing platform for CE[4], based on the Solid protocols, another emerging set of web standards. However, it is important to note that the prototype, including ontology modules, will certainly change in the current (second) and third iterations of the project.

[3] https://w3id.org/CEON/
[4] https://github.com/KNowledgeOnWebScale/open-circularity-platform

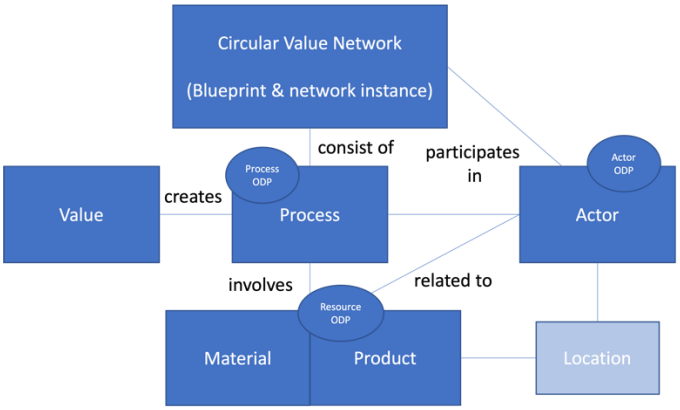

Figure 20: Informal conceptual overview of the topics covered by CEON modules.

The Digital Twin of circular value networks

While semantic interoperability, and ontology-based data documentation, are essential enablers for large scale CE, they are not enough in themselves. Semantically described data also need to be put into use, in automated processes. Today, there is limited data collaboration within industry domains and even less across domains, consequently new circular value networks are only created between known actors that have a certain degree of comfort working together – limiting the possibilities of more high value circulation scenarios, and novel innovative configurations being discovered. Open collaboration could remedy this, but data and ontologies cannot solve the problem alone. To facilitate open collaboration in a data driven circular economy a new entity is needed, the digital twin of circularity.

The concept of digital twins has been used for many use cases and in many industries and the fundamental theory behind the concept is not a new thing. But the idea of constructing digital twins of circular value networks, with the value network itself, and related 'flows', as the objects in focus, is a novel idea and has not been explored before. If digital twins are built upon shared ontologies, i.e. the ontology network, once defined, their blueprints are also reusable as templates for a certain circular value network. These blueprints could be shared with a different set of actors or used within a different industry domain to instantiate new value networks.

4. Validation through industry use cases

The core project outcomes are tested and evaluated in the three project use cases, i.e. in the textiles, electronics and construction domains respectively. In the project a research dataset, incorporating data structures and attributes relevant for CE decisions and value network execution in one example circular flow in each of these industry domains have been developed. Together with scenarios, representing information needs of actors in the value network, this sets the ground for establishing feasibility and evaluating the efficacy and quality of the project outcomes. So far the first platform and ontology network release have been evaluated, rendering a basic confirmation of feasibility and a set of necessary points of further work and improvements have been noted.

Regarding the ontology network, the validation more concretely meant to test the ability for the core ontology modules to be extended into more (industry) domain specific ontologies and concepts. Hence, as a test case, three industry specific ontologies were created, by specialising the core modules and patterns, and thus assessing their ability to document the data needed in those three use cases.

5. Conclusions and outlook

When analysing existing ontologies, we note gaps in coverage of central CE concepts, such as the Circular Value Network itself. In other domains on the other hand, e.g. materials and manufacturing, there are instead many overlapping ontologies and/or partly competing conceptualizations. Our proposed solution is to create a set of Ontology Design Patterns, i.e. a "pattern language", and ontology modules that represent core concepts related to CE, to provide a core to which existing ontologies can be aligned, and in addition complement missing CE concepts. Alignments to existing ontologies are still part of future work, and validation of the core CE concepts against emerging standards such as the CE terminology and definitions by ISO/TC 323. However, we can still conclude that the approach has proven feasible and useful, in initial modelling exercises of the project, c.f. the use case validation described above. Together with the extended methodology, FAIR publishing, and the high degree of modularisation we see this as a step towards true ontology reusability, even in cross-domain scenarios such as CE.

Ongoing and future work includes the creation of alignment modules, to connect our network to other ontologies, and to perform a more extensive evaluation, involving actual data exchange through the Solid-based Onto-DESIDE data exchange platform, and to extend the evaluation to encompass cross-sectorial data exchange.

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openLCA and OpenSemanticLab - Build a Digital Bridge between Material Science and Life Cycle Assessment (LCA)

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Safety and sustainability by design (SSbD) is nowadays an important aspect in material science. Nevertheless these key aspects are seldom included in early stage development, where critical decisions about the paths to explore are made. This is due also to the disconnection of both the human experts and the data structures in the material science and sustainability domains. To overcome the lack of a common language we have created a linked data schema for an electronic lab notebook which is compatible to the openLCA data schema.

The approach is based on JSON-LD shaped with JSON-SCHEMAs which are also used to generate a web user interface with the OpenSemanticLab software stack.

The user interface enables any material scientist to feed data (processes/materials) directly from the lab, requiring only a web browser and no specific know-how neither on JSON-LD nor on openLCA.

The interface to openLCA is based on simple python app that allows to query and select process entities, automatically maps them to the target format and downloads the result as openLCA ZIP-Archive. While doing so, existing openLCA definitions like properties, units and existing flows are referenced and not duplicated by using mapping terms or user annotations.

This allows materials researchers to create a knowledge graph of their experimental setups which can be converted automatically to openLCA flows and processes. Semi- or fully automated predefined assessments by LCA experts can then evaluate various scenarios and provide an early and fast feedback to the materials researcher. In this talk we demonstrate this approach for the use case of paper-based electronics and elaborate on the potential of a strong coupling between materials and sustainability research from an early development stage.

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Session 4: Digital Transformation - Computational Tools & Platforms for Materials R&I Acceleration

This Session discusses the (potential) implementation of the most recent technology trends in the materials R&I process. Advanced modelling methods and Artificial Intelligence (AI) are already finding numerous applications in innovation processes, ranging from the autonomous discovery of components to the design of new substances and composites and their deployment in advanced devices. Moreover, such accelerated R&I processes are supported by advanced data analytics, robotics, and high-performance computing.

Presentations (oral and poster) will also cover the following topics:

- Materials R&I supported by materials acceleration platforms, autonomous robotics platforms, AI-driven design and advanced simulations, theory and multiscale modelling (High-Throughput Experimentation, Digital Simulation of Test Methods/Materials),
- Digital twinning of and use of AI in materials characterisation and fabrication technologies,
- AI-based data handling and workflow optimisation,
- Business models for platforms and best practices, and
- Digitalisation of materials modelling and characterisation and test methods.

Detailed Programme

Start	End	Title	Presenter
09:30	09:45	Harnessing the power of automation and machine learning with a modular material acceleration platform – an illustrating example	Simon Stier
09:45	10:00	Advancing Material and Chemical Development through Innovative Computational Modelling in the PINK Project	Haralambos Sarimveis
10:00	10:15	Experimental synthesis of safer nanomaterials through computational modelling and design	Richard Harris
10:15	10:30	First Principles In Silico Characterisation of Advanced Materials and Bio-Nano Interface	Vladimir Lobaskin
10:30	10:45	Advancing Materials Development through Multiscale Modelling and Data-Driven approaches in the Safe and Sustainable by Design Framework	Andrea Lorenzoni

Posters

S04_P01	Efficient Workflow Automation for Materials Modeling: Towards Predictive AI Systems using Synthetic High Throughput Dataset Generation	Mario Vozza

S04_P02	A Combination of Computational Modelling, Simulation and Experimental Work: Titanium dioxide nanoparticle toxicity with different shapes and sizes evaluated based on solution pH.	Shanaaz Witbooi
S04_P03	Computational assessment of the environmental transport and fate of small molecules and PFAS using the SimpleBox4Planet web-application	Dimitra-Danai Varsou
S04_P05	GrapheNet: A Novel Deep Learning Model for Predicting Physical and Electronic Properties of 2D Materials Using Images	Tommaso Forni
S04_P06	Size-dependent study of water adsorbed iron oxide nanoparticles: a computational and experimental study	Danell van Wyk
S04_P07	ProtoNANO: assessing the toxicity of inorganic nanomaterials using nano-QSAR models	Salvador Moncho
S04_P08	Grouping of advanced multi-component nanomaterials: can machine learning help?	Georgia Tsiliki
S04_P09	A local search approach to predict and optimize nanomaterial toxicity in early stage nanomaterial design.	Kostas Blekos
S04_P10	Molecular mechanisms and potency for ENM grouping	Marcella Torres Maia
S04_P11	Toxicity assessment of metal-ions binary mixtures: new computational approach for calculation toxicity indexes	Dawid Falkowski

Oral Presentations: Session 4

Harnessing the power of automation and machine learning with a modular material acceleration platform – an illustrating example

Matthias A. Popp[1], Shahbaz T. Bandesha[1], Simon Stier[1]

Materials research includes variation and optimization of synthesis routes including sequences of parametrized steps such as dosing, mixing, heating, transport and many others. The huge combinatorial space spanned by combinations of elementary steps and their parametrization can be overwhelming and puts a strong limitation on labor-intensive research tasks accompanied with high cost in terms of time and money for the development of new materials. Therefore, it is desirable to speed up the iterative research loop by the use of automation and robotics. In addition, utilization of modern machine learning techniques can decrease the number of iterations needed to reach optimal results. The concept of a material acceleration platform (MAP) therefore includes automated synthesis, automated analysis and automated decision-making.
In this presentation we demonstrate a minimal viable example utilizing our modular MAP developed in the context of the project BIG-MAP. We elaborate key concepts both on the hardware and software side as well as data management. Last but not least we showcase the interplay between our robotics platform and the Open-Source software stack OpenSemanticLab to orchestrate and visualize the experiments in a human friendly way.

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Advancing Material and Chemical Development through Innovative Computational Modelling in the PINK Project

Haralambos Sarimveis[1], Steffi Friedrichs[2], Francesca L. Bleken[3], Anna L. Costa[4], Francesco Mercuri[5], Antreas Afantitis[6], Antonino Marvuglia[7], Tommaso Serchi[8], Dario Greco[9], Penny Nymark[10], Martin Himly[11], Karin Wiench[12], Philippe Jacques[13], Iseult Lynch[14], Andreas Karwath[15], Georgios Gkoutos[15], Roland Hischier[16], and Thomas E. Exner[17]

1. Introduction

The PINK project represents a groundbreaking initiative at the forefront of material and chemical innovation. Positioned within the landscape of contemporary scientific research and industry needs, it aims to revolutionise the way advanced materials and chemicals are developed. By harnessing the power of cutting-edge computational modelling techniques and aligning with the principles of Safe-and-Sustainable-by-Design (SSbD), the project seeks to create a computational infrastructure for materials and chemicals that are not only functional but also inherently safer and more sustainable.

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2. PINK Modelling and Decision Support Framework

Central to the PINK Modelling Framework is the harmonization of diverse data models and software tools, aimed at addressing complex multi-objective optimization challenges. These challenges encompass balancing functionality, cost-efficiency, safety, and sustainability in material and chemical development. In line with the recently proposed SSbD framework, a detailed library of data analytics and machine learning models is under development. This library is crafted to predict the functionalities and impacts of materials and chemicals across their entire lifecycle, encompassing all stages from production through to disposal.

A crucial element of the PINK project's modelling work is data-driven and AI-based methodologies, such as QSAR and QSPR models, which are employed to predict material properties and impacts. Complementing this, multi-scale modelling is offering essential insights into material properties across various scales, from atomic to macroscopic. Incorporating life-cycle assessment (LCA) methods further enriches the project, enabling an evaluation of the environmental impact of materials across their entire life cycle. The integration of both exploratory and prospective LCA approaches allows understanding of sustainability impacts at various developmental stages. Moreover, the project will incorporate advanced methods in toxicogenomics, which involves using omics technologies to understand the molecular mechanisms underlying the toxicity of substances. Mechanistic models, notably Physiologically Based Kinetic (PBK) models, will play a pivotal role in risk assessment and biokinetics simulations.

For the development of safe production processes, data-driven multi-objective optimization algorithms like Bayesian optimization will be utilised. These techniques help in identifying optimal conditions in production processes, balancing factors like yield, environmental impact, and product consistency. Generative learning and explainable AI are also key components of the project. Generative models will be used to explore vast chemical spaces and propose novel structures, thus driving innovation in material and chemicals design.

The PINK project's decision-support strategy is built on an iterative approach, which effectively narrows down potential material and chemical candidates through successive iterations. In each iteration, a vast array of candidates is evaluated and filtered based on a multitude of factors, including functionality, safety, sustainability, and cost-efficiency. As the process advances, the number of candidates reduces, and the focus intensifies on those with the most promising profiles. Explainable AI will ensure that the decision-making process in the material development is transparent and understandable, crucial for gaining trust and acceptance in the industry.

3. Conclusions

The PINK project aims to establish a new benchmark in material and chemical development by integrating diverse, advanced modelling methods into a unified and coherent framework. It aligns the goals of enhanced functionality with environmental responsibility and safety, paving the way for a more efficient and sustainable approach to material and chemical innovation.

4. Acknowledgement

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Experimental synthesis of safer nanomaterials through computational modelling and design

R.A. Harris[1]

1. Introduction

Iron-oxide magnetic nanoparticles (NP) have extensive applications in many different fields such as biomedicine and biochemistry, high density data storage, magnetic resonance (MR) contrast enhancement and immunoassay analysers to name a few [1,2]. These NPs have been approved by the food and drug administration for clinical applications as MRI contrast enhancers and are a biocompatible material. However, the study of the toxicity of these NPs mainly focusses on particles with tens to hundreds of nanometres while little is known about the toxicity of ultrasmall magnetic NPs [3]. The safe application of magnetic NPs to these various fields is therefore highly dependent on the ability to control the particle's physicochemical properties.

Two common phases of iron-oxide NPs which are magnetite (Fe_3O_4) and goethite (α-FeOOH). Whereas magnetite is commonly used as a contrast agent in MR-imaging [4], goethite (iron-hydroxide) has wide application in material science, manufacturing and environmental pollution remediation [5].

One of the easy and cheap approaches to fabricate Fe_3O_4 NPs, is coprecipitation, where surfactants are always used to control the particle size and shape. Nonetheless, to obtain single-phase, monodisperse, lowly-aggregated NPs with a specific morphology remains a challenge.

Since it is known that ultrasmall Fe_3O_4 (<10 nm) NPs display a high toxicity *in vivo* due to the distinctive capability in inducing the generation of hydroxyls in multiple organs [3], and that this toxicity is related to both the iron element and size of the NP, the need of comprehensive evaluation of their physicochemical properties under different conditions of size, shape, phase and coating, cannot be over emphasised.

Thus, in this investigation we report on how computational modelling and complementary experimental work, can lead to the design and synthesis of safer nanomaterials. We show how computational modelling and simulations can lead to a fundamental understanding of how to control the particle size and shape and the phase that ultimately control the NP's physicochemical properties and consequently its cytotoxicity.

2. Computational modelling and simulations.

For this work, a combination of molecular dynamics (MD) and Monte-Carlo-based simulated annealing adsorption was performed on small and ultrasmall magnetite (Fe_3O_4) NPs and various surfactants. This was done for sizes ranging from 1.0 to 7.0 nm. Shapes were also varied from spherical to cuboidal to observe the changes in binding

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energy (BE) and to qualitatively determine the change in pH of a solution. Furthermore, density functional theory (DFT) was used to analyse the different surfactants and draw conclusions on their reactivity with these NPs. The resulting simulated predictions were then used to synthesize (experimentally) the various NPs and to investigate their physicochemical properties.

3. Experimental setup

Co-precipitation and thermal decomposition were used to synthesize Fe_3O_4 NPs according to the predictions and schemas gained from the computational modelling and simulations. These NPs were further characterized with high-resolution transmission electron microscopy (HR-TEM), powder x-ray diffraction (PXRD), Fourier transform infrared spectroscopy (FTIR) and vibrating sample magnetometer (VSM).

4. Results and discussion

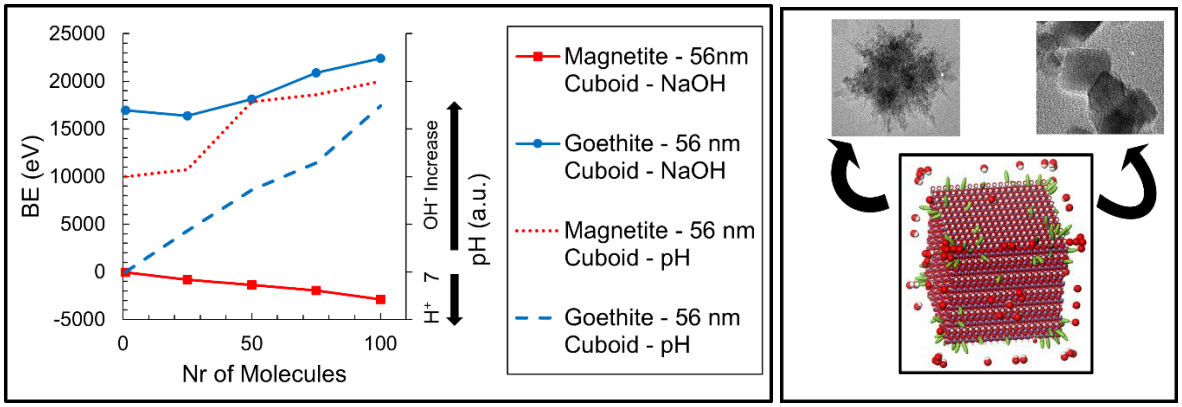

Figure 21: (Left) Calculated Binding Energy (BE) for magnetite and goethite NPs after simulated structures (bottom right) were obtained. Experimental HRTEM images (top right) were obtained to validate the simulated results.

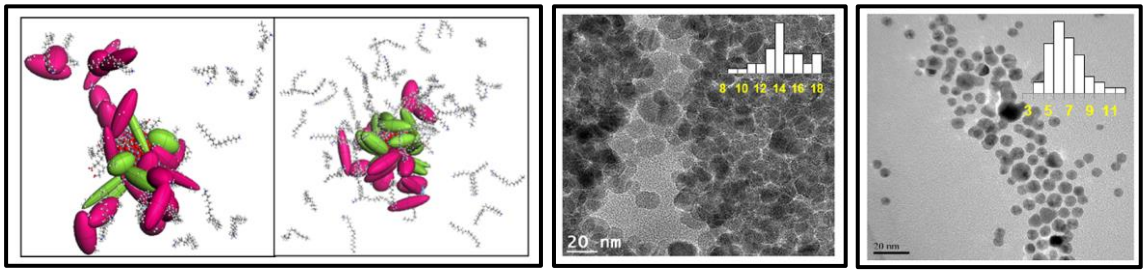

Figure 2: (Left) Simulated geometries of Fe_3O_4 NPs with different ratios of OA and OLA adsorbed leading to NPs with different hydrodynamic sizes. Insights gained from these computational simulations allowed us to synthesise these small NPs with a mixture of cuboidal and spherical shapes that were highly agglomerated (figure 2 middle) *versus* the ultrasmall spherically shaped NPs with a very low polydispersity index (figure 2, right).

Figure 1 shows the calculated BE for the simulated magnetite and goethite NPs after the adsorption of different amounts of surfactants. This was done to gain a qualitative understanding of the role that a change in the pH may play in the stability of these various nanostructures. This allowed us to fine-tune the pH during a real-world experiment (figure 1, right) wherein we successfully synthesised both magnetite and

goethite by only varying the pH and observing the exact point where the phase changed occurred.

Furthermore, we simulated the optimized geometries and calculated the resulting BEs of spherical and cuboidal magnetite NPs with different surfactants (oleic acid (OA), oleylamine (OLA), NaOH, NH_4OH) and observed the effect that the change in size and shape has on the BE (figure 2, left). This descriptor was used a predictor of the stability of these NPs and, consequently, we used these simulation results to successfully synthesize ultrasmall NPs with controlled size, shape and polydispersity index (figure 2, middle and right).

The correlation between NP stability and the number of dispersion medium acid–base complex pairs and free proton concentration was investigated and it was concluded that (as advocated) combinations of OA and OLA play an important role when synthesizing magnetic iron oxide NPs. OLA molecules act as proton acceptors and help to regulate the electrostatic pressure, responsible for OA desorption, caused by an excess of free protons. Too much OLA may also lead to the desorption of the stabilizing OA molecule from the NP surface to form acid-base complex pairs; therefore, an ideal ratio of OA/OLA is to be used that allows for a perfect fit between the NP surface charge, free proton concentration in the dispersion medium, and zeta potential. The fluctuating dynamic kinetic conditions allow for the engineering of specific shapes and sizes of magnetic nanoparticles.

5. Conclusions

MD simulations have revealed that the binding energy of OA to the NP is maximized at an acid/amine ratio of 3. As a result, a better control of the reaction and growth of the NP was obtained, theoretically. We then successfully (in a real-world experiment) demonstrated that at an optimized OA/OLA ratio of 3, the NPs show the lowest monodispersity without a need for any post synthesis size-selective precipitation.

Furthermore, MD were used to predict the more favourable phase when NaOH is used to control the pH, to grow magnetite and goethite NPs. The role of pH was investigated qualitatively by noting the ratio of desorbed/excess hydroxyls to free protons (hydrogen ions) in the solution. BE was used as an indicator of the stability of the cuboid magnetite versus goethite systems. It was predicted that neutral to low pH values (i.e., neutral to acidic solutions) will lead to the formation of cuboid goethite NPs that are stable. Conversely, a more basic solution will lead to the formation of stable, cuboid magnetite. This was used to employ the co-precipitation method in a real-world experiment to successfully synthesize more stable and therefore safer nanomaterials through modelling and design.

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First Principles In Silico Characterisation of Advanced Materials and Bio-Nano Interface

Vladimir Lobaskin [1], Ian Rouse[1], Julia Subbotina[1], Parinaz Mosaddeghi Amini[1], Anais Colibaba[1]

1. Introduction

Advanced materials (AM) represent a new paradigm in materials science: substances with highly specific features and enhanced target properties derived from precise control over their structure and composition. A particularly relevant set of examples of these materials are nanomaterials, which may exhibit properties that significantly differ from the expected behaviour of the same bulk material due to the high surface-to-volume ratio. The large surface implies high specific reactivity and capacity for steering complex processes at the molecular level. New materials, however, come with new risks: these same desirable properties may also lead to unwanted behaviour when these novel materials come into contact with the environment or living beings. As with the benefits, these risks are high for nanomaterials, since their small size enables rapid uptake by the body through multiple pathways, e.g. inhalation, ingestion, or skin contact. Consequently, it is important to be able to predict whether a given material is toxic or biocompatible early at the stage of the material's development. Given the vast range of materials used in modern technology or considered as candidates for applications, and in light of the general need to reduce the amount of in vivo and in vitro tests performed, this suggests the use of in silico methods to predict complex functionalities of AMs from first principles.

2. Methodology

We present a systematic nanoinformatics approach to generating predictive in silico models of functionalities of AMs. It aims at quantitative description of the materials using a combination of physics-based and data-driven materials modelling methods, focusing on their interfacial properties in complex media. Our multiscale method includes:

- evaluation of detailed properties of the nanomaterial interface with water and parameterization of the atomistic force field for the material using electronic structure methods [1]
- calculation of interactions of the biomolecule building blocks (amino acids, lipid segments, DNA bases) with the surface of the material and interaction between the building blocks at the atomistic level at the specified conditions [2,3]
- parameterization of the coarse-grained (CG) force field for biomaterial building blocks and construction of the sample of arbitrary size and shape [3]
- CG modelling of interaction of entire biomolecules with the nanomaterial surface and calculation of preferred orientation and the mean adsorption energy [1]
- modelling competitive adsorption of molecules onto NPs and prediction of the biomolecular corona [4]
- generation of NP descriptors covering intrinsic and extrinsic properties [5]

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- construction of machine-learning models for the prediction of complex NM functionalities.

In the multiscale scheme, these modelling techniques are coupled to each other thus forming a robust characterization pipeline. The overall concept of the nanoinformatics approach is sketched in Fig. 1.

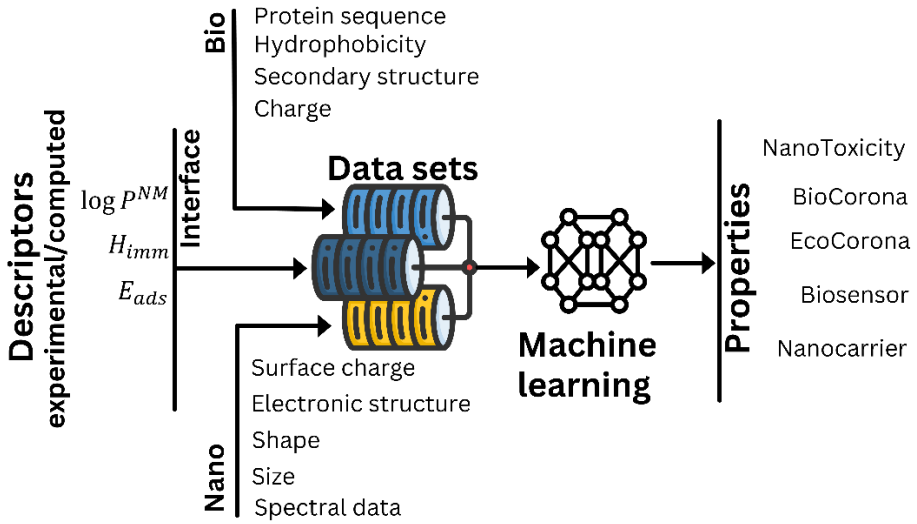

Figure 22: A concept of the nanoinformatics approach combining physics-based and data-driven methods for predicting complex functionalities of AMs [3].

3. Results

We have used the developed theoretical schemes [1-4] to make an open-source software pipeline [6] for in silico AM design and characterisation. In particular, we produced advanced descriptors of multiple common uniform and composite nanomaterials including metals, metal oxides, minerals, carbonaceous materials (carbon nanotubes, graphene, carbon black), polymeric materials and composites. This list features both intrinsic descriptors (ionization potentials, bandgaps, dispersion energy, polarizabilities, dispersion energies) and extrinsic descriptors (immersion enthalpies in water and octanol, adsorption energies for biomolecules, etc.). In this presentation, we demonstrate the outcomes of the advanced in silico characterisation and the predictive power of the nanoinformatics approach using in vitro and in vivo activities of the AMs such as respiratory toxicity or drug delivery.

4. Conclusions

Nanoinformatics approach presents enormous benefits for the modern technology as it allows to screen novel materials for the specific functionality, while saving time and money and avoiding animal experimentation. Although we tested it only in the biomedical field, our methodology is sufficiently flexible to allow for an extension into other applications of AMs and development of safe-and-sustainable-by-design methods at a fraction of wet-lab costs and brute force materials modelling effort. All the code is available for download from [6] together with a library of required input which covers a

wide range of nanomaterials and biomolecules of interest, and further NP materials or adsorbates can be straightforwardly added by the user as required.

5. Acknowledgements

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Advancing Materials Development through Multiscale Modelling and Data-Driven approaches in the Safe and Sustainable by Design Framework

Andrea Lorenzoni[1], Francesco Mercuri[1], Ivana Burzic[2], Christoph Jocham[2]

In recent years, the design and development of materials with enhanced properties and reduced environmental impact have become paramount in various industries. Achieving these objectives requires a holistic approach that integrates advanced computational modelling techniques with Safe and Sustainable by Design (SSbD) principles. SSbD emphasizes the proactive identification and mitigation of potential risks associated with materials and products throughout their lifecycle, promoting safety, sustainability, and environmental stewardship.

In this context, multiscale modelling, with its combination of atomistic, mesoscale, and continuum methodologies, plays a pivotal role in elucidating materials safety and sustainability. High-Performance Computing (HPC) infrastructures empower researchers to efficiently perform computationally intensive simulations, analysing complex systems with unprecedented accuracy. This allows for rapid exploration of materials design space, accelerating the discovery of novel materials with tailored properties and performance. Automation of computational tools and workflows, including the integration of artificial intelligence (AI) methods, further enhances efficiency, enabling intelligent decision-making and optimization of design strategies.

In this work, we present the application of this approach in the context of the Horizon Europe project BIO-SUSHY. Our objective is to apply atomistic and coarse-grain molecular dynamics simulations to comprehensively understand toxicity mechanisms in advanced materials. Specifically, we have conducted simulations to explore leaching mechanisms in cellulose surfaces coated with the thermoplastic polymers poly(butylene succinate) (PBS) and poly-β-hydroxybutyrate-co-β-hydroxyvalerate (PHBV). We aim to compare these simulation results with experimental data to provide valuable insights into coating materials for realistic processes. Additionally, we highlight the importance of data integration and automation, combining experimental data, computational results, and predictive AI models to create a unified framework for materials analysis. This research aims to provide insights into coating materials for realistic processes, addressing key challenges for enhanced safety and sustainability.

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European Health and Digital Executive Agency (HaDEA). Neither the European Union nor the granting authority can be held responsible for them.

Poster Presentations: Session 4

Efficient Workflow Automation for Materials Modeling: Towards Predictive AI Systems using Synthetic High Throughput Dataset Generation

Mario Vozza[1,2], Tommaso Forni[1,2], Fabio Le Piane[1,3] and Francesco Mercuri[1]

In the field of materials science, there has been a significant increase in the need for streamlined computational techniques aimed at generating predictive datasets tailored for artificial intelligence (AI) applications. Density Functional Tight Binding (DFTB) simulations serve as a powerful tool for elucidating atomic-scale interactions and material properties. However, the manual preparation of DFTB simulations can be time-consuming, hindering the rapid generation of large-scale datasets necessary for training AI models.

This study presents a comprehensive approach to automating the generation and analysis of materials science datasets, specifically focusing on defected graphene structures. This workflow efficiently handles computations for various material properties, including energy and charge transport. By automating these procedures, we can efficiently generate extensive datasets wherein each structure is correlated with its corresponding properties. This tight coupling between structures and properties provides a robust foundation for training predictive models. Additionally, beyond the output properties from DFTB, we have augmented the dataset with synthetic Scanning Tunnelling Microscopy (STM) images generated using the Local Density of States (LDOS). This expansion opens ways for correlating experimental measurements directly with the examined structure in future analyses, enhancing the dataset extension.

With the dataset we created, we employed object detection techniques to identify defects within the graphene flakes. Subsequently, we extracted these defects from the structure's image and utilised classical computer vision techniques to derive features from these defects. The aim was to predict material properties based on the defect geometry using eXtreme Gradient Boosting (XGBoost). Moreover, having access to STM images allows us to correlate images and material properties using convolutional neural networks (CNNs). A pivotal element of this study was the robust integration of data, whereby all outputs from the simulations, including the generated STM images, were stored within a NoSQL database like MongoDB. This integrated approach enhances data management capabilities, allowing for easier scalability and ensuring the consistency and reliability of the dataset. By centralising the storage of simulation outputs and images, researchers could seamlessly access and analyse the data, fostering collaboration and accelerating scientific discoveries in materials science.

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A Combination of Computational Modelling, Simulation and Experimental Work: Titanium dioxide nanoparticle toxicity with different shapes and sizes evaluated based on solution pH

Witbooi S.G[1], Cronjé S.[1] Gulumian M.[2], Wepener V.[2], Harris R.A.[1]

1. Introduction

Nanomaterials (NMs) are at the forefront of modern materials science [1]. The analysis of NMs involves considering the physicochemical properties of the NMs because their biological impact relies on these properties. Size and shape are two of these properties that should be considered [2]. The theory of nanoscience can be translated to practical applications by manipulating these materials on the nanoscale [3]. Titanium dioxide (TiO_2) is regarded as one of the most significant nanoparticles (NPs) due to its abundance in nature and numerous applications such as sunscreens, in drug delivery systems and in food enhancement [4]. The toxicity of TiO_2 as it pertains to its various properties across its various applications has thus become of great interest. In this work, we first investigate the toxicity of TiO_2 NPs qualitatively and *in-silico*. This is done by considering the effect that different simulated shapes and sizes have on the production and/or release of free radicals when they are placed in an acidic, basic and neutral substances. Reactive Oxygen Species (ROS) are highly reactive molecules containing oxygen that can cause damage to cells and tissues in the body. Furthermore, we investigate this, for ultrasmall NPs, since it has been established that these show a high level of toxicity in vivo, however very little is known about their biosafety [5]. We then proceed to verify our qualitative simulation results with experimentally obtained data.

2. Procedure

Nanorods (NRs), nanocubes (NCs) and nanospheres (NSs) were constructed *in silico* and three different sizes between 1.0 nm – 6.9 nm were chosen. Water molecules were constructed. Varying numbers of water molecules were adsorbed onto the different sized and shaped NPs to determine the number of free ions. The number of free ions observed served as an indication of the toxicity of these NPs in water. This was repeated for water molecules with an excess of hydrogen ions (H^+) which simulated the substance with an acidic pH level. This was repeated again for water molecules with additional hydroxide ions (OH^-) to simulate a substance with a basic pH level. These models were then verified by obtaining experimental data where these NPs were synthesised, and their pH correlated to the free-ion concentration in the solution.

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3. Results

A representative example of the simulated spherical TiO_2 NP is shown in figure 1 with the water molecules adsorbed. It can be seen that for the 1.1 nm particle (Fig. 1 (left)) most of the H_2O interact with the NP. The same is true for the 2.0 nm NP where most of the OH-ions interact with the NP (Fig. 1(middle)), but by changing the NP size just slightly (from 2.0 to 2.6 nm) the interaction of OH-ions seizes (Fig. 1(right)).

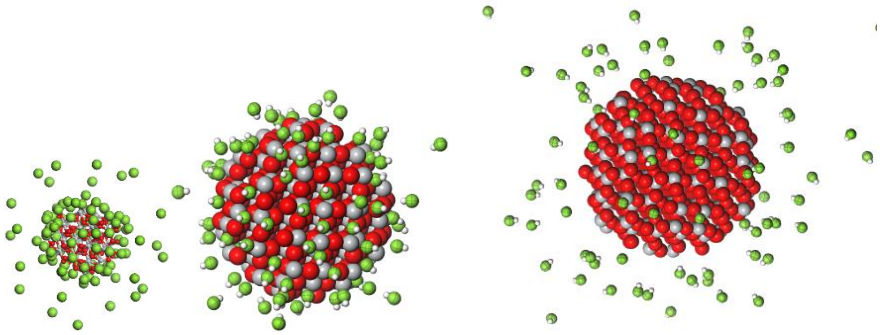

Figure 1: Simulated ultrasmall, spherical anatase TiO_2 NPs with (left) 100 H_20 molecules adsorbed on 1.1 nm NP, (middle) 100 OH-ions adsorbed on 2.0 nm NP and (right) 100 OH-ions adsorbed on 2.6 nm NP.

The corresponding binding energies for the particles with their ligands from figure 1 are shown in table 1. From this we can see that the 2.0 nm particles have the highest binding energy. This implies that this system would be much more stable compared to the slightly larger 2.6 nm system where no bonds between the OH-ions and TiO_2 NP are observed. The consequence of this on the release of Ti-ions will be further explained in this work. Many studies have led to a general agreement about TiO_2 NPs toxicity, in particular for anatase form, but no mechanistic details have been provided yet. In this study, among other things, we evaluate (qualitatively) the role of titanium (Ti) ions released by TiO_2 NPs in different pH conditions.

Table 1: The simulated particle sizes with their corresponding ligand and binding energies.

Size of NP (nm)	Ligand	Total System Energy (eV)	Nanoparticle Energy (eV)	Ligand Energy (eV)	Binding Energy (eV)
1,1	H_2O	-144,88	-59,97	7,25	-92,16
2,0	OH^-	-2442,93	713,14	1240,62	-4396,69
2,6	OH^-	-1194,24	-1194,24	0,00	0,00

Figure 2 shows the number of Ti-ions released, that were found over a 96-hr time period adapted from Matteis *et. al*, [5].

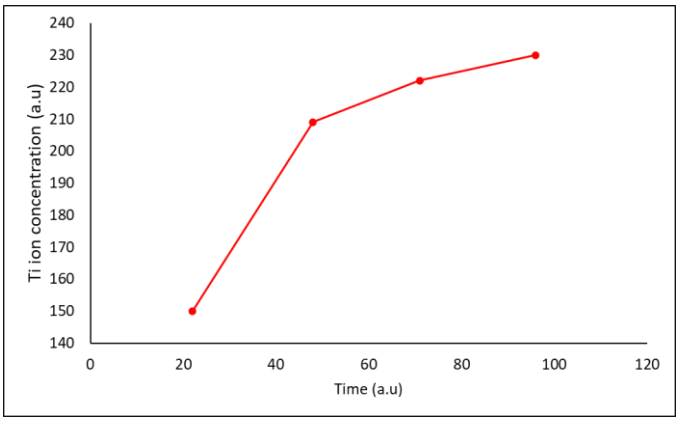

Figure 2: Effects of time and pH on titanium ions released by TiO_2 anatase NPs at a pH of 4.5 [5].

Figure 2 confirms that the TiO_2 anatase NPs are more reactive in an acidic environment and undergoes degradation which indicates a greater toxicity. Furthermore, a greater ion release is observed which results in greater ROS production which is also a descriptor of toxicity.

We observed (from our computational work) that no free Ti-ions were observed for the NP in water. Experimental work confirmed that no free Ti-ions were observed. Furthermore, experimental work by Matteis *et. al*, [5] confirmed this observation for water and reported that they could not detect any Ti-ions that were released into the solution which suggested that the NP degradation did not occur. More free radicals caused by the Ti-ions released were quantitatively observed (both *in silico* and experimentally) for a solution with low pH values. Thus, qualitatively, oxidative stress is higher for low pH values and the NPs may therefore be more toxic.

4. Conclusion

In conclusion, this work aimed to combine computational modelling and simulations with physical experimentation. Firstly, the results obtained from the simulation modelling suggested water (as a neutral substance) played no role in destabilizing specific sizes (i.e. 1.1 nm) of TiO_2 (anatase) NP and therefore no oxidative free radicals were observed. The simulations were experimentally verified.

Furthermore, more free radicals were observed *in-silico* for solutions with low pH values. It was established that the more acidic environment leads to major ionization and consequent free radical release. The effect that the NP size and shape has on this ionization was qualitatively determined *via* computational modelling and simulation and then confirmed experimentally by observing the change in pH and other physio-chemical characteristics of the synthesized NPs.

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Computational assessment of the environmental transport and fate of small molecules and PFAS using the SimpleBox4Planet web-application

Dimitra-Danai Varsou[1], Nikolaos Cheimarios[2], Dimitris G. Mintis[2], Andreas Tsoumanis[2], Antreas Afantitis[2]

1. Introduction

Per- and polyfluoroalkyl substances (PFAS) are present in a wide variety of industrial processes and consumer products. Nonetheless, they are increasingly being identified as environmental pollutants, and some have been associated with adverse effects on human health. Their structure includes carbon-fluorine bonds, which are among the strongest chemical bonds; thus, they are resistant to degradation both during use and upon release to the environment ("forever chemicals"). In fact, PFAS are regularly found to contaminate groundwater, surface water, and soil[1–3]. In this scope, the PROPLANET project supports the development of safe and sustainable by design (SSbD) coatings that will substitute the PFAS-type coatings used in the textile, food packaging and glass industrial sectors[4]. To support the SSbD principles, the PFAS alternative substances are explored *in silico* to assess their environmental transport and fate. A customized SimpleBox[5] model, incorporating the specific properties of the PROPLANET candidate PFAS alternative substances, is used to simulate their concentration in air, water, sediment, and soil. The produced results can be later supporting the assessment of potential risks throughout the coatings' lifecycle. To ensure the use of the SimpleBox model from the wider community (including industry and regulators) the Excel version of the model is incorporated into the SimpleBox4Planet tool where all the necessary input parameters are streamlined in a user-friendly interface. The SimpleBox4Planet tool is also available through Application Programming Interfaces (APIs) for integration with the PROPLANET Replication tool enabling simulation of coating behaviour under various conditions and supporting SSbD.

2. Development of the SimpleBox4Planet tool

The SimpleBox[6] is a nested multimedia mass balance model that simulates the transport of chemical substances between different homogeneous environmental compartments (e.g., air, water, soil, etc.) in different landscape settings, developed as an MS Excel® spreadsheet. The SimpleBox4Planet tool provides a user-friendly environment (Figure 1, https://www.enaloscloud.novamechanics.com/proplanet/simplebox4planet/) without compromising the capabilities of the original SimpleBox Excel-based version. Furthermore, the SimpleBox4Planet is available through APIs (https://www.enaloscloud.novamechanics.com/proplanet/swagger-ui/) so that it can be easily integrated into the PROPLANET Replication tool. The user can select the substance of interest from the available list of PFAS alternatives and one of the available

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exposure scenarios and calculate the environmental fate of the substances (mass flows between air, water, sediment, and soil) on regional, continental, and global spatial scales.

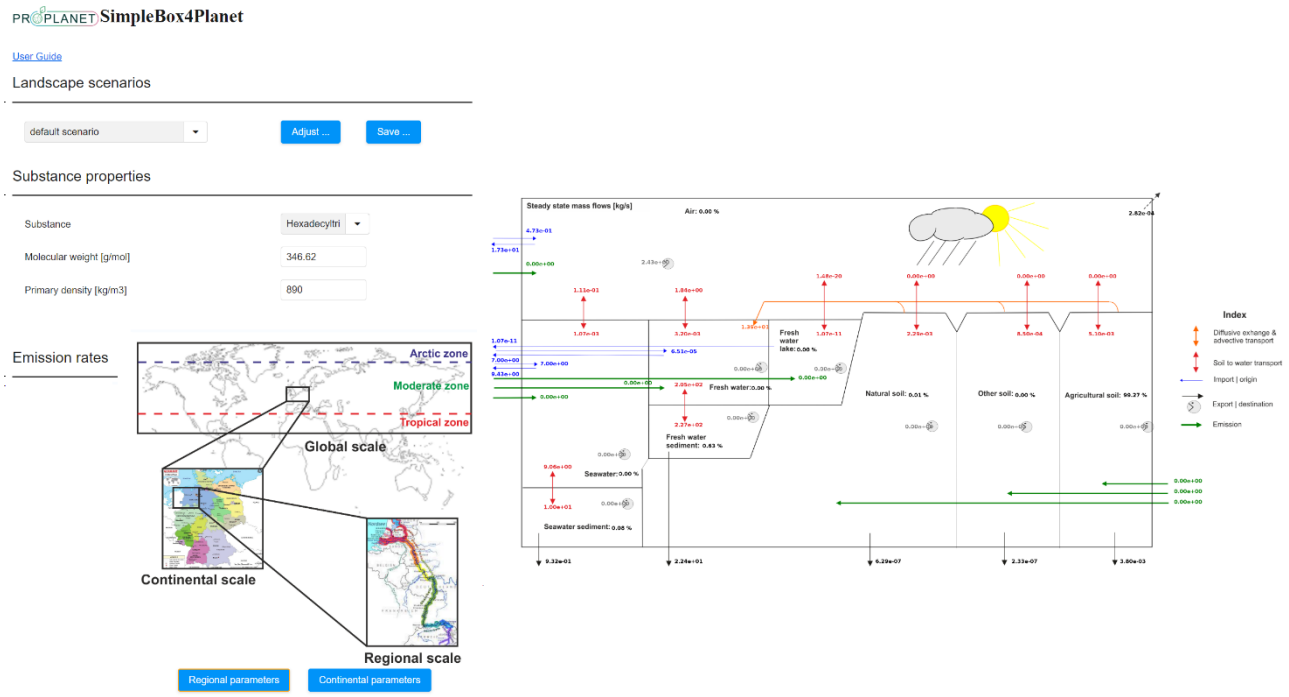

Figure 23: Screenshot of the SimpleBox4Planet tool input and output.

The candidate PFAS alternatives assessed under the PROPLANET project and incorporated into the SimpleBox4Planet tool are:

- Acetic acid,
- Hexadecyltrimethoxysilane,
- Octyltrimethoxysilane,
- Hexamethyldisiloxane,
- Methyltrimethoxysilane,
- Trimethoxyphenylsilane,
- 2-Octenylsuccinic anhydride,
- Dodecyltriethoxysilane,
- Polysiloxanes, di-Me, hydroxy-terminated,
- Polysiloxanes, di-Me (Silicon oil),
- Starch (Corn starch),
- Zinc oxide (ZnO),
- Sodium alginate,
- Chitosan,
- Glycerol,
- 2-Oxetanone, 3-C12-16-alkyl-4-C13-17-alkylidene derivs. (AKD).

The SimpleBox4Planet tool includes an updated database with the properties of the candidate PFAS alternative compounds collected through an extensive database search in PubChem database (https://pubchem.ncbi.nlm.nih.gov/), CAS registry (https://commonchemistry.cas.org/), the ECHA Chem (https://chem.echa.europa.eu/) registration dossiers and the substances safety data sheets. To fill the potential data-gaps, properties were estimated using in-house Quantitative Structure-Property Relationship (QSPR) models for the prediction of the substances' water solubility, vapour

pressure and octanol/water partition coefficient. To use these models, the substance's structure is only needed as input (e.g., in SMILES or SDF format), and the necessary molecular descriptors are automatically calculated using the Mold2[7] software. For comparison purposes three PFAS substances are also included in the SimpleBox4Planet tool; the Perfluorobutanoic acid (PFBA), the Perfluoropentanoic acid (PFPeA), and the Perfluorobutane sulfonic acid (PFBS). Their relevant properties were extracted from the Interstate Technology and Regulatory Council (ITRC) online documents (https://pfas-1.itrcweb.org/).

3. Conclusions

The ability to predict the exposure of chemicals including PFAS in the environment is crucial in assessing their potential risks. However, conducting exposure assessments for chemicals can be expensive and time-consuming, especially when dealing with large numbers of substances. Screening level environmental exposure models such as the SimpleBox model, provide a cost-effective and efficient solution to this problem, as they are designed to provide conservative estimates of exposure without the need for complex data requirements, making them a valuable tool in regulatory environmental risk assessment. However, the stakeholders, including industry professionals, regulators, and consultants, are not typically experts in modelling or software development. Therefore, it is essential that these screening level exposure models have intuitive and user-friendly interfaces. To address this issue, the SimpleBox4Planet web-tool based on the SimpleBox Excel version was developed. It is also available through APIs, making it accessible to anyone interested in using it directly or integrating its functionality into their own software. The development of user-friendly screening level exposure models is a critical step in facilitating the responsible use and regulation of PFAS and other chemicals, helping to ensure their safety and minimize their potential risks to the environment and human health.

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The study of amorphous materials with AI-based multiscale approaches

Stephan Roche[1,2]

1. Introduction

Amorphous materials such as boron nitride (aBN) and amorphous graphene (aG) are becoming prominent materials for many different applications due to their good properties such as thermal stability, mechanical properties, insulating behavior, and ultralow dielectric constant in aBN (<2). Moreover, amorphous films are more suitable to large area deposition compared to clean hBN or graphene since it can be grown at low temperatures (about 400 °C) and on various substrates [1-3]. However, their properties depend on the nature and degree of disorder, which needs a well-defined metrics for benchmarking materials. Having such metrics in place will allow to tune the properties and performance of these films during the fabrication for desired applications. In this context, revealing the relationship between fabrication strategies and the material properties of the film is also crucial.

Capturing the key features of the amorphous nature of materials requires theoretical characterization to understand how material properties change with the microstructure. Since simulations of amorphous materials need large structural models, density functional theory (DFT) is not a suitable tool despite the high accuracy it offers. On the other hand, molecular dynamics (MD) simulations with empirical interatomic potentials require much less computational cost; however, they are not accurate enough to correctly describe the local environment of amorphous materials. Machine learning-driven interatomic potentials (ML-IP) can describe the local environment with a similar accuracy to DFT and at a much lower cost [4,5]. Here, we introduce Gaussian approximation potentials (GAP) for atomistic simulations of aBN incorporating different contaminators and doping materials, which are trained on a large dataset of atomic structures generated by DFT calculations [6-8]. We will present a systematic analysis to screen out possible realistic morphologies as a function of growth parameters, such as temperature, quenching rate, and the presence of a dopant, and their corresponding material properties using GAP-driven MD simulations. The extensive simulations of a large quantity of possible structures presented in this work will guide experimental research and provide trends of scaling behavior as a function of experimentally controllable parameters. The impact of amorphousness on dielectric properties will be also discussed for aBN and aG [9,10].

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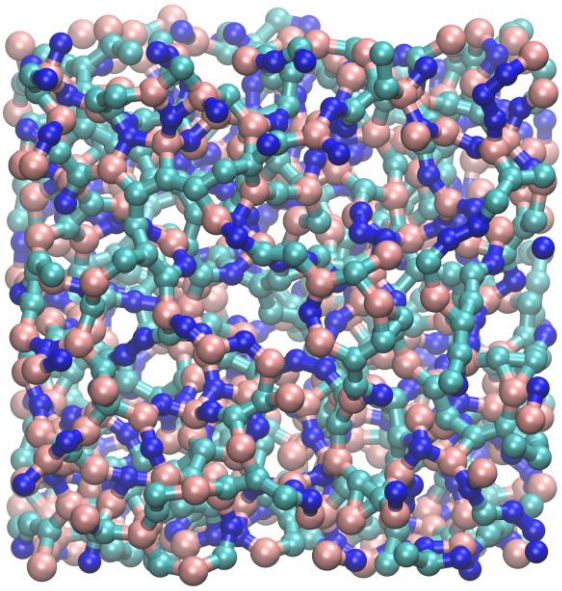

Figure 24: Typical amorphous structure of aBN:C compounds, namely an amorphous BN structure with a certain density of carbon atoms, affecting the overall system properties (thermal stability, mechanical and dielectric properties, etc)

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GrapheNet: A Novel Deep Learning Model for Predicting Physical and Electronic Properties of 2D Materials Using Images

Tommaso Forni[1,2], Matteo Baldoni[1], Fabio Le Piane[3] and Francesco Mercuri[1]

The quest to represent complex advanced materials and nanostructures has been a persistent challenge in the field of chemistry and materials science. Traditional methods of representing small molecules, such as SMILES, have proven to be insufficient to represent more complex systems. In recent years, the use of 2D images to represent the structure of materials has gained popularity, especially with the development of artificial intelligence (AI) tools and deep learning algorithms [1].

In this study, we present a novel approach to represent the structure of 2D based materials, such as graphene [2] and graphene oxide nanosystems [3], and an advanced predictive AI-based framework. Our proposed deep learning model, GrapheNet, is based on an Inception-ResNet architecture consisting of multiple blocks of convolutional layers with different kernel sizes. The GrapheNet model can be trained to make predictions about the physical and electronic properties of graphene-based systems using PNG images as structural representations. The efficacy of the approach was tested on datasets of graphene oxide and defected graphene systems, built starting from repositories of computed structure/property data. Structural data of the nanosystems in the dataset, encoded in standard structural formats, are transformed into threedimensional (graphene oxide) or two-dimensional (defected graphene) tensors, converted into RGB (graphene oxide) or grayscale (defected graphene) PNG images and pre-processed (cropping, resizing, recentering, padding). Upon training, the GrapheNet framework yielded very accurate results in predicting phyisico-chemical properties of graphene oxide and graphene nanostructures, with low mean prediction errors for all target properties considered, also exhibiting a significant computational efficiency. Being based on highly-efficient frameworks borrowed from state-of-art computer vision technologies, the approach proposed demonstrates the potential of using image-like representations of 2D and low-dimensional nanostructures in connection with deep learning predictive models, predicting the chemico-physical properties of nanographenes with great accuracy and outperforming the computational efficiency of current methods.

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Size-dependent study of water adsorbed iron oxide nanoparticles: a computational and experimental study

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1. Introduction

The significant growth in nanotechnology has resulted in the formation of various nanoparticle (NPs) types. These NPs have diverse applications, making them attractive for use in drug delivery, cosmetics, medicine, electronics, and as contrast agents for magnetic resonance imaging (MRI), among other fields. Iron oxide magnetic NPs may be used as MRI contrast agents and as vehicles for targeted drug delivery, angiogenic therapy, and chemotherapy [1]. Their small size allows them to actively travel intravascularly or intracavity for drug delivery [2].

Despite their advantages, the toxicity of iron oxide NPs (IONs) remains largely unexplored, especially for ultra-small IONs. Several studies have indicated that the potential toxicity, including cytotoxicity and genotoxicity, caused by IONs are due to the generation of reactive oxygen species (ROS) [3]. Therefore, it is essential to investigate their toxicity, especially considering that different types of NPs exhibit size-dependent toxicity. In recent studies, it has been observed that ultra small NPs (i.e. <5 nm in size) specifically Fe_3O_4, is able to stimulate cells to produce ROS. However, larger NPs (>5 nm) do not exhibit a significant induction of ROS. Therefore, the generation of ROS appears to be influenced by the size of the NPs. The toxicity of ultrasmall Fe_3O_4 NPs is thought to be related to ferroptosis, a form of programmed cell death characterized by the excessive accumulation of iron and the buildup of lipid peroxides [4].

Furthermore, under certain specific conditions, these IONs can release iron ions (Fe^{2+} or Fe^{3+}) into the environment with which it interacts. These ions can react with water to form hydroxide ions (OH^-) and protons (H^+), affecting the pH. Thus, we hypothesise that there might be a correlation between the pH of a solution containing IONs, and the resulting toxicity. It is necessary to investigate and provide a detailed explanation of IONs toxicity and potential risks to human health [5]. The toxicity of NPs is attributed to their specific physico-chemical properties, including their high surface-to-volume ratio, chemical composition, size, dosage, retention in the body, shape, organ-specific toxicity, breakdown, and elimination from the body [6].

In this study iron oxide (Fe_3O_4) NPs of different sizes and shapes were modelled and simulated (different ultrasmall sizes (1.2 nm, 2.6 nm and 5.6 nm)) where 100 H_2O molecules were absorbed. We qualitatively determined the change in pH of the solution

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and how this affected the release of Fe-ions (which could lead to the generation of ROS). The corresponding binding energies were then calculated and used as a descriptor of these NPs stability.

2. Atomistic computational modelling and simulation and experimental setup.

Spherical, cuboidal, and rod-like shapes of IONs (Fe_3O_4) ranging from 1.0 nm to 6.5 nm in diameter were simulated *in-silico*. These shapes represent the most common geometries found for these kinds of NPs in experimental literature. The NPs were simulated in an aqueous environment, where different concentrations of water molecules were allowed to interact with the IONs in a simulated absorbance scheme.

This setup allowed for the investigation of how the different shapes and sizes of IONs interact with water molecules and may influence the generation of free radicals – particularly Fe^{3+} and Fe^{2+} ions. The generation of free radicals is a crucial aspect to consider, as it can lead to oxidative stress and potentially harmful effects in biological systems. Additionally, the interaction of IONs with water molecules can lead to changes in pH. By comparing the effects of various shapes and sizes of IONs on the generation of free radicals and pH changes in an *in-silico* environment, we attempted to qualitatively described the toxicity of these NPs.

3. Experimental setup

Co-precipitation was used to synthesize these NPs and the resulting pH was measured for different sizes. The qualitative results were compared with the simulation results. Further characterization of the physicochemical properties was performed, in particular PXRD and FTIR.

4. Results

Figure 1 illustrates a spherical model of Fe_3O_4 with different sizes which shows the water molecules attached to the NP.

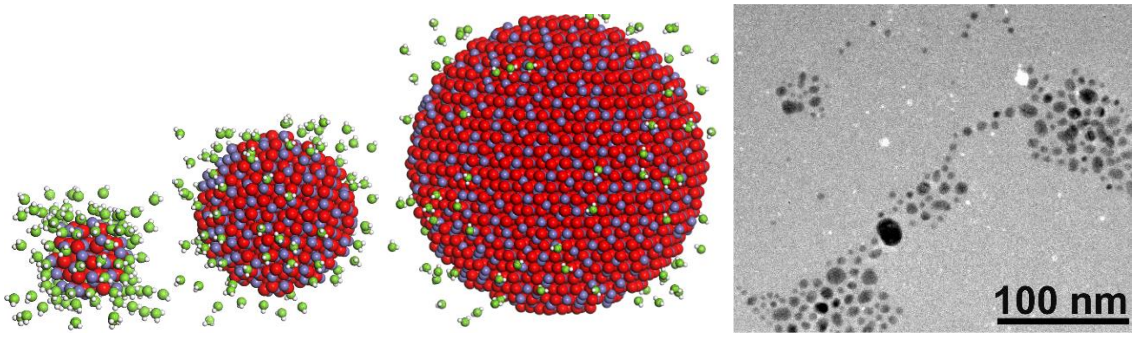

Figure 1: Simulated ultrasmall, spherical and bare magnetite (Fe_3O_4) NP with the adsorbed H_2O molecules. From left to right the sizes are 1.2, 2.6 and 5.2 nm respectively. The image on the right shows a representative TEM image of the experimentally prepared NPs.

NP Size (nm)	Total System Energy (eV)	Nanoparticle Energy (eV)	Ligand Energy (eV)	Binding Energy (eV)
1.2	267,89	700,74	58,66	-491,52
2.6	-2918,90	-2812,85	11,09	-117,15
5.2	-32392,80	-32390,26	0,08	-2,62

Table 1: The different simulated particle sizes 1.2nm, 2.6nm, 5.2nm with the corresponding total system energies, NP energy and ligand energy with the calculated binding energy.

Figure 1 shows the simulated magnetite NPs and the adsorbed H2O molecules. By using the insights gained from the simulation study, the same NPs could be synthesized experimentally (Figure 1, right).

In Table 1 it is observed that as the NP size increases the binding energy decreases. Thus, more H_2O molecules interact with smaller sized NPs than the larger sized ones. This interaction may lead to the desorption of Fe-ions which in turn could result in the generation of ROS. Furthermore, this could lead to the generation of hydroxyls. Wu *et al.* [6] observed that, after intravenous injection, a significantly elevated OH level in the heart, serum, and multiple organs was detected. Among these organs, the heart showed the highest OH level due to the high distribution of ultrasmall Fe_3O_4 NPs, leading to the acute cardiac failure and death. Therefore, in our study, the correlation between the generation of OH groups, H-ions and pH was qualitatively studied to aid in our mechanistic study of the NP toxicity.

5. Conclusions

Through computational modelling we could observe that ultrasmall Fe_3O_4 NPs showed high toxicity. This was done by qualitatively determining the correlation between pH and the release of Fe-ions, OH-ions and H-ions. Now since we know that the toxicity was related to both the iron element and size [6] these findings may provide a novel insight into the toxicology of ultrasmall Fe_3O_4 NPs, and highlight the need of comprehensive evaluation which could be done with Molecular Dynamics, i.e. computational modelling and simulations.

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ProtoNANO: assessing the toxicity of inorganic nanomaterials using nano-QSAR models

Salvador Moncho[1], Co-Authors: José Luis Vallés-Pardo[1], Eva Serrano-Candelas,[1] Rafael Gozalbes[1,2]

1. Introduction

Development of new chemicals and materials focuses in enhancing a few properties of interest, such as potential therapeutical effects (pharmaceuticals) or tribological properties (lubricants). However, it is essential to assess the risks that those materials pose for the safety of humans and the environment. Computational assessment is a very convenient way to consider the safety of substances with reduced economical, ecological and ethical impact. Among those methods, the most outstanding are mathematical models to relate the structure of chemicals with a biological/physicochemical property or activity: the QSAR models (from Quantitative Structure-Activity Relationships). QSARs for discrete organic molecules are widely used and are accepted for regulatory purposes. In recent years, QSAR models on nanomaterials (NMs), from herein labelled as nano-QSARs, are being developed and improved [1].

2. Nano-QSAR

Usually, QSAR models describes substances by their chemical structure, often represented by the SMILES code. However; this approach is insufficient for NMs, because a key component of their definition is their size. Furthermore, often they are characterised by complex compositions which affect their physicochemical and biological behaviour. In addition to develop specific calculated descriptors for NMs, experimental properties and/or conditions are being used as descriptors, due to their ability to capture insights on the real structure. We recently reviewed the range of numerical descriptors used in the literature for NMs [2], and proposed a classification for descriptors considering if they are direct descriptions of the structure (composition of the core/surface and geometry of the particles) or indirect experimental parameters (related to the NM properties, its synthesis or the endpoint measurement). However, the use of experimental data creates another challenge for the nano-QSAR models, the lack of consistence among the methods and parameters used to characterize and evaluate NM in the literature that hinder the creation of modelling databases.

ProtoNANO [3], which is one of the modules in the *in silico* prediction server ProtoPRED®, facilitates the use of a series of nano-QSAR models developed for different inorganic NMs, such as noble metals, metallic oxides and quantum dots (QDs). The

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models concern toxicity (to humans through *in vivo* or *in vitro* models, such as *E. coli* or *cell-lines*), ecotoxicity (adverse effect on plants and animals) and physico-chemical properties. The later includes those with a key role in risk assessment (related with physical hazards or with exposure and environmental fate, such as partition coefficient) but also properties used to characterize and group materials, such as the Zeta potential.

3. Case study: Cytotoxicity of QDs

From the different models existing in ProtoNANO, this presentation will use the cytotoxicity of QDs to exemplify the particularities of applying this technique to nanomaterials. In this case, we will explore the dataset compiled by Bilal et al.[4] which includes cytotoxicity data against both tumoral-based cell-lines and primary cells. QDs are a particular group of materials which are characterized by their unique optical and electronic properties caused by their semiconductor nature which makes noticeable certain quantum mechanics (QM) behaviours. For example, their discrete electronic levels lead to UV-visible emission patterns which depend on the size of the particle (Figure 1). In this case, the database describes inorganic, Cd-based QDs which composition is distributed among four different categories: core, shell, ligands and modifications. Interestingly, the database also provides information on experimental data such as the size, wavelength of emission and experimental conditions.

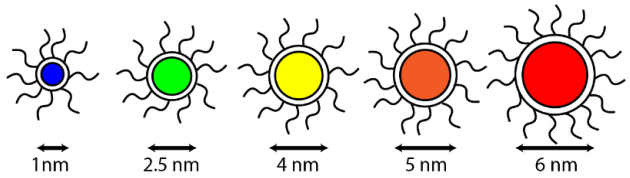

Figure 25: Graphical representation of the UV emission wavelength change with the QD size.

In this presentation, we analyse the contents of the database and present the development of a series of predictive models. The examples will serve to discuss the effect of different features, including calculated descriptors and experimental measurements. Furthermore, we explore the division of the dataset in two groups, primary cells and cell-lines. The objective is to have two different but complementary models to enrich the interpretation of the data and to explore their potential as antitumoral treatments.

4. Acknowledgements

This project has received funding from the European Union's Horizon 2020 research and innovation programme under the Marie Skłodowska-Curie grant agreement No 896848 (NanoQSAR).

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Grouping of advanced multi-component nanomaterials: can machine learning help?

Georgia Tsiliki[1], Alex Zabeo[2], Vicki Stone[3], Danail Hristozov[2]

1. Introduction

Multi-component nanomaterials (MCNMs) can be manufactured featuring many different physico-chemical properties. Unlike mono-component nanomaterials (NM), MCNMs consist of multiple components that may interact with one another, and for that reason their safety profile should be clearly characterised. Traditionally evaluating MCNMs is expensive and time-consuming. Similarity assessment methodologies specifically designed for MCNMs could be valuable tools to justify that existing safety-related information can be re-used between group members, thereby reducing the need to generate new hazard data and improve their sustainability. In the case of MCNMs, it is expected to evaluate the differences and similarities to their mono-components NMs aiming to assess their functionality and potential hazard.

We suggest a two-step grouping approach for identifying similar MCNMs, which allows researchers to quantify similarities between nanomaterials and then use this information to read-across safety information from well-studied materials to new ones. The two procedures can be used as standalone approaches for grouping and read-across. Depending on the quality and the quantity of the data available, the method can adjust to various scenarios using both scalar and dose-response data. The methodology is applied to two use cases from industry to demonstrate the method's effectiveness.

2. Methods

A sequential workflow is presented to identify groups in the data and read-across unknown hazard or toxicity endpoint values. The method first normalizes intrinsic and extrinsic properties, calculates MCNMs similarity scores for each of the properties, and finally suggest a unique grouping ranking across data sets. The output is then used for reading across toxicity endpoints. Specifically, Gaussian mixture modelling is employed to describe parameter- and MCNM-specific distributions and compare them in a probabilistic manner. The agility of the method is that it can adopt to any format or range of the raw data by breaking the input data into distinct components and then combine them to describe a data-specific mixture distribution. The method primarily calculates pairwise comparisons of interest to allow researchers to focus on specific parameters of interest and evaluate their biological relevance. To determine the mixture model, we initially consider an arbitrary set of k Gaussian distributions and calculate the mean vector and covariance matrices from all the data points. An iterative process using an Expectation-Maximisation (EM) algorithm is used to find the optimal k and corresponding distributions' parameters. Preliminary work on pairwise similarity analysis

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is used as the basis of model comparison to identify the optimal *k* groups in the data (Tsiliki et al., 2022). Additionally, a clustering topology is included in the analysis to visualize the groups of similar MCNMs formed.

We demonstrate our method's performance comparatively to hierarchical agglomeration clustering and to k Nearest Neighbours (kNN) algorithm. Applications to use case data following integrated approaches to testing and assessment (IATA) for inhalation exposure are shown (Tsiliki et al., 2024).

The workflow includes a final step for data gap filling for toxicity or hazard endpoints using the grouping results. The data gaps are filled individually using a weighted average between the neighbours' mean value and the class mean value. To help the user judgement for the acceptable uncertainty for read-across regulatory purposes, we enforced the algorithm with an uncertainty estimate.

3. Conclusions

Toxicological properties of a material are often driven by their physico-chemical properties. This principle is the basis for many existing in silico predictive models. However, for grouping advanced materials, more information should be collected and analysed for a robust similarity assessment and a grouping decision. We propose a similarity assessment method and grouping approach that can be applied to one- and two-dimensional data and identifies common groups across data sets accompanied with an uncertainty score for ease of decision making in terms of regulatory purposes. Although the suggested method is less computationally intensive compared to most Machine Learning (ML) algorithms (e.g. Support Vector Machine) and it is easy to implement, it is highly influenced by the size of the available data. When rich toxicity data or high-quality biological activity data are available, more consistent and accurate will be produced.

The workflow is demonstrated on MCNMs, however the method can be extended to any advanced materials reducing the burden of testing the safety of chemicals and therefore contributing to improving their sustainability.

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A local search approach to predict and optimize nanomaterial toxicity in early stage nanomaterial design

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1. Introduction

The rapid advancement of nanotechnology has led to the development of a wide range of engineered nanomaterials with unique properties and applications. Potential risks associated with human health and the environment remain largely unknown (Marcoulaki2021, Mancardi2023). To address this challenge, we propose a novel approach that utilizes local search techniques to predict and optimize nanomaterial toxicity during the early stages of nanomaterial design.

2. Nanomaterial Representation

Our approach leverages our recently proposed general and extendable representation for nanomaterials (Blekos2023), to greatly facilitate similarity assessments between components, which is crucial for calculating nanomaterial affinities. This representation forms the backbone of our local search methodology, which utilizes existing data on nanomaterial composition, structure, and toxicity to drive the identification and design of new nanomaterials with optimized safety profiles.

3. Local Search Approach

The local search approach is particularly well-suited for the complex and high-dimensional design space of nanomaterials. By efficiently exploring the neighborhood of known nanomaterials with desirable safety profiles, the algorithm can identify promising candidates that strike a balance between functionality and reduced toxicity. This targeted search strategy allows for the rapid discovery of safer nanomaterial designs, reducing the need for extensive experimental testing and accelerating the development process.

4. Bayesian-based Predictive Model

By integrating this local search framework with a Bayesian-based predictive model, we forecast the toxicological profiles of novel nanomaterials but also guide the iterative design process towards safer alternatives. As new data on nanomaterial toxicity becomes available, the model can be updated to refine its predictions and guide the search towards increasingly safer designs. This iterative feedback loop between the local

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search algorithm and the predictive model ensures that the approach remains robust and responsive to the latest advancements in nanotoxicology research.

5. Funding

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Molecular mechanisms and potency for ENM grouping

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1. Introduction

Engineered nanomaterials (ENMs) have unique physicochemical properties that have led to a widespread interest for diverse industrial applications. The variability of the produced ENMs pose challenges for their efficient hazard assessment. Grouping along with read-across strategies have been proposed to overcome this obstacle to allow for generalizability of hazard for existing and emerging ENMs.[1] However, present grouping approaches often lack sufficient consideration of the impact of individual studies, not encompassing a wide range of experimental conditions and materials tested. Furthermore, existing strategies have been largely centered around chemical aspects and use of apical endpoints. Toxicogenomics, on the other hand, offer a system level understanding. It has been used to characterize early molecular mechanisms of action (MOA) in the context of adverse outcome pathway (AOP) framework.[2] This framework has also been allied with benchmark dose (BMD) modelling[3] to determine dose-dependent effects elicited by ENM exposure.[4] It is known that direct effects typically exhibit a dose-dependent trend. Transcriptional derived BMD values has been linked to ENM potential of triggering a response. Here, we hypothesized that AOP-based direct molecular effects and ENM potency[5] derived from BMD modelling could be used to group ENMs.

2. Statement of contribution and methods

In this work, we applied an AOP-based strategy for ENM grouping. A collection of genome-wide expression data of ENM exposures with 51 experimental conditions, defined by the combination of GEO accession number, material tested, and exposure time was used. We focused on direct MOA triggered by ENMs represented by differentially expressed genes that respond in a dose-dependent manner. Before the grouping, we investigated the influence of time and dose of the exposure in the biological response. To achieve this, we analysed how often a molecular initiating event, or an adverse outcome is enriched within the AOPs. Additionally, we investigated enrichment frequency of different levels of biological organization, such as molecular, cellular, and tissue, are enriched key events (KE). This included examining the effects of both low and high doses. Furthermore, we examined the distribution of BMD values, all analyses being conducted over time. After determining relevant aspects to be

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considered in the grouping, hierarchical clustering was performed considering direct MOA induced by ENMs within the AOP framework and their potency based on transcriptional BMD modelling to group ENMs with similar hazard profiles at different exposure ranges. Distinct similarity metrics were used to obtain a consensus grouping. Then, a decision-tree based ensemble classifier was used to predict the pre-defined clusters enabling to determine exposure features that contributed to the grouping.

3. Results & Discussion

Mechanistic knowledge was successfully incorporated into the ENM-induced MOA through key event-AOP enrichment analysis. BMD modelling of toxicogenomic data allowed to determine direct MOA of ENM exposures. Time wise analysis of biological response and ENM potency highlighted relevant KEs within the AOP framework. Our results demonstrate that there are time and dose-dependent mechanisms triggered by distinct exposures. These findings suggest that exposure time should be considered to capture common mechanisms across distinct exposures. Genotoxicity related KEs were highlighted in longer exposures. In contrast, higher potency was found particularly associated with less advanced phase of the biological response. The opposite was observed for lower potency, which suggests that system complexity may play a role on the attenuation. Considering the influence of time, biological response and ENM potency in a consensus hierarchical clustering, 5 and 3 clusters were identified at shorter and longer exposures, respectively, indicating that common molecular responses could be identified by this approach. Relationship between exposure characteristics, such as exposed system and material tested, were considered major drivers of the clustering.

4. Conclusions

Our study suggests that ENM potency and time are important factors to distinguish shared mechanisms induced by distinct ENM exposures. The former was related to the responsiveness and the latter was associated with the type of response. We conclude that the similarity between ENM exposures considering mechanistic insight and potency at different timescales can be an effective way to form a consistent grouping that accounts for ENM complexity, given commonalities in attributes such as ENM features, biological system, and biological response. By exploring the relationship between dose of exposure and mechanisms, we open possibilities for the development of quantitative AOPs. This approach could work as a proxy for ENM grouping in safety assessment to support decision makers.

5. Funding information

This research was supported by the Tampere Institute of Advanced Study, the Horizon Europe Framework research and innovation programme (HORIZON), INSIGHT (grant number 101137742), and the European Research Council (ERC) programme, Consolidator project ARCHIMEDES (grant number 101043848).

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Toxicity assessment of metal-ions binary mixtures: new computational approach for calculation toxicity indexes

Dawid Falkowski[1,2], Alicja Mikolajczyk[1,2], Tomasz Puzyn[1,2]

1. Introduction

Assessing the toxicity of mixtures is crucial these days, as large amounts of innovative Advanced Nanomaterials (AdvNMs) and Multicomponent Nanomaterials (MCNMs) are being produced and released into the natural environment. While laboratory mixtures consist of known ingredients and concentrations, environmental mixtures are complex and mainly multi-component, often with unknown proportions. This fact creates an additional issue: the exact concentrations of the mixture components are unknown. To resolve this problem, we propose a new combined approach to calculate the concentrations of mixture components in a theoretical mixture that causes an EC_{50} effect. Based on this approach and a dataset containing nanomaterials-ions mixtures, we calculate several types of mixture toxicity indices: Sum of Toxic Units (STU), Additivity Index (AI), Mixture Toxicity Index (MTI), and Model Deviation Ratio (MDR).

2. New approach for calculate toxicity indexes

In our work, we propose a computational approach to support the prediction of the joint effects of AdvNMs and MCNMs at the early design phase, prior to synthesis. To address the lack of knowledge about the concentrations of individual components in EC_{50} mixture samples, we utilized the known concentrations of the individual components in the binary mixtures used to determine the EC_{50} dose and effect (e.g., immobilization). Based on these parameters, two dose-response curves were obtained for each component of the binary mixture. The individual concentration in the mixture samples was used as the dose, while the response of the binary mixture was used as the response. Using these curves, we determined the concentrations of the mixture components necessary for calculating mixture toxicity indexes in the next step. The calculations were performed using a combined Python and R script with the 'drc' package.

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[2] Laboratory of Environmental Chemoinformatics, Faculty of Chemistry, University of Gdansk, ul. Wita Stwosza 63, 80-308, Gdansk, Poland

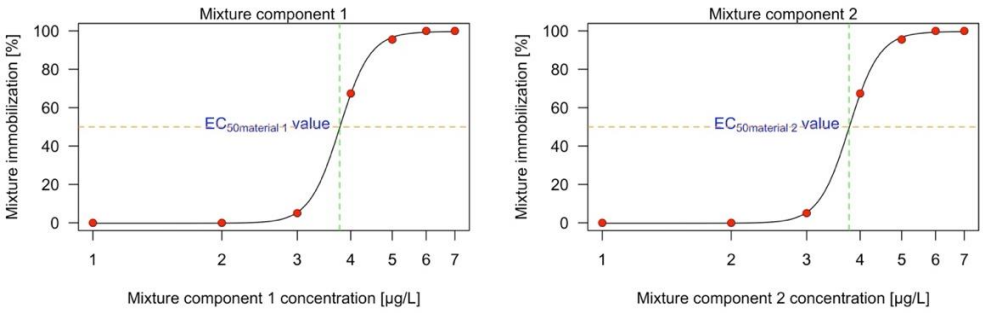

Figure 26 Graphical explanation of two DRC curves method

3. Mixture toxicity indexes calculation

Based on the compositions of binary mixtures of nanoparticles with metal ions available in the literature, the developed approach was utilized to obtain the values necessary for calculating toxicity indices. Four toxicity indices were calculated: Sum of Toxic Units (STU), Additivity Index (AI), Mixture Toxicity Index (MTI), and Model Deviation Ratio (MDR) to assess modes of action (additivity, synergism, and antagonism) for specific samples. In the next step, the indices were compared and displayed graphically.

4. Conclusions

As a result, we obtained a set of 17 binary mixtures of nanoparticles (NPs) and metal ions, characterized by four toxicity indices: Sum of Toxic Units (STU), Additivity Index (AI), Mixture Toxicity Index (MTI), and Model Deviation Ratio (MDR). Primarily, the binary mixtures of nanoparticles with ions exhibited an antagonistic effect, but in four analyses, the effect was synergistic. The effects of toxicity as characterized by these indices were also compared. In 11 of the 17 samples, different types of indices yielded the same toxicity results.

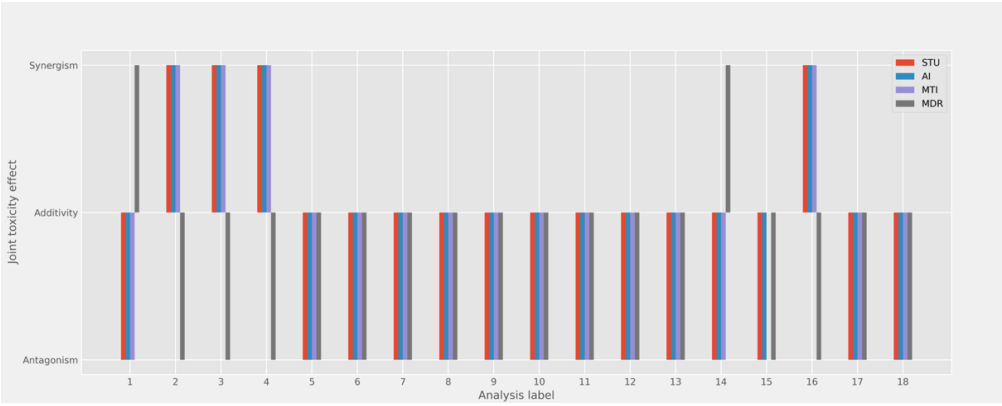

Figure 27 Joint toxicity effect indicate by 4 types of toxicity indexes (STU, AI, MTI, MDR)

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Session 5: Digital Transformation – Towards a common Materials' Data Ecosystem

Knowledge sharing and information transparency is a prerequisite to meet the requirements for SSbD innovative and advanced materials by supporting co-innovation, better and faster decisions, accelerated development, and the ability to handle complexity. This session will discuss key elements and innovations towards a common material's data ecosystem include building the foundations of data documentation, the data sharing framework and its governance, ensure that harvesting and exploiting data from digital systems and technologies, such as modelling and simulation, is advanced and integrated along the value chain.

Presentations (oral and poster) will also cover the following topics:

- Materials digitalisation and data management in trusted data spaces,
- Federated governance across distributed data spaces,
- Harmonisation and automation of data documentation and FAIRification across all areas of materials innovation and SSbD,
- Reporting standards and provenance documentation as part of trust building in integrated approaches of data and software solutions applied for decision support, and
- Stakeholder-centric data documentation and aggregation to support e.g. cross-domain interoperability, regulatory applications or dissemination to the general public based on the digital material / product passports.

Detailed Programme

Start	End	Title	Presenter
16:40	16:55	Workflow for digital twin creation for secondary aluminium alloy in automotive parts	Eugen Gazenbiller
16:55	17:10	Normalised similarity assessment to inform grouping of advanced multi-component nanomaterials by means of an Asymmetric Sigmoid function	Georgia Tsiliki
17:10	17:25	Domain ontology for sharing data related to sustainable metallurgical and manufacturing industry	Jesper Friis
17:25	17:40	IUPAC International Chemical Identifier (InChI) – the compound identifier that makes molecule recognition FAIR	Gerd Blanke
17:40	17:55	How can we unambiguously refer to materials and their corresponding data?	Thomas E. Exner
17:55	18:10	Database generation workflow for supporting SSbD risk assessments	José Luis Vallés-Pardo

18:10 18:30 24/7 Poster Presentations

Posters

S05_P01	From CHADA to CHAMEO: a reference system for characterisation data management	Gerhard Goldbeck
S05_P02	Linked Data Schema Repositories for Interoperable Data Spaces	Simon Stier
S05_P03	Enalos Cloud Platform: A Unified Cheminformatics, Nanoinformatics and Advanced Materials Platform	Dimitra-Danai Varsou
S05_P04	Using machine learning to fill data gaps in the toxicity characterization of chemicals for life cycle assessment	Tianran Ding
S05_P05	Data management for image-based characterisation of 2D materials	Pascal P. Ankli
S05_P06	Domain-Specific Language (DSL) for Nanomaterial Representation	Kostas Blekos
S05_P07	NanoPharos: Collection, curation & organization into machine-readable format of NMs data	Dimitrios Zouraris

Oral Presentations: Session 5

Workflow for digital twin creation for secondary aluminium alloy in automotive parts

Eugen Gazenbiller[1], Lukas C. Jarren[1], Markus Apel[2], Janin Eiken[2], Franz Roters[3], Sharan Roongta[3], Daniel Höche[1], Mikhail Zheludkevich[1]

1. Introduction

The utilization of secondary aluminium, derived from post-consumer scrap, plays a pivotal role in the sustainable practices of the industrial sector. While recycled aluminium is instrumental in the production of various automotive and engineering components, challenges arise as impurity elements accumulate during the recycling process. [1] The presence of iron, even in small amounts, impacts the characteristics of aluminium alloys, influencing factors such as strength, ductility, fracture toughness and corrosion properties. The effects are governed by the alloy microstructure, especially by the presence of additional secondary particles like β-AlFeSi, which are reported to be harmful for mechanical and corrosive properties. [2,3] The aim of the project is the development of a digital workflow, which facilitates the prediction of mechanical and corrosive properties from the impurity content in the utilized aluminium scrap. The approach will enable fast assessment of scrap quality and suitability for specific car components.

2. Schematic workflow structure

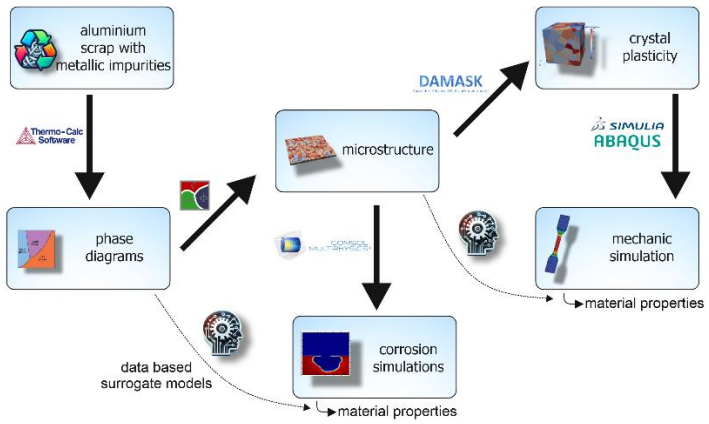

Figure 28: Schematic workflow for digital twin creating including utilized software packages.

The workflow utilizes a combination of free and commercial software packages (Fig. 1) to simulate the formation of the secondary alloy microstructure and its effects on the final mechanical and corrosive properties. [4,5] The approach combines phase field models with regular FEM models and Machine Learning techniques for surrogate model creation. Each of the steps requires dedicated data transfer between the generated and required formats to ensure a flawless transition between the simulation steps. An important step between all steps is the experimental validation of the obtained results.

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3. First selected results

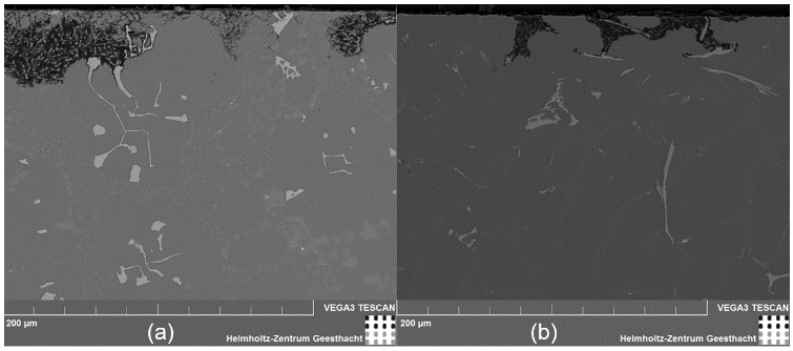

Figure 29: SEM of cross-section after potentiodynamic experiment of artificially impurified AlSi7Mg0.3 with (a) 1.0% Fe, 0.6% Cu, 0.6% Mn and (b) 0.5% Fe, 0.05% Cu, 0.2% Mn

In this work, the workflow will be demonstrated on the example of a AA6063-based secondary alloy with Fe and Cu impurities. The impurity content was artificially adjusted and the effects on the microstructure and corrosion characteristics were analyzed. The corrosion characteristics of AA6063 are highly dependent on the amount and kind of intermetallic particles. Due to reported cathodic potential of both AlFeSi phases compared to Al-matrix, the formation of microgalvanic cells leads to elevated localized corrosion tendency. Moreover, Mg+Si-containing phases are anodic and dissolve preferentially, whereas Mg is removed via dealloying, and Si-remnants can act as a cathode afterwards.[3] This interplay between the electrochemically active phases leads to complicated corrosion mechanisms, as can be seen in SEM cross-sections in Fig. 2. The different intermetallic phases and resulting geometries due to intergranular and trenching corrosion indicate impurity-dependent mechanisms. First solidification simulations (Fig. 3) based on thermodynamic data revealed that the occurrence of the β-AlFeSi phase can be prevented by adding Mn to the melt.

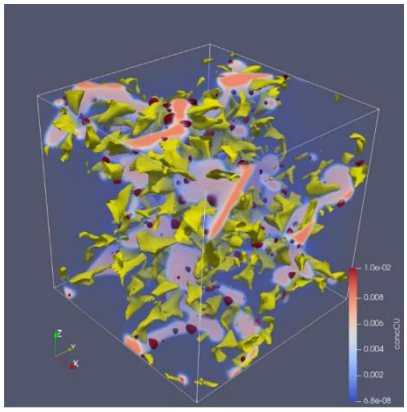

Figure 30: Exemplified result of a MICRESS simulation.

4. Conclusions

The first part of the project lead to promising results which reveal the occurrence of Fe-containing phases in impurified alloy. The precipitation of detrimental β-AlFeSi phases can was simulated via MICRESS software and validated experimentally. The next steps will involve the calculation of the mechanical properties with DAMASK package and FEM corrosion simulations based on the calculated microstructures. The proposed digital workflow is a valuable tool for transformation towards accelerated material design with sustainable recycled alloys.

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Normalised similarity assessment to inform grouping of advanced multi-component nanomaterials by means of an Asymmetric Sigmoid function

Alex Zabeo [1], Matteo Carisi[1], Fabio Rosada[1], Lisa Pizzol[1], Georgia Tsiliki[2], Danail Hristozov[1]

1. Introduction

Due to the increasing use of advanced multi-component nanomaterials (MCNMs) in various industries, there's a growing need to increase the efficiency of their safety testing while reducing the use of experimental animals. In this context it is relevant to adopt similarity-based grouping approaches as a basis for read-across of existing data for both safe by design and risk assessment purposes.

This document proposes a novel similarity assessment methodology specifically designed for MCNMs. This method groups similar MCNMs, allowing researchers to read-across safety information from well-studied materials to new ones. This reduces the need for extensive testing and animal experiments.

The methodology is implemented in a user-friendly software script and web application accessible to industry users, especially from small and medium-sized enterprises (SMEs). The document also presents a real-world example from the construction sector to demonstrate the added value of the proposed methodology.

2. Methods

A new method for assessing similarities between nanoforms is presented, particularly suited to the more complex identity of the advanced MCNMs. The method considers all available information on the materials' physical and chemical properties, as well as their toxicity. It incorporates a special scaling technique to ensure consistent comparisons across different properties.

This method allows for comparing MCNMs to each other, to groups of MCNMs, or even to single-component nanomaterials. The approach involves several steps: i) transforming data for consistency by application of the Arsinh function (i.e., Inverse hyperbolic sine); ii) scaling of properties to make them comparable by applying asymmetrical Logistic scaling function for scalar properties and full curve shape comparison by application of a modified Kolmogorov–Smirnov metric for bivariate properties; and iii) calculating similarities for each property, and then combining these to get an overall similarity score by the use of Ordered Weighted Average (OWA). To

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make it easier to use, the authors created a software script that automates these steps which was delivered as a web application.

3. Conclusions

A new way to compare properties of materials is introduced which is especially tailored to safety (toxicity). This method uses a special S-shaped curve (sigmoid function) to transform data into a format that's easier to compare and combine. This new approach ensures that comparisons remain consistent even when adding new materials for evaluation.

The authors tested their method on a real-world example from the construction sector: SiO_2-ZnO nanocomposite composed of SiO_2 core coated by ZnO. This material is used to ensure photocatalytic decontamination (NO_X gases removal) of construction materials such as mortar.

The results of applying the proposed method in the case study has demonstrates its effectiveness to identify similarities between multicomponent nanoforms, making it a valuable tool to support grouping as basis for safety assessment. The approach was helpful to point out that using different dispersion media has a propound effect on dissolution-related similarity. Although distance matrices for dissolution in different media are quite distinct, they all show a high dissimilarity for ZnO. Additionally, while the Zeta potential values are all similar, Size shows higher distances for ZnO too. The overall aggregated similarity further confirms these differences by displaying high dissimilarity for ZnO.

4. References

Zabeo, A., Basei, G., Tsiliki, G., Peijnenburg, W., & Hristozov, D. (2022). Ordered weighted average based grouping of nanomaterials with Arsinh and dose response similarity models. *NanoImpact*, *25*. https://doi.org/10.1016/j.impact.2021.100370

Domain ontology for sharing data related to sustainable metallurgical and manufacturing industry

Jesper Friis[1], Sylvain Gouttebroze[1], Astrid Marthinsen[1], Stephane Dumoulin[1], Tomas Manik[2]

1. Introduction

An overview is given of the ongoing work of developing a new domain ontology for metallic microstructures based on the Elementary Multiperspective Material Ontology (EMMO) [1]. This ontology is developed in the context of European Materials Modelling Council (EMMC) [2] and the Norwegian *Centre for Sustainable and Competitive Metallurgical and Manufacturing Industry* (SFI PhysMet) [3], for which the overall objective is to enable and accelerate the transformation of the national metal industry towards more sustainable and cost-efficient production, future material products, solutions, and improved processing methods.

2. The microstructure domain ontology

Ontologies have been successfully used for more than two decades in biomedical sciences to categorise and structure scientific data, to facilitate the description of the human genome and for the rapid development of new vaccines. Until recently there have been very few successful attempts towards ontologies in the domain of material sciences. The main reason for this is the large complexity of materials science, which consists of many scientific communities and has a large variety of characterisation techniques and modelling tools producing and requiring very heterogeneous types of data. However, during the last years, especially in Europe, an increasing interest in utilising ontologies for materials sciences has been observed. These developments to a large extend are driven by the EMMO.

Figure 1 shows a few selected concepts from the microstructure ontology and how they connect to EMMO.

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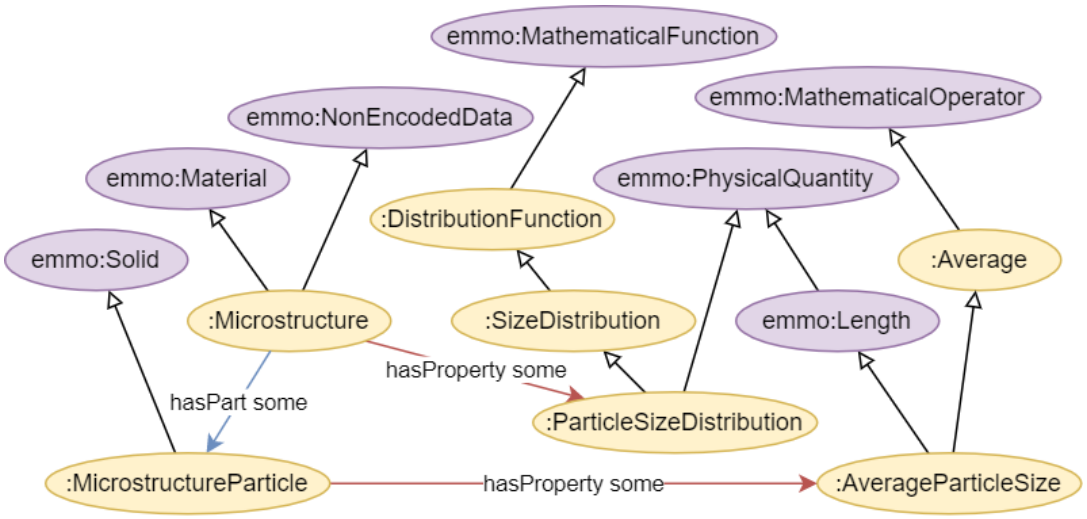

Figure 31. Some selected classes from the microstructure ontology (yellow) and how they connect to EMMO (purple). Three different types of relations/class restrictions are also shown; `rdfs:subClassOf` *(open arrows),* `emmo:hasPart` *(blue arrow) and* `emmo:hasProperty` *(red arrows).*

A microstructure is here described as an `emmo:Material` (real world object representing an amount of a physical substance), which is also an `emmo:NonEncodedData`. EMMO defines data in accordance with Floridi [4], as the variation of properties of a physical object that can be recognised and eventually interpreted, where non-encoded data is data that occurs naturally with no intentional encoding by an agent. A microstructure has (among others) a `MicrostructureParticle` part and a `ParticleSizeDistribution` property.

3. Enabling interoperability

Ontologies provide a common language and enables semantic interoperability, i.e. the ability to connect different models and data sources that have been developed independent of each other into complex workflows. The key is to create simplistic data models describing the underlying datasets and map them to ontological concepts. A simple example of this is shown in Figure 2, which also makes use of the Function Ontology (FNO) [5] to ontologically describe how the `mean_size` property of a data model for a simulation automatically can be instantiated from an experimental dataset of the precipitate size distribution in an aluminium alloy.

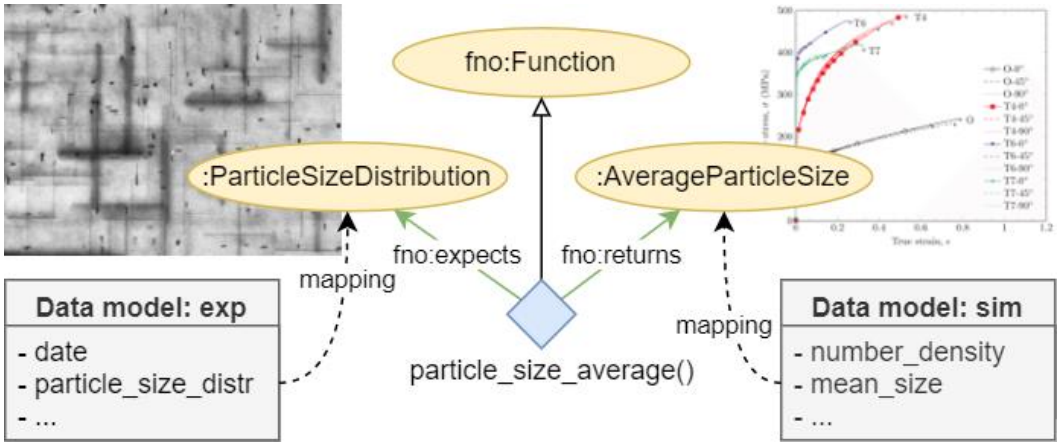

Figure 32. Example of two data models with properties mapped to ontological concepts. FNO is used to ontologically describe how an average particle size can be calculated from a particle size distribution.

4. Conclusions

The microstructure domain ontology provides a straightforward way to semantically document of physical metallurgical data and enable exchange of digital data between characterisation and modelling, across scales and processes and between physical metallurgy and other domains. An example is given on how this ontology can be used in practice to enable semantic interoperability.

5. References

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IUPAC International Chemical Identifier (InChI) – the compound identifier that makes molecule recognition FAIR

Gerd Blanke[1,2], Jonathan M. Goodman[3,4]

1. Introduction

The InChI (IUPAC International Chemical Identifier) is the unique identifier for chemical compounds that allows the precise identification of any molecule in each research step. The unique identification of compounds makes InChI the central pivot point for FAIR data handling in the pharmaceutical and chemical R&D. Recent developments of the InChI enhance the handling of inorganics and organometallics, add extended stereochemistry functionality, and will introduce additional normalization rules for tautomeric functional groups. InChI applications extend the usage of InChIs to reactions, mixtures, formulations, and nano materials.

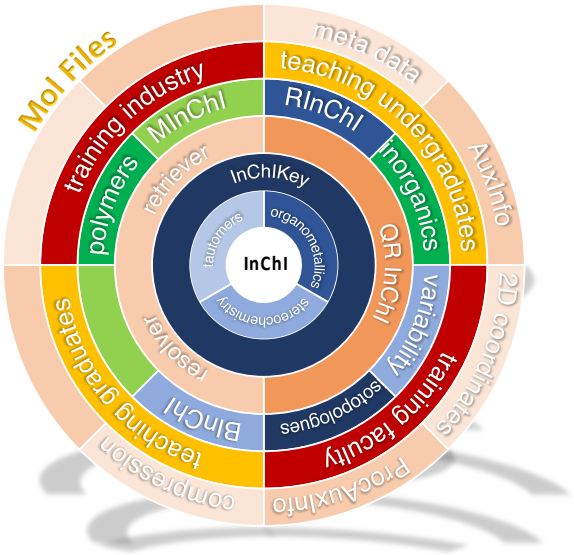

Figure 33: The InChI universe

2. How do I find compound XYZ?

To search, compare, and analyse molecules over multiple sources from different resources you have to ensure the compound identifier follows the FAIR (Findable,

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Accessible, Interoperable and Re-Usable) principles. Independent of the actual compound depiction, the goal of an identifier for the chemical compound is to provide unique identification, making the compound findable and accessible within different research contexts. The accessibility and utility of public databases like PubChem relies on the unique identification of compounds. Research collaborations make it necessary to exchange data. Data interoperability is not possible without unambiguous compound IDs.

InChI fulfils all of these conditions. In the current version it handles more than 99.9% of all organic compounds correctly. (Goodman, Pletnev, Thiessen, Bolton, & Heller, 2021) The current development is focussed on the better representation of inorganics and organometallics and to fill open issues in the area of stereochemistry like MDL enhanced stereochemistry or atropisomers. In a second step, new transformation rules will be implemented to improve the unique representation of tautomeric groups. The support of polymers is already in the test phase. Last, but not least, InChI will provide the registration functionality supported by molfiles.

The InChI application framework addresses the needs of chemical reactions, mixtures and formulations, and nano materials. In all of these cases the identification is based on multiple compounds with each of them being represented by InChIs. In the case of reactions, InChIs represent each of the reactants, products and agents (catalysts, solvents). Additional string sorting rules make it possible that a unique identification called Reaction-InChI or RInChI is created. (IUPAC-InChI/RInChI) (Goodman, Blanke, & Kraut, Analysing a billion reactions with the RInChI, 2022) Mixtures and formulations seen as ordered mixtures consist of the InChIs of each component, the order of the component during the creation of the mixture and may be extended by other physical data and ensure that the unique identifier Mixture-InChI (MInChI) is built. (IUPAC/MInChI) With Nano-InChIs (NInChIs) the usage of InChI is extended to the world of materials where multiple material layers must be described together with physical data in a way that a unique identifier can be created out of it.

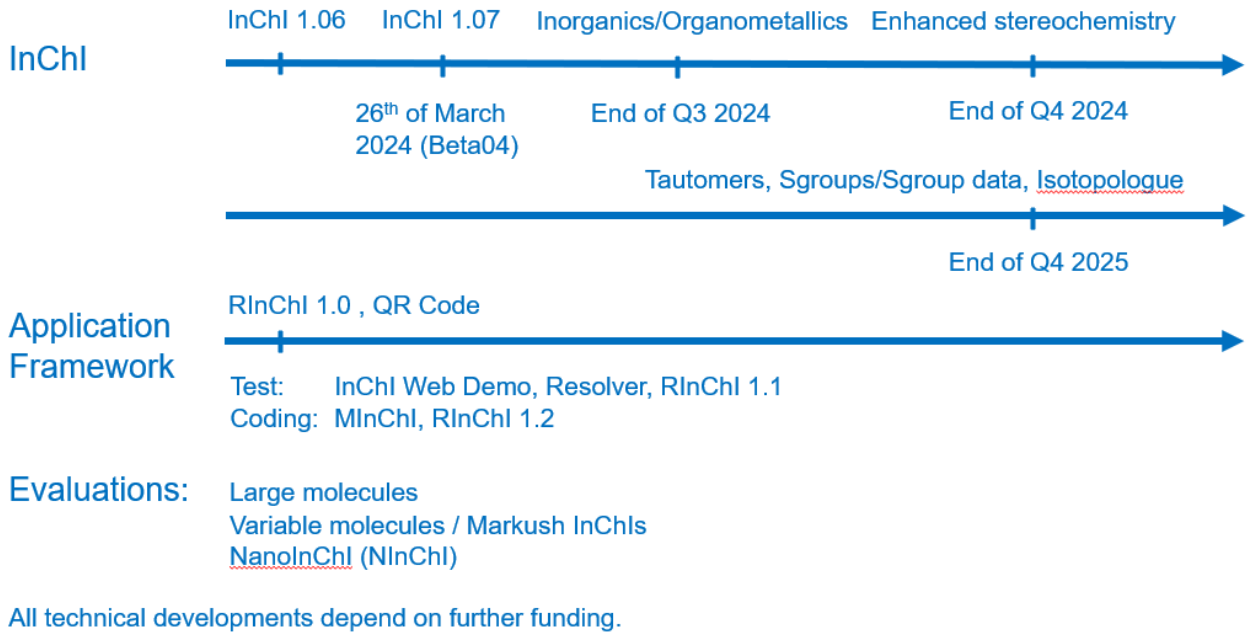

Figure 34: The InChI roadmap, status beginning of April 2024

InChI is an open-source application available on GitHub (/IUPAC-InChI/InChI) under the MIT license.

InChI is used in industry to identify compounds during the R&D processes,

InChI and its InChIKey are found in most of the publicly available databases like PubChem, CAS and ZINC. All together you find far more than one billion compounds that are publicly available via InChIs.

3. Conclusions

InChI has been developed as a unique universal identifier for molecules. The recent developments improve the treatment of inorganics, organometallics, complex stereochemistry and structure normalization. The InChI application framework extends the usage into reactions, mixtures, formulations, and nano materials.

That makes InChI to an integral part of FAIR data handling in R&D of chemical compounds.

4. References

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How can we unambiguously refer to materials and their corresponding data?

Thomas E. Exner[1], Gerd Blanke[2], Jaleesia Amos[3], Mark Wiesner[3], Joh Dokler[1], Maja Brajnik[1], and Iseult Lynch[4]

1. Introduction

Nanosafety research has clearly demonstrated that chemical composition is not enough to represent a nanomaterial and to differentiate it from similar materials, which can show very different properties and toxicities. This has led to the concept of nanoforms and sets of nanoforms, defined by a limited number of physicochemical properties to group materials, which can be handled together e.g., under REACH [1]. For the relatively limited number of commercially relevant nanomaterials, such a classification might be enough, but this changes already if complex nanomaterials are considered. Moving from nano to advanced and innovative materials, this much larger group should be handled from the start in a common materials data ecosystem, and provide data to many emerging modelling applications as applied e.g., in Safe-and-Sustainable-by-Design. Materials undergo multiple transformation steps during their production, which lead to distributions (e.g., particle size distributions in nanomaterials, distributions of polymer chain lengths) or complex, random bonding networks (e.g., coatings synthesised by sol-gel processes, cross-linked polymers) rather than homogeneous entities.

2. Material, sample and data provenance

The FAIR (Findable, Accessible, Interoperable and Re-Usable) principles stress that data can only be understood and therefore re-used if metadata is provided documenting the full provenance trail of the data, describing all manipulations from its creation to its current state including collection, processing, curation and storing. In the same way, documentated material and sample provenance trails are often the only possibility to fully understand what the object under consideration is, how it is related to other, similar materials, why it shows differences to these and even to identify batch-to-batch variations. In this talk, we will present multiple new data management ideas to document such material and sample provenance trails and integrate these as part of data provenance. Instance Maps [2] are used to structure and visualise the material manipulations including production and other life-cycle stages (e.g., use and end-of-life scenarios), and sample preparation and data collection steps (see Figure 1). In combination with existing metadata schemas for data provenance like PROV [3], improved structural representations like the InChI for nano (NInChI) [4] and unique identifiers such as the European Registry of Materials (ERM) [5], a new material

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[4] School of Geography, Earth and Environmental Sciences, University of Birmingham, Birmingham, UK

representation system can be developed, which provides chemical information as precisely as possible but acknowledges the production-specific aspects of materials properties, providing this information for the current life-cycle stage and any past stages and transformations. Documentation in this way provides (i) a description of the real material or specific sample of it (if sample provenance is added) and the collection (distribution) of specific particles or substructure of the material; and (ii)enables all this information to be easily used to create input for data-driven or physics-based modelling, which need to use a specific structure or a small subset of these.

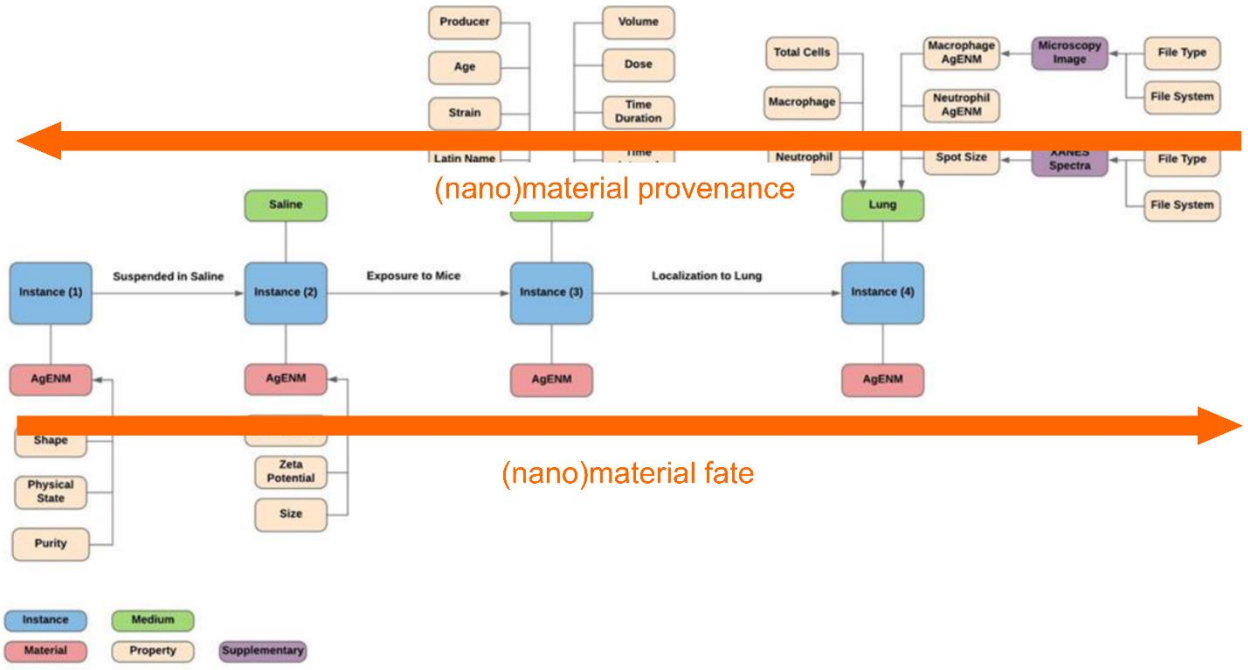

Figure 1: Instance map visualizing the fate of a nanomaterial in a mesocosm experiment looking at effects on mice lungs. Following the instance map backwards, the material provenance can be extracted giving a detailed description of the material and its previous life cycle stages (production and formulation for example).

3. Conclusions

Current identifiers cannot capture the complexity of materials research, leading to cases where (I) different materials or batches of materials lead to different experimental outcomes yet are referred to by the same identifiers (like CAS registry numbers) or (ii) different materials are shown to have the same basic physicochemical properties leading to misclassification as the same material. Thus, current materials characterisation as provided by many studies (and stored in databases) are not enough to prove sameness or similarity. To remove this ambiguity, we suggest using a life-cycle approach, which includes the history of previous stages as material and sample provenance trails. However, such a change of information management will require further developments for tools re-using the data starting with advanced non-structural similarity measures and input generation for modelling.

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5. Acknowledgement

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Database generation workflow for supporting SSbD risk assessments

José Luis Vallés-Pardo[1], Salvador Moncho[1], Eva Serrano-Candelas[1], Rafael Gozalbes[2]

1. Introduction

The new paradigm of green toxicology aims to make chemicals safer by design, focussing on hazard issues earlier during development stages and keeping track on them during their whole life cycle. This evolves in the development of Safety and Sustainable by Design (SSbD) frameworks [1], defining how to perform the risk assessment, from the raw materials until the final disposal and degradation in the environment. The risk assessment on the SSbD framework requires a big amount of information about physical and (eco)toxicological properties of substances used or released along the production, processing and application of the product. However, the green toxicology paradigm includes the reduction of experimental tests [2]. Under these premises we have started different European projects, such as BIO-SUSHY[3], SiToLub[4] and CheMatSustain[5], including data-based approaches for SSbD assessment. For this reason, an automatic workflow for the creation of specific databases for each project, combining experimental data together with QSAR predictions, will become an interesting tool to help in the SSbD hazard statement.

2. Database structure

For the generation of these databases, existing experimental data and QSAR predictions will be used. The automatised workflow to build the databases extracts information from three different kinds of sources (vendor-provided data, public databases and QSAR predictions), as shown in Figure 1.

Vendor's information will be gathered using their safety data sheets (SDSs). Automatic text scrapping will be used to gather the information from the PDF documents and organise it into tabulated data.

Data from a series of reliable public databases will be also extracted, including databases coming from regulatory entities (such as ECHA and EPA). Our databases will include not only the parameters/endpoints values, but also other information about the experimental records -as the sources and experimental protocols- to facilitate the selection among multiple records and to evaluate the reliability and pertinence of the different values. A special treatment will be applied for the mixtures, including data about both, the materials of interest and their constituents. In addition to experimental records for specific properties, our databases will also gather previous safety

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assessments, such as CLP harmonized categories and data from the ECHA list of substances of very high concern.

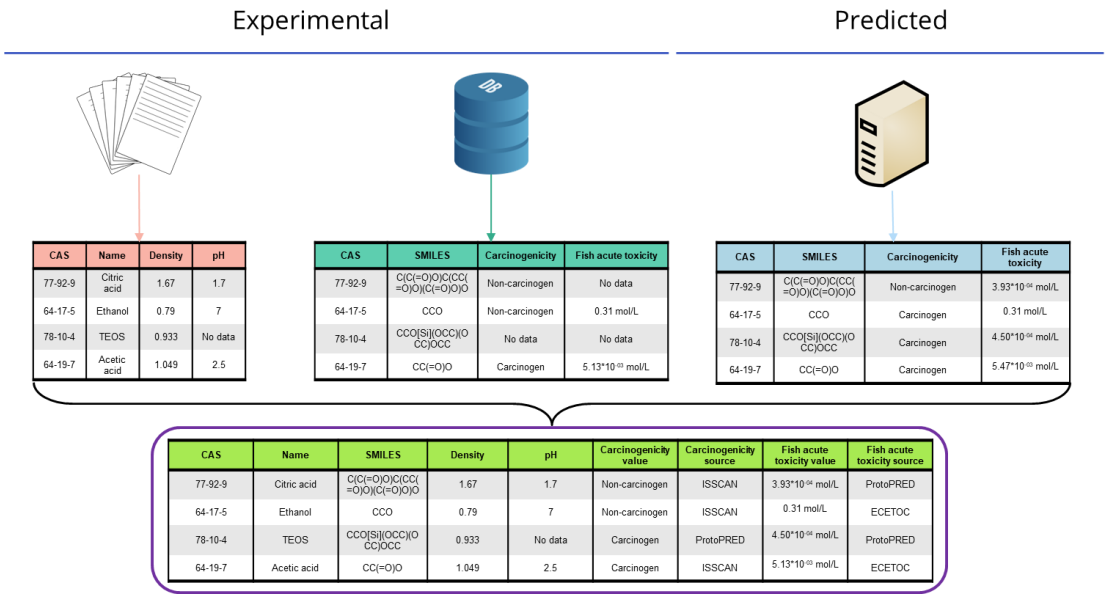

Figure 35. Databases sources.

Predicted data will be obtained from QSAR models. Several prediction tools will be explored to use the most appropriate one, –including our own in-house models available at the ProtoPRED® platform [6]–, keeping track of the selected tool, together with the metrics of the model and other relevant information.

Once the tables with experimental and predicted data will be compiled, they will be combined into a single one for each project, using tailored selection rules to select the information when more than one record exists.

3. Conclusions and future steps

Following the aforementioned protocol, comprehensive databases will be obtained without performing any new experimental test, and therefore without the costs and the ethical considerations when *in vivo* tests are involved.

To broaden the range of this approach, several steps will be taken in the future:

- The number of public databases and QSAR models included will be expanded.
- An automatic process to transform the data obtained into regulatory-based categories used in SSbD risk assessment will be developed.
- Additionally, the remaining gaps will be filled up with *ad hoc* tests.

4. Acknowledgements

The BIO-SUSHY project is funded by the European Union under the Grant Agreement number 101091464. The SiToLub project is funded by the European Union under the Grant Agreement number 101138807. The CheMatSustain project is funded by the European Union under the Grant Agreement number 101137990. Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of

the European Union or the European Health and Digital Executive Agency (HaDEA). Neither the European Union nor the granting authority can be held responsible for them.

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Poster Presentations: Session 5

From CHADA to CHAMEO: a reference system for characterisation data management

Gerhard Goldbeck[1], Pierluigi Del Nostro[1], Daniele Toti[1]

1. Introduction

The CHADA (Characterisation Data) template was developed and standardised (CWA) [1] as a common format for documentation materials characterisation, with a view to generality across any type of characterisation method.

In order to provide a machine readable and actionable version of CHADA, the CHAMEO (CHaracterisation MEthodology Ontology) [2] has been developed in the NanoMECommons project [3]. CHAMEO includes all terms/metadata of CHADA in a unified, EMMO-based semantic model that describes the classes of metadata and how concepts relate to one another, i.e. it provides context and meaning.

CHAMEO is the overarching reference for sub-domain and application ontologies. It has already been applied to areas ranging from nanomechanical characterisation (nanoindentation, FIB-DIC) (e.g. of coatings) to partial discharge testing of batteries [4].

2. Towards FAIR documentation of characterisation experiments

The CHADA document template has a structure of sections with generic guidelines to drive the users to providing information about materials characterisation experiments. This template has the goal to provide a standard format, but the generated documentation is only human readable. Though there are indications on how to fill the template, when collecting CHADAs from different operators it arose that different users filled in differently, making the documentation hard to exchange.

To address these issues the CHAMEO ontology has been developed, as a building block towards a machine readable, FAIR documentation of characterisation experiments.

The ontology design process started from the concepts in the CHADA template, then adding classes, relationships and definitions in order to improve the expressivity of the ontology. CHAMEO has been developed and refined through an iterative process involving domain experts on different characterisation techniques, to realise a common framework for the development of technique or application specific ontologies.

Based on EMMO [5] the CHAMEO ontology provides the basic constructs to describe the different kinds of activity that are performed during a characterisation process (e.g. sample preparation, sample inspection, calibration, measurement, data analysis) the experiment itself, which can be simple or a complex workflow, with information about the laboratory and the operator, the sample (e.g. material, physical and chemical

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properties), the hardware involved and the different types of data produced (raw, primary, secondary, characterisation properties).

Ontologies related to specific techniques or applications can be then developed by specialising the basic constructs of CHAMEO. This follows a modular approach for ontology development which also facilitate the interoperability across different characterisation techniques. Figure 36 depicts the modular approach adopted for CHAMEO and CHAMEO-based ontologies.

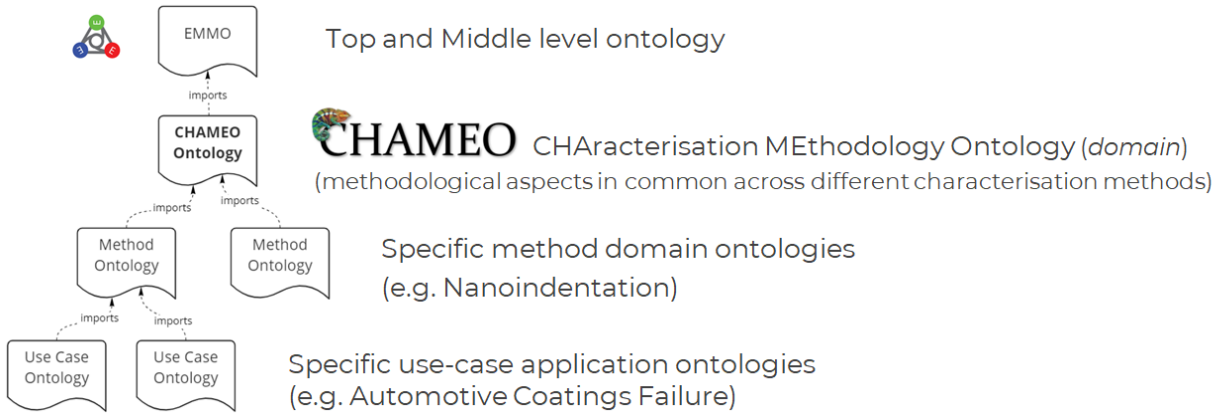

Figure 36 - Ontology design modular approach

The FAIR score of CHAMEO has been measured through the FOOPS validator (https://foops.linkeddata.es/FAIR_validator.html) and is 92%.

3. Conclusions

A reference ontology for all fields of characterisation has been developed. It provides the basis for curated metadata, harmonised documentation of materials characterisation protocols and a commons data space that supports queries across currently disparate sub-disciplines.

4. References

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[3] NanoMECommons project: https://www.nanomecommons.net/

[4] https://github.com/emmo-repo/battery-testing-ontology

[5] EMMO: https://github.com/emmo-repo/EMMO

5. Acknowledgments

The NanoMECommons project has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 952869.

Linked Data Schema Repositories for Interoperable Data Spaces

Stier, S.[1]; Gold, L.[1]; Popp, M.[1]; Räder, A.[1]; Triol, A.[1]

In this talk we discuss the improved interoperability and enlarged tool landscape of data spaces by stronger coupling between semantic web, general web technologies, and programming languages and give insights into a pilot data space for battery research.

In a material science context, metadata models need to cover all relevant levels, including data acquisition, processing, interpretation, publication and documentation and should be subject to harmonization within a data space community. For this purpose, both IDS and GAIA-X propose [1][2] RDF and it's JSON-LD serialization as a common data representation, and consequently RDFS, OWL, and SHACL for data schemas and validation. While the expressiveness of RDF is theoretically unlimited and thus fulfills all requirements, there are practical limitation and barriers in its practical and scaled application.

We therefore propose the closer integration between RDF/SHACL and object orientated programming by a modular hierarchical self-description of data assets by JSON-LD annotated JSON-SCHEMAs in combination with direct coupling with object-oriented programming through a linked data schema repository. In addition, a search index, visual renderings and auto-generated edit forms provide a human-centered interface. A published and maintained python package [3] allows the add-hock generation [4] of data classes from data schemas and vice versa, enabling conformance by design of programmatically generated and used data through an abstract knowledge graph interface. This includes not only pure data classes, but also mapped controller classes that provide corresponding functions/methods with a strong link to data space services/apps via automatically generated APIs.

By providing a JSON-SCHEMA for OWL classes the documentation, visualization and graphical editing of large and linked ontologies also becomes an important use case [5] for both their development and governance. Thereby OWL classes and data schemas are regarded as complementary and linked concept combining their strength in formal logic on the one hand and closeness to concrete implementations on the other hand. With respect to the existing reference architectures this approach integrates the hierarchical concept of GAIA-X with the graph structure of IDS and provides a user and programmer friendly toolset to extend their application to detail/domain levels beyond the core metadata models.[6][7]

[1] https://internationaldataspaces.org/wp-content/uploads/dlm_uploads/IDSA-Position-Paper-GAIA-X-and-IDS.pdf

[2] https://library.oapen.org/handle/20.500.12657/57901

[3] https://github.com/OpenSemanticLab/osw-python

[4] https://opensemantic.world/wiki/Item:OSW659a81662ff44af1b2b6febeee7c3a25

[5] https://onto-wiki.eu/wiki

[6] https://gaia-x.gitlab.io/gaia-x-community/gaia-x-self-descriptions/core/core.html

[7] https://github.com/International-Data-Spaces-Association/InformationModel

Domain ontology for sharing data related to sustainable metallurgical and manufacturing industry

Jesper Friis[1], Sylvain Gouttebroze[1], Astrid Marthinsen[1], Stephane Dumoulin[1], Tomas Manik[2]

1. Introduction

An overview is given of the ongoing work of developing a new domain ontology for metallic microstructures based on the Elementary Multiperspective Material Ontology (EMMO) [1]. This ontology is developed in the context of European Materials Modelling Council (EMMC) [2] and the Norwegian *Centre for Sustainable and Competitive Metallurgical and Manufacturing Industry* (SFI PhysMet) [3], for which the overall objective is to enable and accelerate the transformation of the national metal industry towards more sustainable and cost-efficient production, future material products, solutions, and improved processing methods.

2. The microstructure domain ontology

Ontologies have been successfully used for more than two decades in biomedical sciences to categorise and structure scientific data, to facilitate the description of the human genome and for the rapid development of new vaccines. Until recently there have been very few successful attempts towards ontologies in the domain of material sciences. The main reason for this is the large complexity of materials science, which consists of many scientific communities and has a large variety of characterisation techniques and modelling tools producing and requiring very heterogeneous types of data. However, during the last years, especially in Europe, an increasing interest in utilising ontologies for materials sciences has been observed. These developments to a large extend are driven by the EMMO.

Figure 1 shows a few selected concepts from the microstructure ontology and how they connect to EMMO.

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[2] NTNU, Dept. of Materials Science and Engineering (Norway)

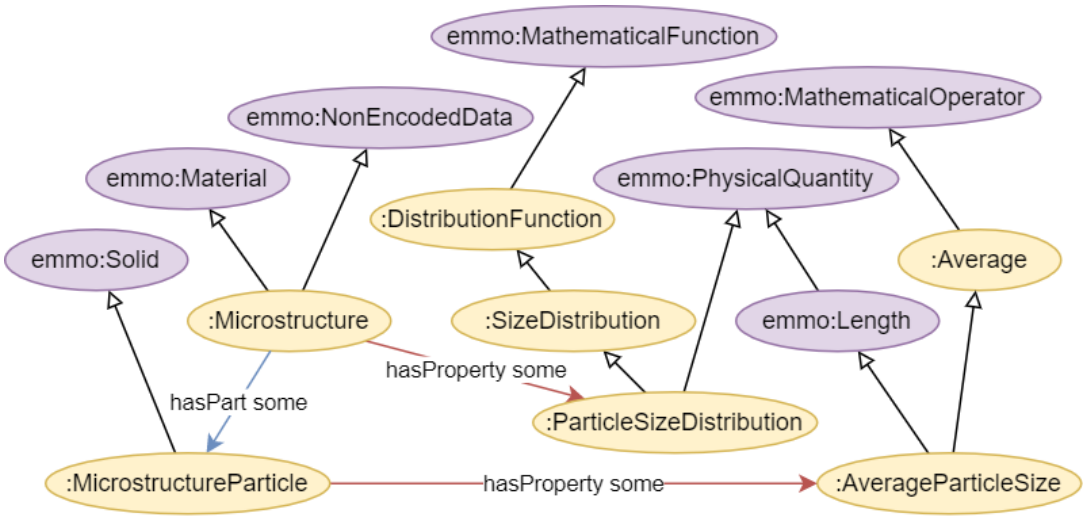

Figure 37. Some selected classes from the microstructure ontology (yellow) and how they connect to EMMO (purple). Three different types of relations/class restrictions are also shown; `rdfs:subClassOf` *(open arrows),* `emmo:hasPart` *(blue arrow) and* `emmo:hasProperty` *(red arrows).*

A microstructure is here described as an `emmo:Material` (real world object representing an amount of a physical substance), which is also an `emmo:NonEncodedData`. EMMO defines data in accordance with Floridi [4], as the variation of properties of a physical object that can be recognised and eventually interpreted, where non-encoded data is data that occurs naturally with no intentional encoding by an agent. A microstructure has (among others) a `MicrostructureParticle` part and a `ParticleSizeDistribution` property.

3. Enabling interoperability

Ontologies provide a common language and enables semantic interoperability, i.e. the ability to connect different models and data sources that have been developed independent of each other into complex workflows. The key is to create simplistic data models describing the underlying datasets and map them to ontological concepts. A simple example of this is shown in Figure 2, which also makes use of the Function Ontology (FNO) [5] to ontologically describe how the `mean_size` property of a data model for a simulation automatically can be instantiated from an experimental dataset of the precipitate size distribution in an aluminium alloy.

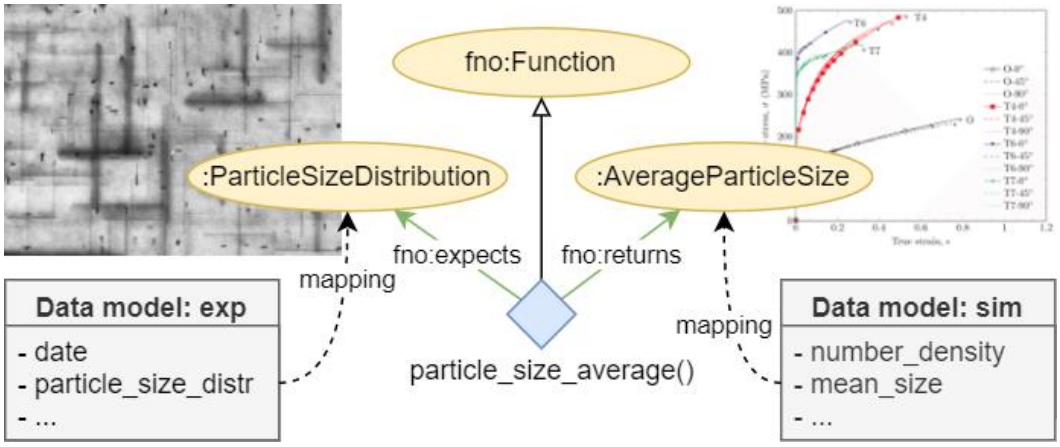

Figure 38. Example of two data models with properties mapped to ontological concepts. FNO is used to ontologically describe how an average particle size can be calculated from a particle size distribution.

4. Conclusions

The microstructure domain ontology provides a straightforward way to semantically document of physical metallurgical data and enable exchange of digital data between characterisation and modelling, across scales and processes and between physical metallurgy and other domains. An example is given on how this ontology can be used in practice to enable semantic interoperability.

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[2] European Material Modelling Council: https://emmc.eu/

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[4] Luciano Floridi, "Information - A very Short Introduction", Oxford University Press., (2010) ISBN 978-0199551378.

[5] The Function Ontology (FNO): https://fno.io/

Using machine learning to fill data gaps in the toxicity characterization of chemicals for life cycle assessment

Tianran Ding[1], Gustavo Larrea-Gallegos[1], Antonino Marvuglia[1], Thomas Schaubroeck[1]

1. Introduction

With the increasing number of marketed chemicals, understanding their effect on different dimensions of sustainability has become a priority. Since chemicals can be found along the different stages of the supply chains of most products and services, it is important to understand their sustainability from an holistic perspective. For this purpose, Life-Cycle Assessment (LCA) has been commonly selected as the suitable tool to quantify the impacts associated with the life-cycle of a product or chemical. The mapping between environmental flows and the affectation to the environment is done through the use of coefficients known as characterization factors (CF). While CFs are developed to address different types of environmental impacts, in this study we focused on toxicity-related impacts.

In the literature, different methods were proposed to develop toxicity-related CFs for numerous chemicals, such as USEtox and Environmental Footprint (EF) (Saouter et al., 2018). Nevertheless, not all chemicals are characterised in these methods. For instance, USEtox provides CFs for around 3000 chemicals and a recent update of this method (i.e., EF version 3) expanded the chemical coverage to around 6000. However, the provided CFs are still not enough to cover the whole range of chemicals, especially the ones newly developed. In these methods, calculating new CFs requires collecting various data concerning chemical properties to calculate factors related to fate, exposure, and effect. However, some of these data are not always available since they traditionally come from experimental tests that are cost- and time-consuming, confidential or non-transparent, and could face legislation restrictions on in-vivo tests on animals.

To address this, recent literature has adopted the use of data-driven approaches such as machine learning (ML) to predict parameters or metrics that are later fed into the USEtox method, such as fate and intake factors (Marvuglia et al., 2015), species sensitivity distribution (SSD) (Song et al., 2022), hazard concentration 50% (HC_{50}) (Hou et al., 2020a, 2020b; Li et al., 2024). These works rely on the use of USEtox database to train their models, but they have not been updated or improved using novel toxicity datasets, such as the one provided by the new version of the EF 3 method (Saouter et al., 2018).

The aim of this study is to fill these gaps by exploring different ML algorithms to produce off-the-shelf models of toxicity prediction. For this, the models are trained to predict hazard concentration 20% (HC_{20}) of chemicals using only SMILE representation as input, so it can be used later in the pipeline of the novel EF 3 methodology. The novelty of our

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study relies on the use of a new dataset that contains almost two times more data entries if compared to the formerly used USEtox dataset.

2. Materials and methods

Based on the different types of approaches found in the literature, we have identified two main methodological pathways that are commonly explored (see Figure 1). In this study we selected the first pathway that looks towards predicting HC_{20}. The predicted HC_{20} are then used to calculate the effect factor (EfF) that measures the potentially affected fraction (PAF) of exposed masses in the freshwater ecosystem in the EF method.

HC_{20} is predicted using two algorithms: the eXtreme Gradient Boosting (XGboost) and Gaussian processes. Molecular descriptors were obtained from SMILE labels using an open source cheminformatics library (i.e., RDKit) and HC_{20} were collected from the EF dataset. The final dataset contains 5540 observations with one predicted variable (i.e., HC_{20}) and 256 characteristics as initial predictors.

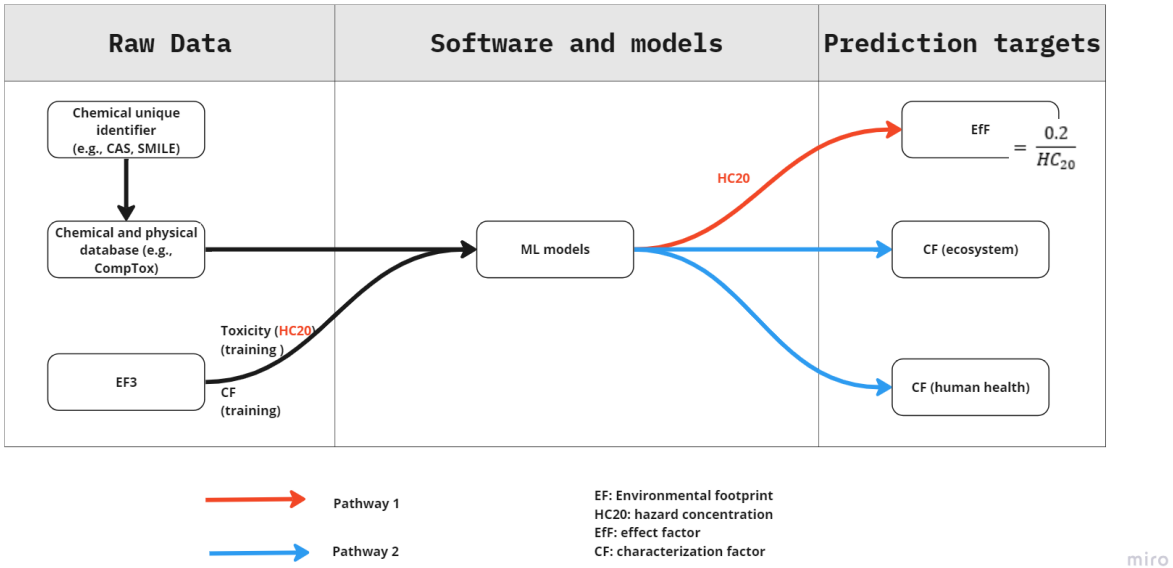

Figure 1. Illustrations of two methodological pathways common in literature. This work follows pathway 1.

The data were split into training (70%) and testing (30%) sets. Three-fold cross-validation was used to choose the best hyperparameter combination from a grid search. The best model was then used to predict the test set using the coefficient of determination (R^2) as indicator of performance of the model.

3. Results

In our preliminary results, the XGBoost model yielded an R^2 of 0.46 (see Figure 2), which sets a new benchmark for this training dataset. With respect to the Gaussian Process, a similar R^2 of 0.47, suggests that this model has a similar capacity of capturing the underlying complexity of the dataset.

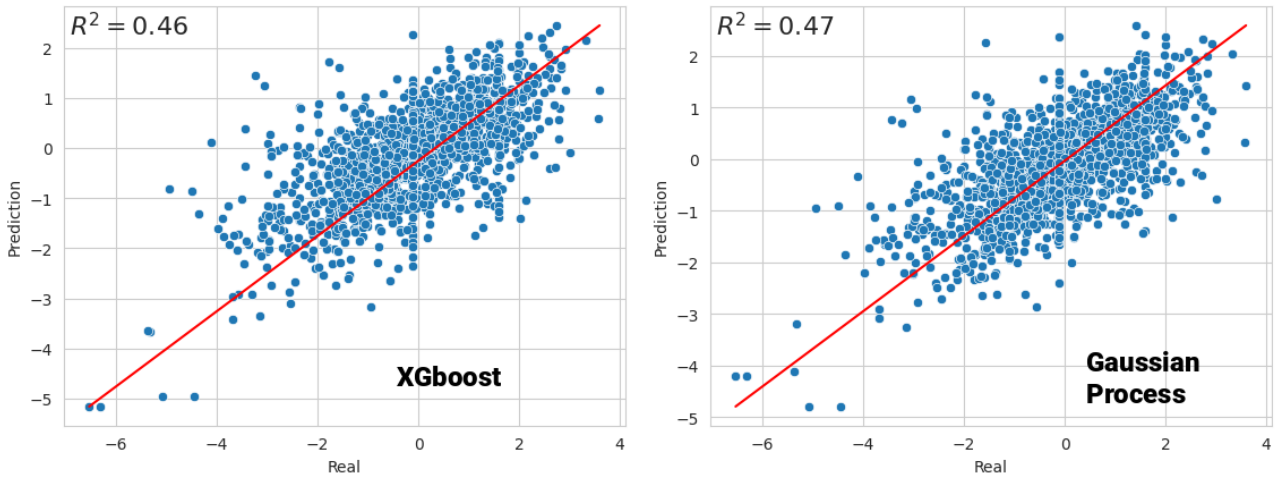

Figure 2. Performance of predictions obtained from the XGBoost and Gaussian Process model using coefficient of determination as indicator.

4. Conclusions

This study embarked on a required quest to harness ML in bridging data gaps inherent in the toxicity characterization of chemicals, a pressing need amid the burgeoning array of chemicals in the market. Through the adept application of ML algorithms, namely XGBoost and Gaussian processes, this research is working on predicting chemical toxicity more accurately, leveraging on the latest EF data and methodologies.

While preliminary, our results indicate that a further improvement of the algorithms is required. This may suggest that further research should be oriented to the adoption of more sophisticated algorithms such as deep learning. Finally, further steps in this study will include the exploration of the methodological pathway 2, which would imply the delivery of a completely off-the-shelf tool to be used in LCA studies.

5. Acknowledgements

This study is part of the CALIMERO project, funded by the European Union with the grant number: 101060546.

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Data management for image-based characterisation of 2D materials

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1. Introduction

ACCORDs is a Horizon Europe project with the goal to develop an image-based characterisation (ACCORDs) framework for the holistic and correlative assessment of Graphene Family Materials (GFMs) as a representative of 2D materials to assess and predict the 2D material's risk on health and environment.

During the development of the ACCORDs framework, a data management workflow and infrastructure guarantees the organisation of data which has been used and generated throughout the project, thereby adhering to Findable, Accessible, Interoperable and Reusable (FAIR) principles. This data includes protocols, SOPs, generated images, results and collected metadata from partners, which is correlated to parameters throughout the project to ensure proper characterisation of the materials in the end. In particular, the infrastructure includes:

1. A data management and Knowledge Infrastructure (KI).
2. An image repository which allows the uploading of image data and image data sets in an organised and FAIR manner.
3. Metadata collection forms associated with the submitted data, including images, within the knowledge infrastructure.
4. An analysis tool, which characterises materials based on images.

This infrastructure allows the easy as well as user-friendly organisation of data within the ACCORDs project.

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[8] University of Oxford, UK
[9] Wageningen Food Safety Research, Netherlands
[10] Fundación Idonial, Spain

2. . Objectives

Our objectives are separated into the following categories:

The Knowledge Infrastructure

The knowledge infrastructure allows users to upload, share, search and download data. It includes:

- A Content Management System (CMS).
- A Database Selection using a relational database such as PostgreSQL.
- A Search Functionality.
- An Access Control using Django's authentication system.
- A User Interface using HTML and CSS.
- Continuous Integration/Continuous Deployment (CI/CD) to automate testing and deployment of updates to our knowledge base.

Image repository

We use OMERO as the image repository. It allows users to upload and organise image data, annotate metadata, access the images for analysis and to prepare them for publication.

Data collection forms

To ensure data to be FAIR, it is crucial to collect and annotate datasets with comprehensive metadata. This includes detailed annotation of image datasets to capture essential parameters effectively. To facilitate this process and enhance user experience, we have developed an easy-to-use submission form, aligning with the Recommended Metadata for Biological Images (REMBI)[2] guidelines. This approach streamlines the metadata collection process, ensuring that the datasets are both rich in information and standardised across the project.

Image analysis

For feature extraction from images, we aim to analyse these images to identify and quantify various components such as graphene, functionalized graphene and the supporting film. The analysis is designed to detect features such as particle sizes and their distribution, edge roughness of particles, porosity of materials at a granular level, particle overlap and various artefacts including overcharging artefacts, preparation artefacts and issues related to morphology characterisation.

3. Ongoing activities

Knowledge Infrastructure

The KI was established as visualised in Figure 1 and above mentioned features are being implemented.

Fig. 1: The ACCORDs knowledge infrastructure portal.

OMERO image repository

The OMERO image repository is set up as visualised in Figure 2 and can be accessed through the ACCORDs KI. First datasets have been uploaded. We are currently working on standardising data to make it more «FAIR» and to implement automated uploading of images and annotated metadata.

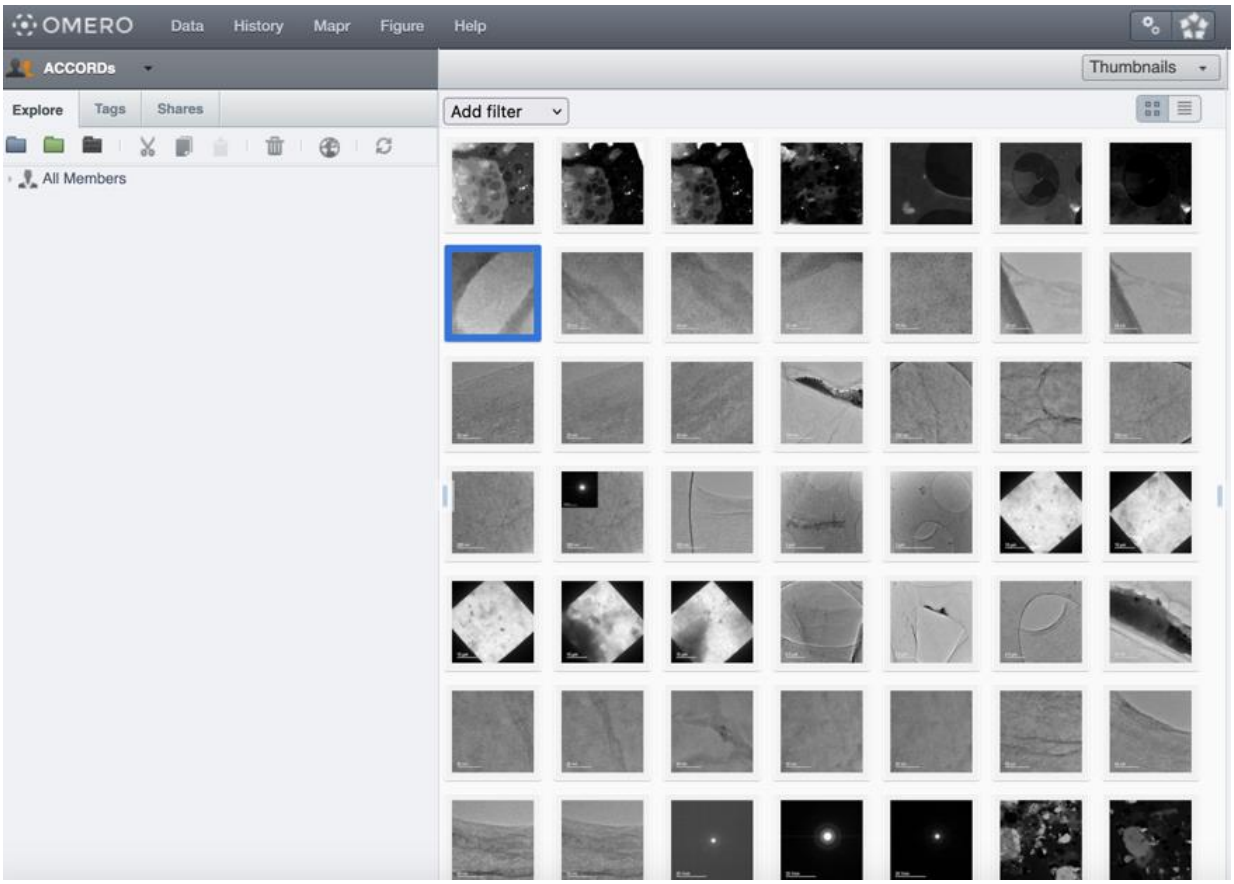


Fig. 2: Initial image dataset generated on ACCORDs and uploaded to the OMERO image repository.

Data Collection Forms

We streamlined the data collection process by implementing REMBI guidelines and incorporating partner feedback to ensure all essential details are captured. Our method involves analysing REMBI guidelines, categorising them into distinct, non-redundant entities for a database schema, and adding unique identifiers. We then structured the data collection into phased, related entries, creating Google Forms for each phase to gather partner feedback , illustrated in Figure 3. Next, we plan to integrate these forms into the ACCORDs knowledge Infrastructure for data submission by partners.

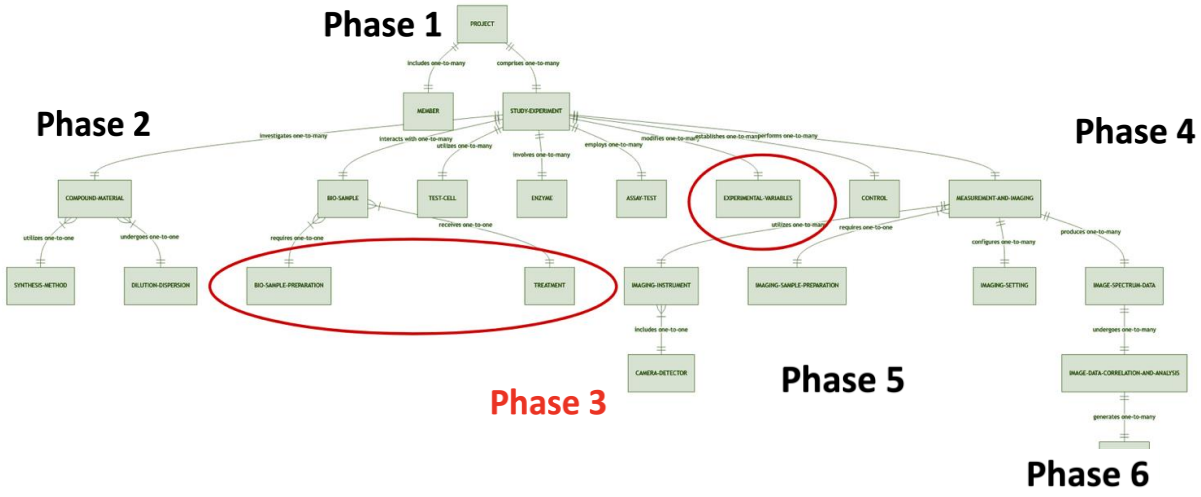


Fig. 3: Identification of the different entities throughout the project. Related entities are grouped into phases, which are then implemented in online forms.

Image Analysis

We started with thresholding methods for segmentation to create a dataset with labelled pixels, facilitating the training of machine learning segmentation models. This technique is valuable for developing a small, labelled dataset for trainable segmentation, utilising pixel labelling techniques and region labelling techniques. In scenarios where the dataset is unlabeled or when facing increased complexity, unsupervised deep learning becomes a viable option. This approach requires a substantial number of example images but eliminates the need for pre-labeled data. On the other hand, for more structured and detailed analyses, we plan to adopt supervised deep learning, which depends on a large repository of labelled data for effective training. Examples of results from the ongoing image analysis work are illustrated in Figures 4 and 5.

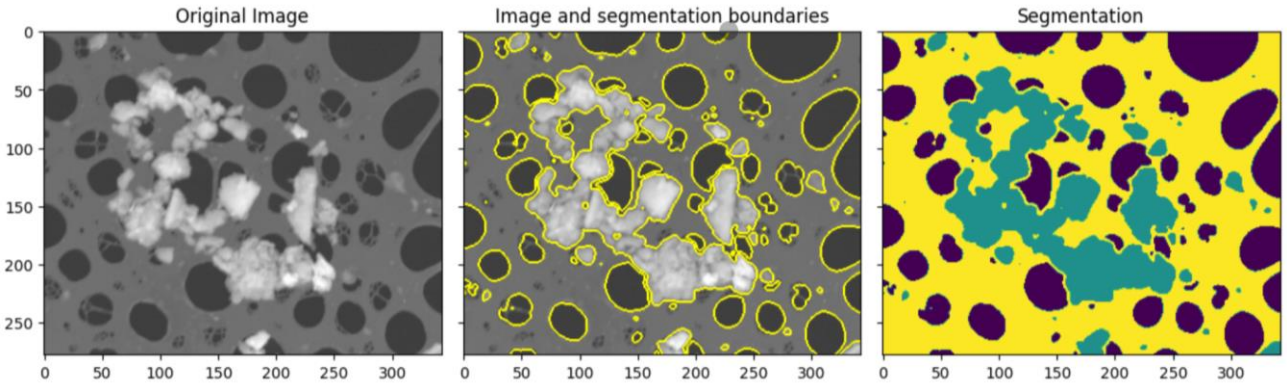
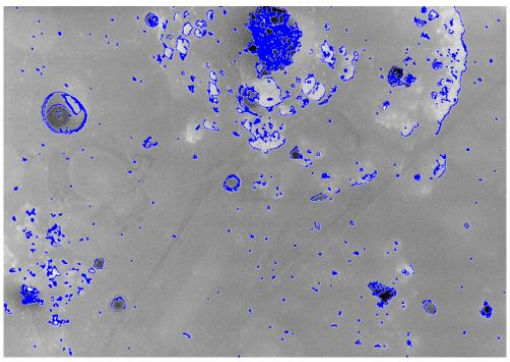
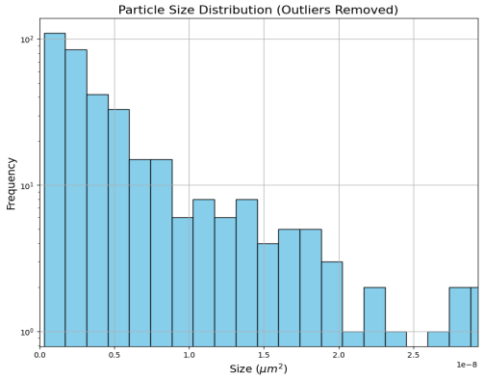


Fig. 4: Results from combining pixel labelling and region labelling techniques using thresholding approaches. Subsequently, trainable segmentation was used to label all pixels in the image to identify the different components within the image.






```
Image: AC_UT_GO_02-01.tif | Magnification: 1KX
Mean size: 1.3698655913978494e-08
Median size: 2.9000000000000003e-09
Standard Deviation: 9.278423533203485e-08
Range: 1.5988000000000003e-06
Mode: 1.4000000000000001e-09
Coefficient of Variation: 6.773236433901169
25th, 50th, 75th, 90th Percentiles: [1.600e-09 2.900e-09 6.725e-09 1.638e-08]
Skewness: 14.980263689027604
Kurtosis: 239.10658261317715
Geometric Mean: 3.768411030672972e-09
Geometric Standard Deviation: 3.026247069018761
```

Fig. 5: Analysis of Scanning Electron Microscope (SEM) images using an automatic thresholding technique. This method finds a threshold that minimises the intra-class intensity variance or, equivalently, maximises the inter-class variance, to detect flakes and obtain the particle size distribution within the image.

4. Expected Outcomes

The outcome of the work will be a knowledge infrastructure where documents such as protocols, SOPs and other data can be uploaded, searched for, shared and downloaded in a FAIR way. Data will be annotated to images which are stored in the OMERO image repository where they can be processed for publication and accessed for analysis. An overview over the workflow and infrastructure is given in Figure 6.

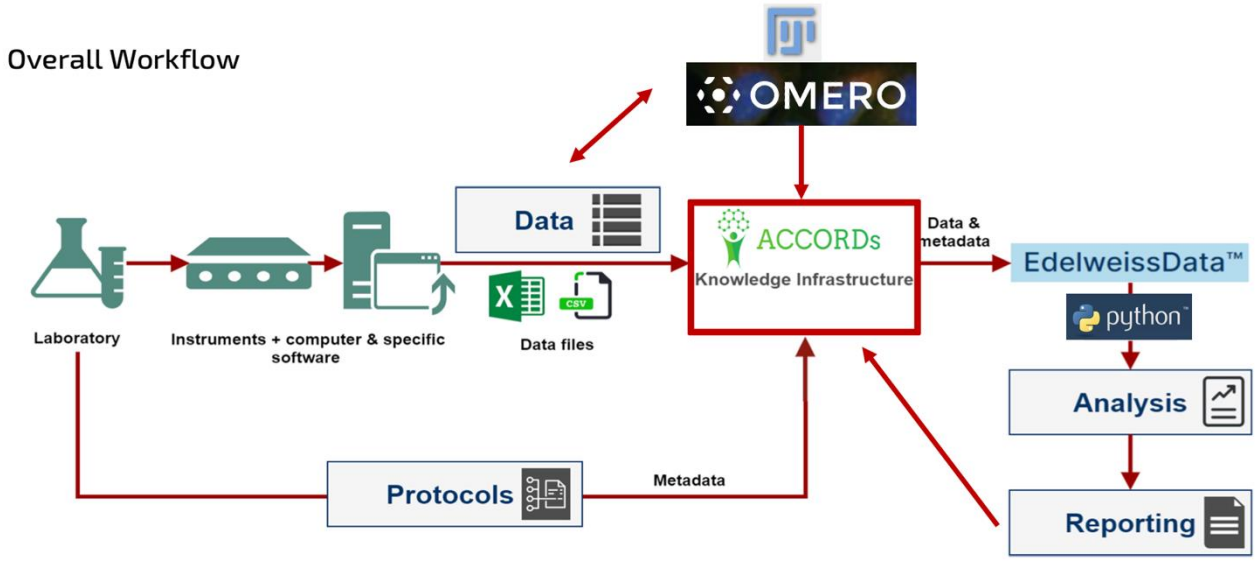


Fig. 6: ACCORDs workflow and infrastructure: Data is collected and organised in a knowledge infrastructure based on FAIR principles. It is related to images stored in OMERO as image repository. Data will also be accessible with computational tools for analysis and reporting.

5. Acknowledgements

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Funded by the European Union. Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union or European Health and Digital Executive Agency (HADEA). Neither the European Union nor the granting authority can be held responsible for them.

Associated Partners (i.e. (a) Swiss Partners and (b) UK Partners) have received national funding from (a) the Swiss State Secretariat for Education, Research and Innovation (SERI), and (b) Innovate UK.

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Domain-Specific Language (DSL) for Nanomaterial Representation

Kostas Blekos[1], Effie Marcoulaki[1]

1. Introduction

Nanoinformatics can benefit from standardized nanomaterial representations to depict the unique complexity and variety of possible nanoforms and their dynamic nature. This work introduces a new metalanguage designed as a domain-specific language (DSL) to address these challenges and support knowledge sharing. Our motivation stems from the limitations of existing NM representations, which struggle to encapsulate the vast diversity of NM compositions, sizes, shapes, surface chemistries, etc. and also address the nanoparticle dynamics.

2. Methodology

We employed a methodology centered around defining specific objectives crucial for the DSL's development, including the accurate portrayal of NMs' structural and morphological features without necessitating major future revisions. The DSL prototype is built upon the essential components identified in [1]. The language's specification, articulated in Backus-Naur Form (BNF), ensures a comprehensive and extensible schema, laying the foundation for detailed nanomaterial descriptions.

3. DSL Capabilities

Our proposal illustrates the DSL's capacity for nuanced representation, able to consider the distributions of NM composition, morphology, size etc., interfaces and hierarchical structuring, modifications, and the relationships among different NM entities. The proposed DSL provides a flexible implementation framework to describe relationships between different states of a NM and information on the transitions between those states, extending to the description of NM dynamics, evolution and interactions.

4. Discussion

The discussion highlights the DSL's potential to advance nanomaterial documentation, offering significant advancements over conventional representation systems, by enhancing data management and query capabilities, and providing a robust framework for representing both fundamental and complex aspects of nanomaterials. This is crucial since NMs are rarely found in their pristine (i.e., as synthesized) forms and they constantly evolve through interactions and through their integration with biofluids, the environment etc. Poor consideration of these dynamic phenomena may reduce the accuracy of predictive nanoinformatics models [2].

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5. Conclusions

This work aims to initiate a discussion for a collaboration to develop and implement a standard representation able to capture the real particle dynamics using the proposed DSL-based approach.

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NanoPharos: Collection, curation & organization into machine-readable format of NMs data

D. Zouraris[1,2], A. Tsoumanis[1,3], A. G. Papadiamantis[1,2,4], G. Melgaraki[5], I. Lynch[2,4], A. Afantitis[1,2,3]

1. Introduction

NanoPharos (https://db.nanopharos.eu/) is a carefully designed database to store and organise data on the environmental health and safety of nanomaterials (nanoEHS). The datasets can be curated from literature, experimentally generated, or computationally derived either from 1st principles (so-called physics-based models) or using data-driven modelling approaches including machine learning, in accordance with the FAIR principles[1] (Fig. 1). The initial rationale of NanoPharos was to create a database to fill a gap for nanoinformatics modelling of nanomaterials properties, interactions, and impacts (adverse outcomes or mechanistic toxicity assessment utilising in vitro or in vivo assays). NanoPharos provides modelling-ready tab-delimited datasets that can be directly imported into computational workflows and software, such as the Isalos Analytics Platform or KNIME using, e.g., the Enalos+ KNIME nodes.

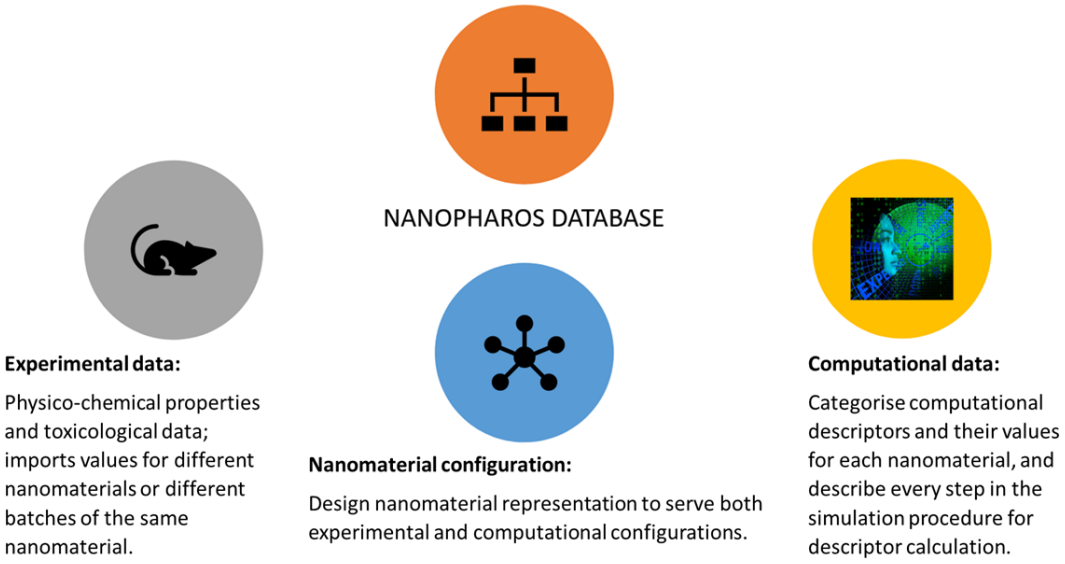

Figure 1: NanoPharos allows capture, storage, harmonisation and programmatic access to experimental and computational datasets relating to nanomaterials environmental health and safety (nanoEHS).

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[5] Division of Physical Sciences and Applications, Hellenic Military Academy, Vari 16672, Greece

2. NanoPharos Features

The NanoPharos database has several features and innovations that distinguish it from other databases, including:

Structured and FAIR-Compliant Framework

NanoPharos streamlines nanomaterials research with a FAIR-compliant framework, accelerating nanoEHS discoveries. Its high-quality ready for modelling datasets bridge a crucial nanoinformatics gap, enabling efficient and accurate analysis through platforms like KNIME (Fig. 2).

Dynamic Nanomaterials Management

NanoPharos adeptly tracks the variability and transformations of nanomaterials by defining separate batches and environmentally altered versions, linking them to a "parent" material. This tracking is supported by the European Materials Registry (ERM)[2] and NanoInChI identifiers which captures key features like composition and morphology[3].

Computational Analyses and Descriptor Enrichment

NanoPharos enhances nanomaterial data with computational descriptors for detailed characterization and facilitates *in silico* cytotoxicity prediction models. For instance, it used a dataset of 14 metal oxide nanomaterials with 62 descriptors to create a validated cytotoxicity model[4].

Inclusion of Omics Data and Comprehensive Data Spectrum

The extension of NanoPharos to include omics data marks a significant advance, covering the full spectrum of data needed for *in silico* exploitation of nanoEHS data. This comprehensive approach enables users to query and group datasets based on various criteria, facilitating detailed studies on nanomaterial impacts.

Iterative Improvement and Curator Engagement

NanoPharos evolves via continuous updates and curator collaboration, incorporating feedback and the latest research methods. An automated system for adding computational results into the database further enriches it with new insights and predictions.

3. Updates and Expansion Plans

NanoPharos plans to enhance its FAIR compliance and usability by introducing application programming interfaces (APIs) and KNIME nodes for better machine findability and actionability. Integrating ontologies like eNanoMapper and CheBI will make data and metadata machine understandable, fostering links between datasets and their corresponding nanoinformatics models, thus enhancing their FAIRness. Efforts are also being made to create a searchable registry for data and metadata, with the aim of certifying NanoPharos as a Trusted Repository under CoreTrustSeal or ISO16363 standards.

4. Recently Added Datasets and their added value to NanoPharos.

The addition of new datasets, including detailed examinations of Log*P* measurements for noble metal nanoparticles (NPs), PFOS adsorption efficiency by Gold NPs under varying pH conditions, reactive oxygen stress (ROS) induction by Gold NPs in HEK293 cells, zeta potential measurements for various NPs, and studies on the cellular uptake of NPs by A549 and HEK293 cells, represents a significant enrichment of the NanoPharos database.

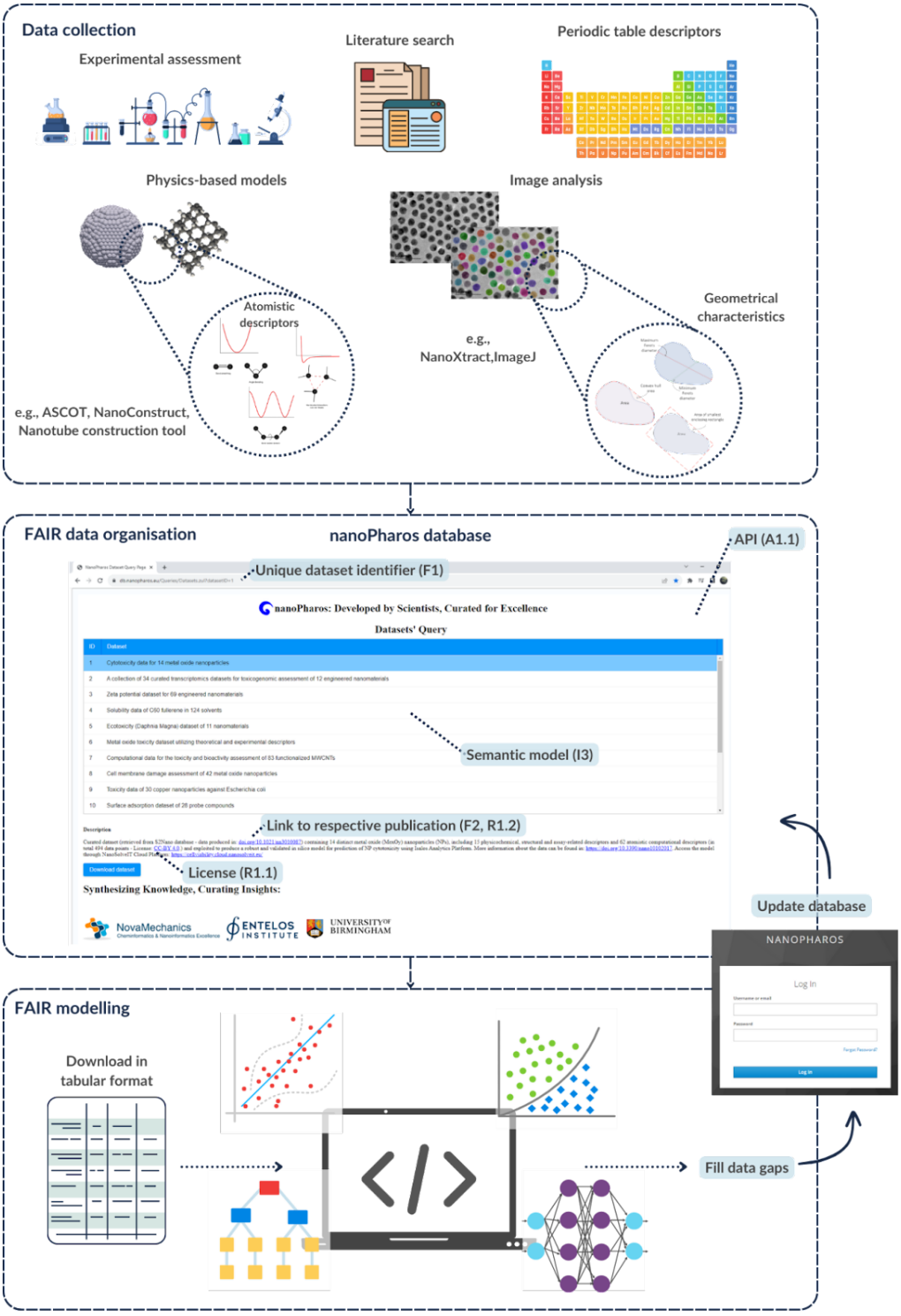

Figure 2: Schematic workflow for FAIRification of experimental and computational nanoEHS data via NanoPharos.

These datasets provide comprehensive physicochemical properties, bioactivity measures, and detailed insights into the interactions between nanomaterials and biological systems, serving several key purposes:

- **Enhanced Predictive Modelling Capabilities**: The computationally enrich datasets, enhance the accuracy of models predicting nanomaterial behaviour in environmental and biological contexts, advancing NanoPharos's support for research across environmental science to nanomedicine.
- **Facilitation of Interdisciplinary Research:** The structured, FAIR-compliant data format ensures their versatility and reusability across computational and analytical studies, reinforcing NanoPharos as a key nanomaterials research tool and promoting the safe development and use of nanotechnologies.
- **Promotion of Data Reusability:** NanoPharos offers open-access, harmonized data ready for modelling, greatly reducing entry barriers for researchers in nanomaterials safety and risk assessment, where gathering experimental data is often expensive and time-intensive.
- **Support for Environmental and Health Safety (EHS) Research**: Incorporating data on PFOS adsorption efficiency and ROS induction by nanomaterials provides essential insights into their environmental uses and potential toxic effects. This information is vital for creating nano-enabled solutions for water treatment, pollution reduction, and understanding of nanomaterials toxicity.
- **Advancement of Nanomedicine**: Datasets detailing the cellular uptake of nanomaterial by A549 and HEK293 cells are crucial for nanomedicine, shedding light on how physicochemical traits affect cellular interactions, essential for crafting efficient drug delivery systems, therapeutics, or diagnostics.

5. Conclusions

NanoPharos is an increasingly important database for nanoinformatics and nanosafety research, adhering to the FAIR (Findable, Accessible, Interoperable and Re-usable) principles for easy data access and sharing. It offers comprehensive tracking, detailed analysis, and diverse data, utilizing unique identifiers like ERM and NanoInChI for accuracy. Recent updates have enhanced its utility across various scientific fields, facilitating collaborative research, data reuse, and safety assessments. As it evolves, NanoPharos increasingly becomes vital for nanotechnology safety efforts.

This research was funded by the European Union's H2020 Marie Skłodowska-Curie Actions via CompSafeNano under (Grant Agreement n° 101008099).

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Session 6: Frameworks & Methodologies for Materials Safety & Sustainability

This session will focus on the requirements to establish the relevant ecosystem for the safe and sustainable materials R&I focusing on (policy) frameworks and their implementation measures. This includes:

1. the upstream conduct of the R&I, scale-up of innovative products and processes, their safety assessment (experimental and in silico) using model and alternative organisms and new approach methodologies (NAMs), and life cycle sustainability analyses (LCSA), or either one of its components, such as environmental LCA, life cycle costing (LCC), and social assessment (S-LCA), material flow analyses (MFAs), and eco-design;
2. the challenges related to downstream (re-)use, and possible re-and up-cycling at their end-of-life; and
3. development, validation, standardisation, and harmonisation of test methods applicable to (advanced) materials and their application in risk assessment.

Presentations (oral and poster) will also cover the following topics:

- Contributions to the implementation of the Safe & Sustainable-by-Design (SSbD) framework: case studies for applications and interdisciplinary insights,
- OECD Test Guidelines & Guidance Document development and implementation Strategies for Advanced Materials,
- Standardisation of methods, materials, models, workflows, definitions (e.g., CEN/ISO),
- Upstream R&I conduct: eco-design,
- Downstream R&I: challenges to LC(S)As, and end-of-life (recycling),
- Scaling-up of R&I best practices,
- Development of (innovative approaches/non-animal assays) methodologies and their incorporation into the hazard identification and risk assessment process, and
- Best practices on LCA screening early in the R&I.

Detailed Programme

Start	End	Title	Presenter
09:20	09:35	PARC roadmap for nanomaterials – exploring how PARC can contribute most usefully	Iseult Lynch
09:35	09:50	NANOMESUREFRANCE: A Single Entry Point for Structuring the Nanomaterials Industry around Comparable and more Reliable Data	Georges Favre
09:50	10:05	Utilizing In vitro cytotoxicity data of advanced material in life cycle assessment and human risk assessment	Peter Wick
10:05	10:20	Making OECD Test Guidelines applicable for Nanomaterials and Advanced Materials – Activities by the Malta Initiative and MACRAMÉ	Elisabeth Heunisch

10:20	10:40	24/7 Poster Presentations	
11:00	11:20	The EC Safe & Sustainable by Design (SSbD) framework: Towards the improvement of its relevance, reliability and operability	Irantzu Garmendia Aguirre
11:20	11:35	Safe and Sustainable by Design Strategies for the H2020 SUNSHINE case studies	Arianna Livieri
11:35	11:50	Decision Support System for SSbD in the early innovation stages	Wouter Fransman
11:50	12:05	Challenges in Predictive Sustainability Assessment of Novel Lubricants following SSbD Principles	Jonas Hoffmann
12:05	12:20	Safe and sustainable by design roadmaps. A glimpse of the ASINA case studies	Furxhi Irini
12:20	12:35	Advances and challenges of Safe-andSustainable-by-Design: The case of high-entropy alloy coatings	Adamantia Kostapanou
12:35	12:50	Towards a nano-specific, quantitative based and human centric-SSbD Approach: Antibacterial nanocoatings case study	Massimo Perucca
12:50	13:00	24/7 Poster Presentations	

Posters

S06_P02	From Science to Regulation – The NanoHarmony White Paper on Test Guideline Development	Eric A.J. Bleeker
S06_P03	Dustiness testing of high aspect ratio nanomaterials and its use for exposure assessment – towards an OECD Test Guideline	Carla Ribalta
S06_P04	Adapting current in vitro ecotoxicity standard methods to allow more realistic and environmentally relevant exposure conditions	Alberto Katsumiti
S06_P05	New approach methodologies (NAMs) for hazard assessment of chemicals and materials at human biological barriers	Beatrice A. Brugger
S06_P06	Testing nanomaterials in complex 3D in vitro lung models	Emma Arnesdotter
S06_P07	An improved ALI exposure chamber for higher deposition efficiency and optimized operations	Pamina Weber

S06_P08	In Vitro Effect Extrapolation for Human Risk Assessment of Advanced materials	Jimeng Wu
S06_P09	Boron nitride nanosheets can trigger lipid-mediated autophagy in lung alveolar epithelial cells	Tina Buerki-Thurnherr
S06_P10	Form-specific prospective environmental risk assessment of graphene-based materials in European Freshwaters	Hyunjoo Hong
S06_P11	Biological reactivity assessment of graphene oxides	Veno Kononenko
S06_P12	Risk management tool	Blanca Maria Pozuelo Rollon
S06_P13	Advancing the development of Safe-and-Sustainably-by-Design toolboxes for advanced materials: similarities between the SUNSHINE Tier 1 SSbD approach and Early4AdMa Tier 2	Lisa Pizzol
S06_P14	Learning from Safe-by-Design for Safe-and-Sustainable-by-Design: Mapping the current landscape of Safe-by-Design reviews, case studies, and frameworks	Akshat Sudheshwar
S06_P15	Applying the SSbD framework for the development of bio-based PFAS alternatives for textile and packaging sectors – The ZeroF case study	Panagiotis Isigonis
S06_P16	Respiratory deposition estimates of airborne perand poly-fluoroalkyl acids (PFAS) powered by Enalos Cloud Platform	Dimitris G. Mintis
S06_P17	Investigating the influence of nanomaterials metal composite ratios on the toxicity and intracellular uptake in epithelial cell lines	Kailen Boodhia
S06_P18	Establishing the methodological basis for environmental, health and safety (EHS) impacts assessment- The SUNRISE approach	Alberto Katsumiti
S06_P19	Implementation of Safe-by-Design (SbD) and Safer and Sustainable by Design (SSbD) within the Health, Safety and Environment (HSE) Risk Research Platform in South Africa	Mary Gulumian
S06_P20	ChemPharos: a comprehensive database of plastic-degrading enzymes, powered by Enalos Tools	Constantinos Papavasiliou
S06_P21	Integrated computational methods for the development of Safe and Sustainable-by-Design Innovative Advanced Materials: the case of surface modified nanophotocatalyst	Tomasz Puzyn

Oral Presentations: Session 6

PARC roadmap for nanomaterials – exploring how PARC can contribute most usefully

Iseult Lynch[1], Susana Loureiro[2]

1. Introduction

The Partnership for the Assessment of Risks of Chemicals (PARC) is an interdisciplinary effort to develop next-generation chemical risk assessment approaches to protect human health and the environment [1]. It supports the European Union's Chemicals Strategy for Sustainability and the European Green Deal's “Zero pollution” ambition with new data, knowledge, methods, tools, expertise and networks.

Building on a previous human biomonitoring (HBM) project (HBM4EU), PARC has prioritised a set of chemicals for evaluation in years 1-3, with additional prioritisation underway for years 4 onwards. Nanomaterials and advanced materials were identified by several stakeholders as an important priority of focus for the coming years. To facilitate this, and ensure that PARC’s efforts enhance ongoing activates (e.g., funded under Horizon Europe, and member states activities) rather than duplicating work, a first step in the process will be to undertake a landscaping exercise and to develop a RoadMap for Nano and Advanced Materials in PARC. As with all major chemical groups and methodologies being addressed in PARC, chemical leads have been appointed to develop the nanomaterials roadmap, and will work with stakeholders, relevant ongoing projects (via the PARC SynNet efforts to drive synergies between PARC and related relevant projects, and beyond) and via the networks of PARC partners, many of whom also work with nanomaterials or advanced materials.

2. Developing the PARC nanomaterials roadmap

Many of the unique properties and applications of nanoscale materials arise from the duality whereby nanomaterials have properties of bulk material (*intrinsic properties*) coupled with properties driven by their highly reactive surface chemistry which are dependent on the nanomaterials surroundings (pH, ionic strength, ion composition, available biomolecules) and are thus *extrinsic* or context dependent properties [2]. Nanomaterials are defined by their chemistry, size, shape, and surface properties, and by a wide-range of calculated descriptors arising from their elemental composition [3].

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The challenges in describing nanomaterials, and making nanosafety research data FAIR arise from a number of sources including: (i) the interdisciplinarity of nanosafety (which spans materials science, chemistry, analytical exposure and toxicology both human and environmental) which results in (ii) an enormous breadth of data types including materials characterisation, environmental transformation and fate and effects data, (iii) the fact that there are many nonstandard (mechanistic-focussed) methods including many which are highly data-intensive such as "omics" and high content screening approaches, (iv) the variety of measurement principles and experimental setups from *in vitro* to *in vivo* to mesocosm and field scale experiments, and (v) the evolving requirements from new research foci such as safe and sustainable by design of materials [4]. Recent example of approaches that require largescale data re-use are materials modelling [5], safe by design modelling of nanomaterials [6], and optimising the safe use of nanotechnologies through re-use of nanosafety data to support the achievement of the UN Sustainable Development Goals [7].

PARC has a number of landscape mappings underway, related to capacities and facilities across PARC partners for example, as well of the data landscapes related to different chemicals. Utilising the methodology and approaches used for mapping of capacities, and building on the experiences of the other Chemical Leads, the PARC nanomaterials leads will establish a working group to perform a landscape mapping of existing nanomaterials and advanced materials knowledge to the PARC activities to identify areas where maximum synergy can be achieved, through collaboration with existing activities and/or through bespoke PARC-led activities to supplement ongoing activities and gap-fill areas where no current activity is occurring and which maps to PARC overarching priorities of regulatory relevance for chemicals risk assessment.

Given the leadership demonstrated by the nanosafety research community in developing tools and solutions to support both FAIR (Findable, Accessible, Interoperable and Re-usable) data and for Safe (and Sustainable) by Design (SSbD), as well as the match of these activities to dedicated efforts in PARC (WP7 for FAIR data and WP8 for SSbD, see also the Tools and Resources section of the PARC website), it is clear that these two aspects will form a key focus for the landscape mapping and synergy development. Demonstration of the translation of research findings *from* nanomaterials safety and tools developed for nanomaterials *to* advanced materials research will also be a key focus. All outcomes of the Nanomaterials Roadmap will be made FAIR and open also, in line with the ambition of PARC to make all datasets accessible and reusable for research and risk assessment purposes, as part of an "Open Science" approach that takes into account ethical, legal and confidentiality considerations, following the "as open as possible, as closed as necessary" principle.

3. Conclusions

The initial inputs and prioritisation for the PARC nano- and advanced materials landscape mapping and roadmap for PARC activities will be presented, and MaterialsWeek participants will have the opportunity to feed into the activity in order to shape the work undertaken in Years 4-7 of PARC and where these can have a strong

focus on nanomaterials and advanced materials. A strong focus on synergies (managed through PARC SynNet will also be facilitated via interactions at MaterialsWeek.

4. References

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NanoMesureFrance: A Single Entry Point for Structuring the Nanomaterials Industry around Comparable and More Reliable Data

Georges Favre[1], François-Xavier Ouf[1]

1. Introduction

Nanomaterials are formidable sources of innovation and are used in all industrial sectors. However, their development is hampered by the fact that the reproducibility of industrial production processes is difficult to achieve [1], a lack of harmonisation in their definition [2], regulatory requirements for which harmonised test methods are not always available, and an often negative perception by society [3].

The lack of traceability [4] regarding the use of these substances, the risks of which are sometimes still poorly assessed, and the relative fragmentation, within the sectors concerned, of the players involved do not favour the establishment of a context conducive to the marketing of products incorporating nanomaterials.

These various obstacles are partly due to the difficulties in obtaining reliable and comparable testing data, while the characterisation of nanomaterials is a complex task.

2. The NanoMesureFrance initiative

The NanoMesureFrance initiative [5] has been launched in 2022 to help moving forward on these issues. It is a French public/private partnership, led by LNE and supported by the French State and the Île-de-France region.

It aims to create a sustainable non-profit association to strengthen confidence in nanomaterials and associated innovations by bringing together interested stakeholders (producers and users of nanomaterials, instrument manufacturers, service providers, academic laboratories and platforms) to build collective answers to the main issues and priorities identified. The association was co-founded by LNE, France Chimie (professional organisation representing companies in the chemical sector in France) and FEBEA (professional association for the cosmetics sector) and already gathers 47 members.

NanoMesureFrance mainly focuses on harmonisation and validation of the tools and methods needed to better identify nanomaterials in a regulatory perspective and to characterise their key physico-chemical properties at different stages of their life cycle. The main actions consist of:

- production of documents proposing harmonized approaches upstream of standardization
- sharing information and best practices
- promoting inter-laboratory comparisons initiatives

[1] NanoMesureFrance Association & French National Metrology and Testing Laboratory (LNE)

- liaising with key players, networks and initiatives working in the field of pre-standardization of characterization and testing methods (VAMAS, EURAMET, OECD/WPMN, Malta Initiative, JRC...).

3. NanoMesureFrance action to improve the identification of nanomaterials

Among the various issues identified within the different Association's WGs, the question of better identification of nanomaterials was seen by members as a key issue. This is indeed the first step in determining the regulatory requirements to be applied, and the corresponding testing methodologies to be implemented.

While this stage is relatively straightforward for a number of particulate substances, there are many cases where difficulties still arise. There are indeed different situations where even the microscopy ***Confirmatory Step*** recommended in JRC guidance when screening methods are inconclusive is not sufficient to draw a definitive conclusion regarding the determination of the potential ***Nanomaterial*** status of particulate substance. Furthermore, the existing documents to help advance the process of identifying nanomaterials are aimed at people who have a technical basis to take them in hand, which is far from being the case when regulatory people interact with their suppliers, potentially outside Europe. These documents are also very often too long for SMEs to be able to absorb their content due to lack of time and/or adequate expertise. It is therefore very complicated for them to judge the relevance of the data provided to support the classification as non-nanomaterial of certain substances and the provision of simple documents allowing them to ask the right questions with a view to challenging their suppliers proves useful. A number of documents are currently being developed within the Association's WGs to help all stakeholders make progress on the subject, and to suggest avenues for improvement.

4. Conclusions

The NanoMesureFance Association works to build harmonized approaches to produce and access improved quality test data on nanomaterials. The diversity of the 47 members of the association in terms of profile (start-up, SME, big companies, academic or government laboratory, etc.) or sectors (materials, cosmetics, nanomedicine, instrumentation, waste treatment, construction , transport, services etc.) shows the relevance of the approach and the benefit of building links between stakeholders to break down barriers.

Significant efforts are being made to improve the identification phase of nanomaterials at the basis of their traceability in value chains, but the characterization of their main physicochemical properties is also the subject of specific actions.

[1] https://nanofabnet.eu/

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Utilizing In vitro cytotoxicity data of advanced material in life cycle assessment and human risk assessment

Peter Wick[1], Jimeng Wu [1,2], Bernd Nowack[2]

1. Introduction

Over the past three decades, the field of advanced materials (AdMa) has evolved significantly, positioning itself as a key enabling technology in the 21st century. Despite acknowledging their benefits, concerns have arisen about potential adverse environmental and health effects, primarily due to the distinctive risks of involuntary exposure and unique toxicity profiles associated with AdMa compared to bulk materials [1]. To address these challenges, the integration of toxicological data with general risk methodologies, such as Risk Assessment (RA) and Life Cycle Assessment (LCA), is crucial for early risk identification [2].

Traditionally, RA and LCA have relied on epidemiological or in vivo toxicological data assessing dose-response relationships. However, the transition from phenomenological to more cell based mechanistic toxicological studies demands a proactive adaptation of risk methodologies to accommodate the newly evolving data sources and types. [3]. The *in vitro* technologies are starting to anticipate this complexity by moving from cancer cell lines to primary human cells, from monocultures to co-cultures, from 2D to 3D systems, and from static to dynamic conditions, creating novel systems such as organs-on-a-chip mimicking the physiological environment of the cells. Thus, this shift requires an adaptation of risk methodologies to accommodate evolving data sources and types, minimizing reliance on animal testing [4].

Despite significant strides, establishing a comprehensive strategy for a quantitative assessment of the hazard impacts of advanced materials, using available non-animal data and in silico models, remains a challenge [5;6]. Our objective is to explore pathways towards quantitative In Vitro In Vivo Extrapolation (QIVIVE) of AdMa, emphasizing the integration of in vitro data into hazard assessment for a next-generation toxicity evaluation.

Building upon our previous work, which identified the combination of in vitro dosimetry and lung dosimetry as a mature approach for QIVIVE, particularly for inhaled particles affecting the lungs (Romeo, et al., 2022), we have developed a simplified model for inhaled spherical nanomaterials and their impact on the lungs to extract toxicity effect factors (Romeo, et al., 2022). Additionally, our research extends to Machine Learning and Quantitative Structure-Activity Relationship (QSAR) models, exploring their potential to predict in vitro activity of Graphene-related Materials (GRMs)(Romeo, et al., 2022).

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Given the development of in vitro techniques, our studies aim to bridge the gap between currently increasing in vitro data pool, RA and LCA.

2. Screening of in vitro to in vivo extrapolation methods

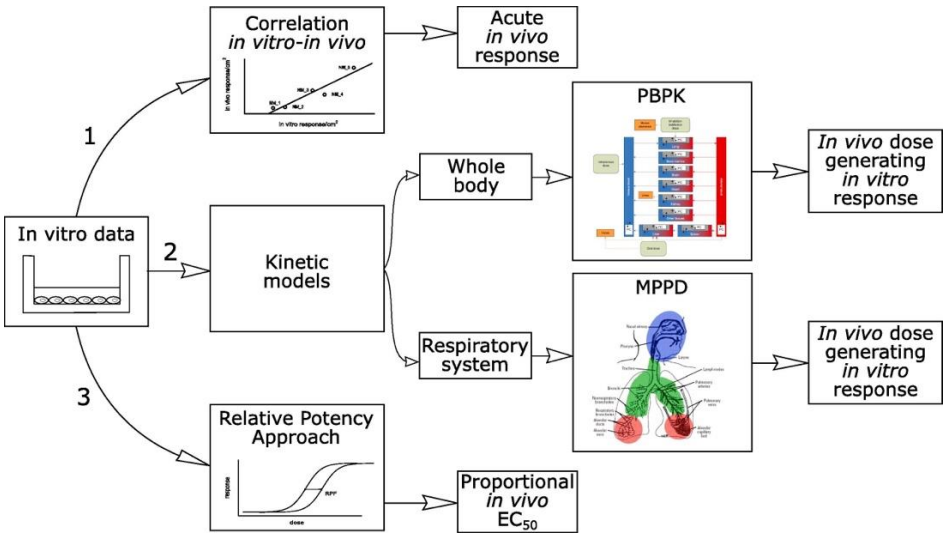

Figure 39: Pathways to extract in vivo information from in vitro data.

Utilizing mechanistic in vitro studies and in silico modelling, our objective is to bridge the gap between cellular responses and whole organism effects, as highlighted in [7]. The challenge lies in linking these two sets of information, for which there is currently no standard method. Our proposed solution involves three options, illustrated in the Fig.1.

We introduce the CoDo model [8](Romeo, et al., 2022), a novel approach that combines in vitro dosimetry and lung dosimetry to establish a link between in vitro doses and human intakes. Illustrated through a case study on titanium dioxide, the CoDo model effectively demonstrates realistic in vitro doses corresponding to exposure levels below 10 mg/m^3, highlighting its efficacy. A step-by-step procedure to calculate in vitro-to-in vivo extrapolation factors for estimating human Benchmark Doses and subsequent in vitro-based EFs for various inhaled non-soluble nanomaterials was developed [8] (Romeo, et al., 2022).

Except for in vivo benchmark dose extrapolation, we also step into the toxicity prediction using machine learning (ML) and QSAR. We have crafted a classification model to assess the viability effects of graphene-related materials (GRMs) [9] (Romeo, et al., 2022). The significance lies in comprehending potential adverse impacts on human health, particularly on the lungs, a sensitive exposure route. Employing ML approaches, we analysed in vitro cytotoxicity data derived from lung cell studies. Multiple regression models were employed to predict this endpoint based on material properties and experimental conditions.

3. Uncertainty space evaluation for hazard extrapolation

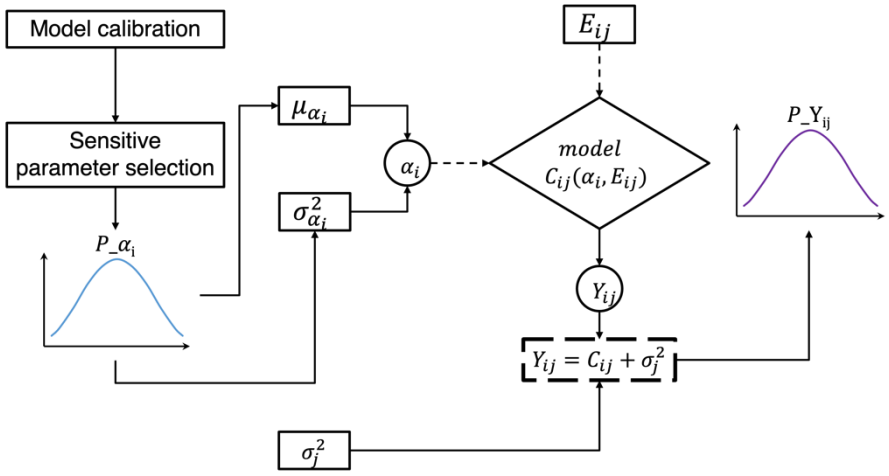

Figure 2: Bayesian Model Structure to evaluate the parameter uncertainties.

Bayesian statistical analysis serves as a crucial tool when dealing with the diversity of in vitro nanotoxicity datasets. Its utility extends to characterizing uncertainties originating from variations in experimental conditions, providing a resilient framework for comprehending the intricate dynamics of result variability. Through this analytical approach, we gain insights into the influence of these uncertainties on the extrapolation of safe AdMa concentration levels, a pivotal aspect of risk assessment. It enables the estimation and evaluation of these uncertainties, allowing for a nuanced examination of their impact on the estimation of in vivo effective doses.

This not only enhances the robustness of risk assessments but also contributes to a more informed and reliable understanding of the potential risks posed by nanomaterials to human health. In essence, Bayesian statistical analysis acts as a guiding compass in navigating the complexities of nanotoxicity assessment, providing a pathway towards more accurate and comprehensive risk evaluations.

4. Advanced in vitro methods as new source

As advancements in in-vitro technologies continue to progress, we anticipate a future where these cutting-edge methods could potentially streamline the existing procedures. The ultimate goal is to leverage advanced in vitro technologies directly for organ-to-human extrapolation, reducing intermediate steps and facilitating a more direct translation of in vitro data into in vivo effects. This paradigm shift envisions a time when in vitro data will be harnessed in a manner analogous to the current utilization of animal data, employing extrapolation methods to directly derive in vivo effects.

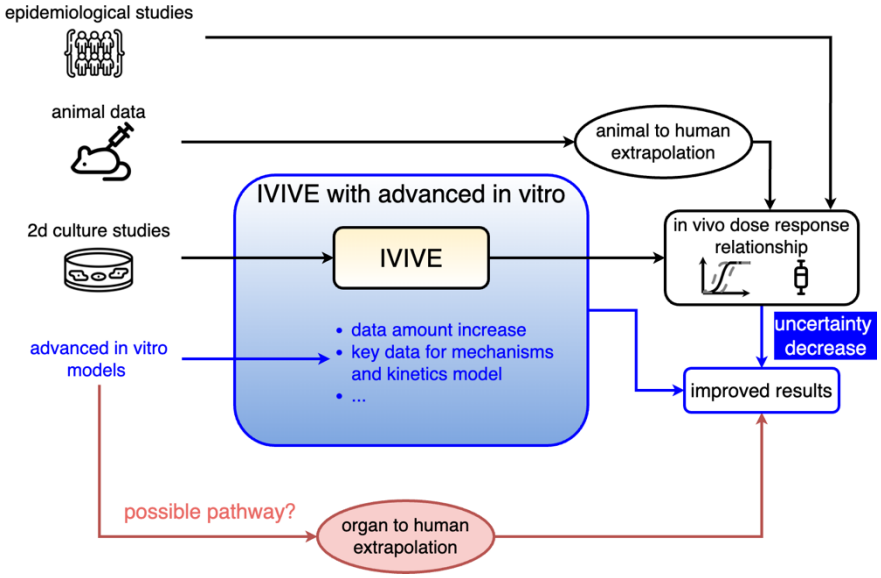

Figure 3: In vivo dose response relationship generation pathways from different data source

5. Conclusions

In conclusion, we are not yet there for a consistent and systematic calculation of in vitro-based EFs. However, we showed promising methods to calculate these factors and identified further steps are needed to reduce the uncertainty, improve and expand the results. Continued studies are needed to address remaining questions, with the future envisioning in vitro data usage comparable to current in vivo data through specific extrapolation steps.

6. Acknowledgment

Funding for this research was received from MACRAME (Grant agreement number – 101092686 and State Secretariat for Education, Research and Innovation (SERI) no 23.00141).

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Making OECD Test Guidelines applicable for Nanomaterials and Advanced Materials – Activities by the Malta Initiative and MACRAMÉ

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1. Introduction

Since 2017 the Mata Initiative has been working to update OECD Test Guidelines (TG) and Guidance Documents (GD). This work aims to ensure that TGs/GDs are applicable to nanomaterials and (other) advanced materials. OECD TGs are essential for industry and regulatory authorities involved in the testing and evaluation of chemicals. They help to ensure that legislation works.

2. The Malta Initiative Priority List

Ensuring that innovations in materials can come to the market and comply with regulations is important. This requires collaboration between experts from science, industry and authorities to set priorities for which test methods are required. In March 2024, the Malta Initiative released its Priority List[11]. This list will help ensuring that the required harmonised methods will become available in the near future for nanomaterials and (other) advanced materials.

The Malta Initiative Priority List is a list of prioritised actions to support the development and amendment of OECD TGs for nanomaterials and (other) advanced materials. It has the following aims:

- Helping make legislation implementable and supporting industry in effective regulatory compliance;
- Providing guidance to funders for the support required for the next generation of Test Guidelines;

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[5] Nanotechnology Industries Association aisbl, Belgium (NIA)
[6] University of Birmingham, UK (UoB)
[7] European Chemicals Agency, Finland (ECHA)
[8] Luxembourg Institute of Science and Technology, Luxembourg (LIST)
[9] TEMAS Solutions GmbH, Switzerland
[10] AcumenIST, Belgium (AIST)
[11] https://malta-initiative.org/what/#MI-Priority-List

- Encouraging scientists to develop the required methods and bring them through to OECD Test Guidelines; and
- Supporting the ongoing work of all Member Countries of the OECD relating to chemical safety.

3. MACRAMÉ contributions towards harmonisation and standardisation

The Horizon Europe project MACRAMÉ[12] develops advanced characterisation methodologies to assess and predict the health and environmental risk of advanced materials. MACRAMÉ focuses on inhalable carbon-based advanced materials, e.g. graphene-related materials and carbon nanofibers. The project aims to provide methodologies to assess the risk of these materials within a product matrix along the life cycle. MACRAMÉ identified 5 areas of test method development. For each of these roadmaps for harmonisation and standardisation were prepared.

The project therefore supports a number of the priorities identified in the Malta Initiative Priority List. Examples include the harmonisation and standardisation of specific dispersion protocols for graphene related materials for (eco-)toxicity testing. Other methods aim at detection of carbon-based materials in complex media, aerosol generation for inhalation studies, and in vitro/ex vivo models for inhalation toxicity testing.

4. Conclusions

The Malta Initiative Priority List clearly shows that the activities for making OECD TGs applicable for nanomaterials is still ongoing. Further research on safety testing for nanomaterials and (other) advanced materials is still needed. Researchers are encouraged to focus their attentions on the priorities identified. This should lead to advancing their research towards method validation, standardisation and harmonisation.

5. Funding

MACRAMÉ has received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No. 101092686.

[12] https://macrame-project.eu/

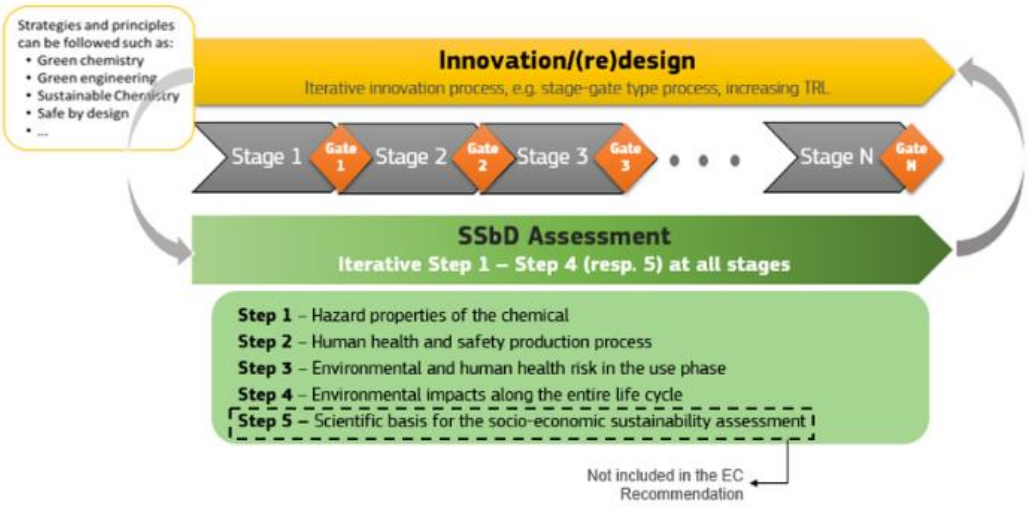
The EC Safe & Sustainable by Design (SSbD) framework: Towards the improvement of its relevance, reliability and operability

Irantzu Garmendia Aguirre[1], Kirsten Rasmussen[1], Hubert Rauscher[1]

1. Introduction

Key for the green industrial transition is the SSbD framework developed by the JRC [1] to ensure the development of chemicals, materials, processes and products that are safe and sustainable by design (SSbD).

The framework puts together safety, environmental sustainability and socio-economic dimensions for the first time. In addition, it requires that the safety and sustainability aspects are addressed together from the beginning, through the entire R&I (research and innovation) process, and with a life cycle perspective, shifting this way the current practice.



In order to improve the relevance, reliability and operability of the framework in R&I activities, the European Commission (EC) published in December 2022 a Recommendation establishing a European assessment framework for safe and sustainable by design (SSbD) chemicals and materials [2]. The Recommendation establishes a two-year testing period in which stakeholders are invited to test the framework and provide feedback.

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2. Conclusions

The 1st period for stakeholders to provide feedback was from 5 May to 30 June 2023. Responses were received from 24 different organisations comprising all relevant stakeholders (including European/national funded project consortia, and NGOs (non-governmental organisations)) to which the recommendation was addressed.

The feedback received from stakeholders reflected challenges based on experience as well as further guidance needs for the implementation of the framework. This includes specific guidance for the definition of the SSbD system in which the framework is applied and for the integration of the safety and sustainability assessment and the functionality in the innovation process.

Based on the experience gained since the publication of the framework and thanks to the feedback received in the 1st reporting phase established in the EC Recommendation, the JRC has published on the 14th of May 2024 the 1st SSbD methodological guidance [3] with the aim of providing support to SSbD practitioners.

3. Acknowledgements

The authors would like to acknowledge the past and present JRC colleagues who contributed to the development of the framework for safe and sustainable by design chemicals and materials, its first application to case studies and the development of the 1st SSbD methodological guidance: C. Caldeira, S. Sala, L. Farcal, L. Mancini, D. Tosches, J. Riego Sintes, A. Amelio, E. Abbate, G. bracalente, M. Bennet and D. Lipsa.

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Safe and Sustainable by Design Strategies for the H2020 SUNSHINE case studies

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1. Introduction

The European Chemicals Strategy for Sustainability and the Zero Pollution Action Plan identify the need to transition towards Safe and Sustainable by Design (SSbD) chemicals and materials. In this context, the H2020 SUNSHINE project has developed an approach to operationalize SSbD, specifically addressing advanced multi-component nanomaterials (MCNMs). The main goal of SUNSHINE is to develop and validate SSbD strategies for products enabled by MCNMs and to facilitate their implementation at an industrial scale. These strategies can be considered as action plans to identify, mitigate, and ultimately resolve hotspots identified through the application of sustainability assessment methodologies. This contribution presents the SUNSHINE SSbD tiered approach and its application to four industrial case studies.

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[13] *EMERGE Ltd, Sofia, Bulgaria*

2. Materials and methods

The SUNSHINE SSbD tiered approach is composed of two tiers. Tier 1 uses a scoring system to calculate indices for the different impacts and plot those on a chart that clearly visualizes safety and sustainability-related 'hotspots of concern' along the lifecycles of the materials/products which can be further assessed in Tier 2. Therefore, Tier 2 consists of LCA (Life Cycle Assessment), LCC (Life Cycle Costing), and S-LCA (Social Life Cycle Assessment) of the MCNMs and the products incorporating them in comparison with selected benchmark materials (Pizzol et al., 2023). The developed tiered approach has been tested on four advanced MCNMs . Since the approach is comparative, the assessed SSbD-modified material is always compared to a benchmark. Such a benchmark could be an alternative design option or a conventional material/product that has the same or a similar function.

The first material consists of a novel PFAS-free anti-sticking coating used in the bakery industry (i.e., coating of baking trays and pans), produced by the company Laurentia Technology SLL, which is compared to a conventional anti-stick coating (Teflon). The second, produced by the company Encapsulae S.L., consists of nano-drops of essential oil anchored at the surface of nano-clays and encapsulated in a polymeric film which keeps the packaged food free of insect pests. It is compared to conventional food packaging (LDPE). The third, produced by the company Avanzare Innovacion Tecnologica SL, consists of a nanocomposite of graphene oxide functionalized with chitosan which provides flame retardant properties and is compared to graphene oxide functionalized with casein, an alternative design option. Finally, the fourth, produced by the foundation CIAC (Centro de Innovación Andaluz para la Construcción Sostenible), is an additive for construction materials (i.e., mortar) based on zinc oxide and silica dioxide with photocatalytic decontamination properties (NOx gas removal), compared to a titanium oxide-based benchmark.

3. Results

Tier 1 is applied at the screening level in the early stages of innovation. Figure 40 shows the results that can be obtained, in terms of percentage of positive impacts to safety, functionality, and sustainability scores, for the innovative material and the benchmark. As a life cycle thinking approach is adopted, the safety, sustainability and functionality assessment is carried out by considering all life cycle stages: from raw materials acquisition up to the end of life (e.g., recycling, incineration). The blue columns report the results for the innovative material while the grey ones those for the benchmark. The light blue and light grey parts of the column show the relative uncertainty for both the innovative material and the benchmark. More specifically, results can be shown by life cycle stages (raw materials and resources needed to produce the material/product, production of the MCNM, production of the product incorporating the MCNM, use of the product, and end of life treatment) or by aspect (safety/environmental, social, economic sustainability/functionality).

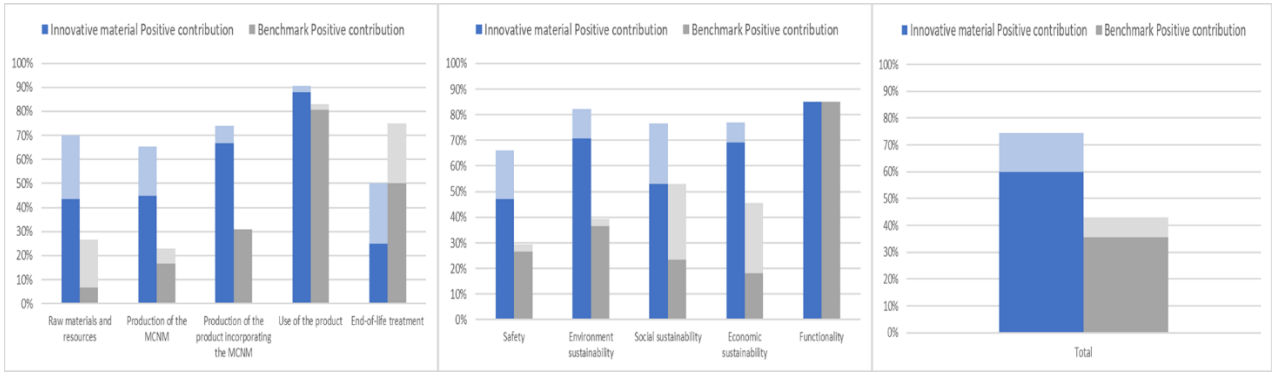

Figure 40 Percentage of positive contributions by life cycle stages, by aspect, and total.

Tier 2 instead, is applied at a more advanced level when the products are already developed and are ready to be released on the market as well as part of post-market evaluations. Example of Tier 2 results are reported in Figure 41.

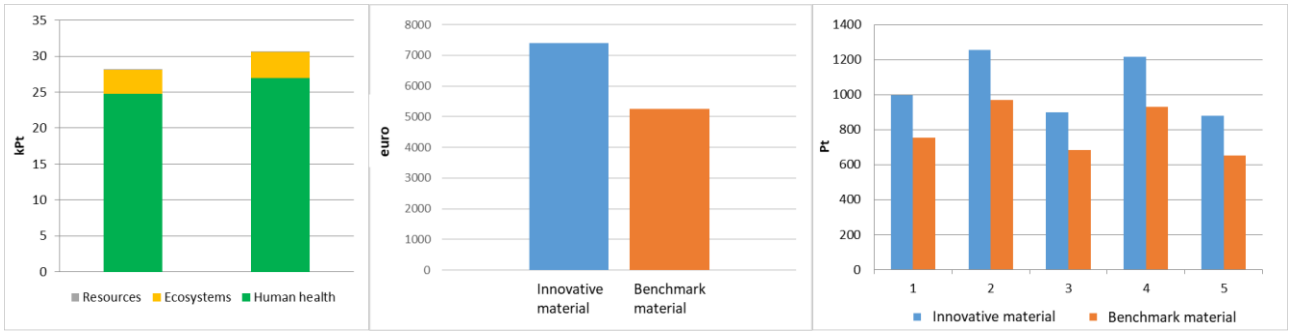

Figure 41 Life Cycle Sustainability Assessment (LCSA) results: LCA single score endpoint results, LCC aggregated results (total cost in euros), and S-LCA weighting categories results.

The application of the tiered approach to the case studies allows to identify safety, sustainability, and functionality hotspots to support the development of materials-specific strategies aimed at mitigating the identified hotspots and at supporting the identification of products' optimisation measures. As far as the case studies results, for each innovative material and product incorporating it, it has been developed a strategy that guided the development during the design phase and pointed out the advantages of such material development.

4. Conclusions

Following the adoption of the EC's SSbD Framework, the SUNSHINE experts have developed a tiered approach to operationalize it. The reason for adopting different tiers for the assessment stems from considerations that the information available for newly developed chemicals or materials could be limited in the early stages of development (e.g., R&D stage), while the availability of data and expertise increases in the later product development and optimization stages, which also demand more thorough assessment of safety and sustainability. The operationalization of the tiered approach proved that the obtained results and information can support decision-making processes, by discriminating between alternatives in a comparative analysis (i.e., an innovative product compared to a traditional benchmark product). In this context, it significantly improves the development of new products, positively affecting the impact of the R&D phase.

Moreover, the results prove the added value of the SUNSHINE SSbD approach in guiding early stages of innovation, along with the opportunity it provides in enabling companies to assess their sustainability performance easily and affordably, which can make them more competitive in the market while leading the design of more environmentally friendly nanotechnologies of high social and economic benefit.

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Decision Support System for SSbD in the early innovation stages

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1. Introduction

Industrial designers have a vast number of tools and methods to choose from when they want to take safety and sustainability aspects into account when making decisions throughout the design process of advanced nanomaterials. Guidance is needed to assist industrial developers which tools and methods for safety and sustainability assessment can support decision making in each stage of the innovation process. Especially during early phases of the innovation process, the tools and methods need to be much simpler to apply with fewer questions and less information required to answer these questions. In addition, most of the existing methods and tools applicable in the lab phase are not sensitive enough to compare the safety and sustainability of different Safe and Sustainable by Design (SSbD) versions of a new material or product. The differences between the SSbD versions are too small to arrive at a different risk assessment outcome with these existing tools.

2. HARMLESS Decision Support System

Within the HARMLESS project we develop an online decision support system (DSS) to support industry in the development of innovative materials in a Safe and Sustainable by Design (SSbD) manner. Based on our experiences from applying existing methods and tools for SSbD to our case study materials, we have made the SSbD-DSS simpler and more sensitive to increase its practical applicability. The SSbD-DSS guides users through a workflow from the ideation phase up to the pilot phase of the innovation process starting with three tools, i.e. AMEA, WASP and ASDI (see Figure 1). First, we have implemented the Advanced Material Earliest Assessment (AMEA) tool for early categorization and advice as an integrated tool and starting point of the DSS. AMEA consists of only 3 questions and is used to check if the developed material or product falls within the applicability domain of the DSS and to provide initial innovation-dependent SSbD advice and early design principles for “exposure during the life cycle”, “hazard” and “sustainability”. If the DSS is applicable, the designer is advised to apply the second tool, named Warning flags, design Advice, Screening Priorities (WASP). WASP is based on the AMEA advice, LICARA innovation scan, Nano Exposure Quantifier and other existing tools, and developed for the ideation and business case phase of the innovation process as a simplified approach that requires less information. This approach consists of 14 questions to identify early warning flags on safety and sustainability and to provide design and assessment advice. To help industrial innovators to make an informed

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decision for the most optimal SSbD version in the lab phase, another approach, named Alternative SSbD Design Inspector (ASDI) was developed. Based on the early warning flags from WASP, ASDI provides a) guidance on which descriptors to measure and b) insight into the differences between the SSbD versions within the various dimensions (safety, sustainability and performance). More deeper analysis tools, including in vivo hazard prediction methods based on physicochemical and in vitro data using, for example, a Bayesian approach, are suggested and directly available in the DSS for pilot phase.

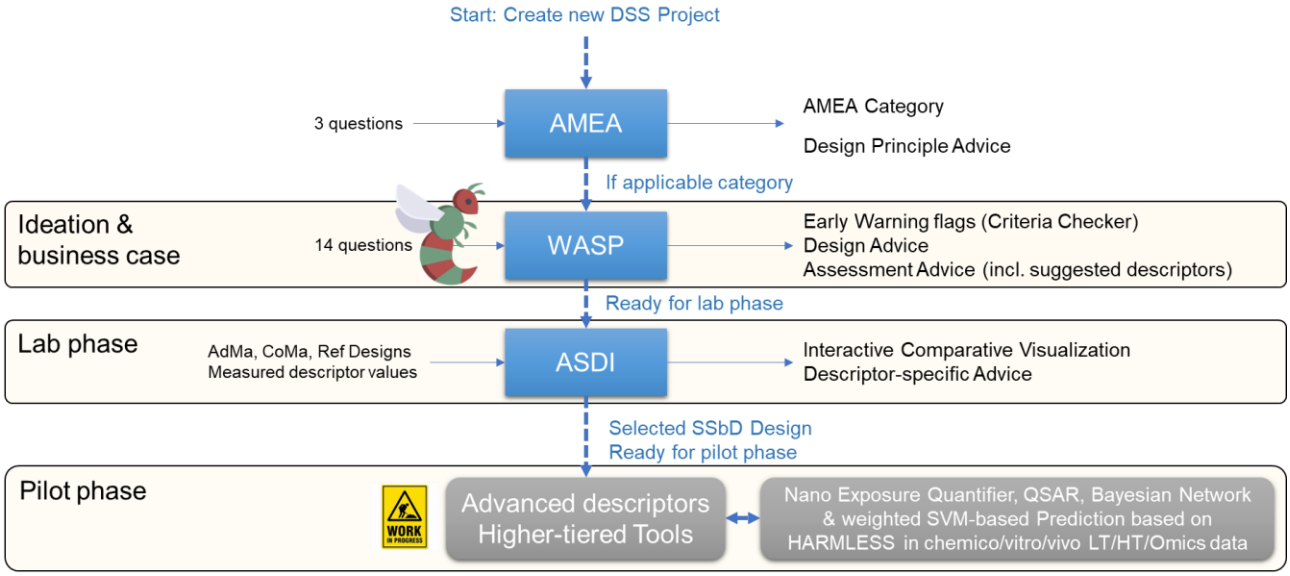

Figure 42: Improved workflow of the DSS: AMEA = Advanced Material Earliest Assessment, WASP = Warning flags, design Advice, Screening Priorities, ASDI = Alternative SSbD Design Inspector.

3. Conclusions

This presentation will describe the development of the new tools and the methods used for data and model integration in the HARMLESS Decision Support System (DSS). The availability of tools, data, and models is a dynamic development process that is changing and developing over time, particularly in a research project like HARMLESS where models and data are becoming available during the whole extent and lifetime of the project. To deal with the broadness of the data and models becoming available as well as to allow for in-depth and more detailed (but also more time-consuming) data and model fusion, we have developed two complementary integration approaches. These two integration approaches are complementary and work seamlessly together, allowing for the necessary broadness of covering important SSbD aspects in combination with more in-depth modelling where needed and possible given available data and models. Future steps will aim for both the AI recommendation engine (which proposes which action to do given the current situation) as well as the AI advice engine (which provides textual advice on the design choices given the current situation) to be able to incorporate decision rules more transparently by adding a functionality that allows experts to see the currently underlying rules.

Challenges in Predictive Sustainability Assessment of Novel Lubricants following SSbD Principles

Jonas Hoffmann[1], Davide Don[2], Sarah Notarfrancesco[2], Salvador Moncho[3], Lucia Pisarova[4], Jakob Kibala[5], Francesco Pagano[6], Andreas Ciroth[1]

1. Introduction

The global imperative to reduce carbon emissions has emphasized the importance of enhanced friction and wear management in tribological applications, potentially mitigating approximately 1460 Mt CO2 and 8.7% of the total energy consumption annually.[1] In low-carbon footprint sectors such as e-mobility and renewable energies, lubricants, play a central role in machinery requiring high durability, efficiency, and tribological performance. Despite their positive impact on reducing friction and wear, the intricate and often environmentally unfriendly composition of lubricants hinders their overall ecological benefits. Stringent regulations (and ecolabels), targeting specific chemicals (lithium-based additives, perfluorinated polymers, chlorinated paraffins), have been implemented by international authorities to address this challenge and are driving trends in the lubricant market. Nevertheless, while staying within the constraints of planetary boundaries, the thresholds for chemical novelties have been already surpassed [2]. Consequently, it is imperative that any novel lubricant is intrinsically non-toxic and environmentally sustainable. A guideline to comply with such criteria has been provided by the European Commission [3], the Safe-and-Sustainable by Design (SSbD) framework. However, with respect to initial testing of said framework in case studies [4], it was found that the framework possesses rather complicated and cost intense approach for the innovation process for already existing products.

2. Challenge and Approach

The challenge at hand involves to develop novel lubricants that comply with the SSbD framework but yet provide competitive function in their respective use cases. The SiToLub Horizon project aims to mitigate risks associated with non-toxic chemical introduction by establishing an integrated multi-functional and cost-effective **simulation environment** in respect to the SSbD framework. Within this environment, we are developing a predictive sustainability assessment tool focusing on all three dimension of sustainability.

The uniqueness of the SiToLub project lies within its interdisciplinary approach to comply with SSbD criteria via simulation tools as well as to foresee the sustainability (Figure 1). To address these challenges comprehensively, we develop a Life Cycle

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[4] AC2T, Vitkor Kaplan Strasse 2, 2700 Wiener Neustadt, Austria.
[5] Ascora GmbH, Birkenalle 43, 27777 Ganderkesee, Germany.
[6] Fundacion Tekniker, Calle Inaku Goenaga 5, 20600 Eibar Guipuzcoa, Spain.

Sustainability Assessment (LCSA) methodology tailored specifically for lubricants and their components. This methodology encompasses the entire lifecycle of lubricants, focusing in particular on use and end-of-life stages. By uniquely incorporating results from toxicity and performance simulation tools, we will capture the environmental performance and impact of lubricant systems comprehensively using our openLCA software platform. The combination with background databases (ecoinvent and PSILCA), allows us to perform the calculation of ecological, cost, and social LCA indicators already in the early product design stage.

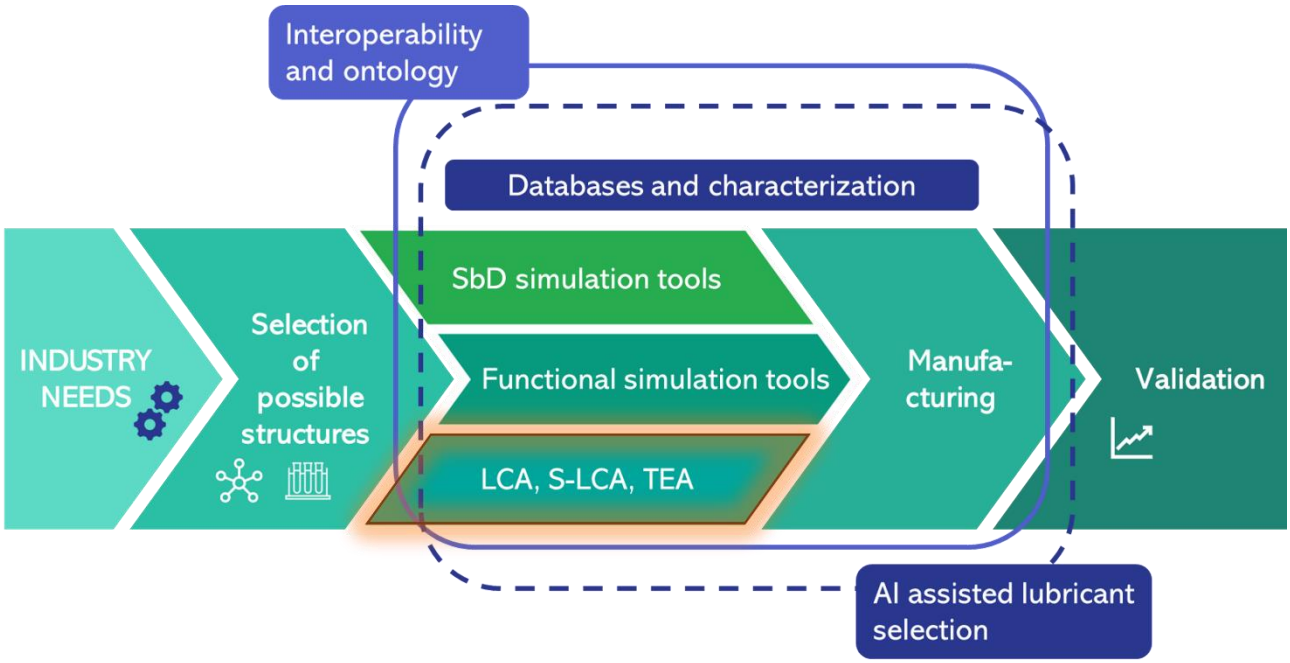

Figure 43: Work flow of SiToLub with focus on the sustainability assessment (ecologic, social and economic).

Although, the SSbD framework [3] focuses mostly on environmental and human health issues, the social impacts have been merely integrated into the assessment as displayed in case studies [4]. In combination with our PSILCA database [5] and system dynamics, we are simulating social impacts for the lubricant fabricant, usage and end of life using quantitative social LCA approaches.

The simulation approaches provided is the project will be finally validated by the production of SSbD-lubricants by industrial partners. (Figure 1). This will allow us to feedback our system dynamics and LCSA models improving the utilized simulation approaches.

3. Initial Results

The initial phase of our research has focused on laying the groundwork for developing a comprehensive LCA methodology for lubricants and integrating results of QSAR and performance modelling into our LCA models. Thereby, we have conducted an extensive review of existing literature, standards, and methodologies, synthesizing insights from diverse sources to inform our approach. For now, connecting QSAR results for (eco)toxicity and biodegradability, with the openLCA software, will require intensive mapping using the UseTox methodology. Yet, the translation of various toxicity values to LCA relevant data remains a challenge. Though, such an approach is eminent as we

focus in particular environmental and health effects of lubricants during their use phase. Nevertheless, the outcome of such an harmonisation will provide a large impact on the SSbD-related simulation approaches.

Looking ahead, our research will focus on refining and validating our LCA methodology through case studies and empirical data collection. By integrating insights from ongoing projects and leveraging advances in computational modeling and data analytics, we aim to develop a robust framework for evaluating the sustainability performance of lubricants throughout their lifecycle. Ultimately, our goal is to provide stakeholders with actionable insights to inform decision-making and drive innovation in the development of energy-efficient and environmentally sustainable lubricant solutions.

4. Conclusions

The results of the SiToLub project serve as indicators for a simulation-based Safe-and-Sustainable by Design (SSbD) approach applicable to specialty chemicals across diverse industries. Additionally, this approach provides important and comprehensive insights into evaluating the sustainability of new materials in the early stages of the design process.

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Safe and sustainable by design roadmaps. A glimpse of the ASINA case studies

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1. SSbD concept

The Safe and Sustainable by design (SSbD) framework from the Joint Research Centre (JRC) seeks the definition of SSbD criteria and evaluation procedures for chemicals, (nano)materials and processes. Developed within the action plan of the European Chemicals Strategy for Sustainability (CSS), the framework foresees the assessment of the entire life cycle of a compound, capturing the human and environmental safety aspects, and the environmental, social and economic sustainability dimensions in the approach. The dimensions covered in the framework are shown in Figure 1 demonstrating the re-design phase supported by a hypothesis formulation and the dimensional targets: functionality, safety across life cycle (e.g., intrinsic hazard, human and environmental safety during production and use phase), and environmental & socio-economic sustainability aspects. For each dimension criteria are envisaged to stimulate sustainable research and innovation, beyond the current regulatory requirements.

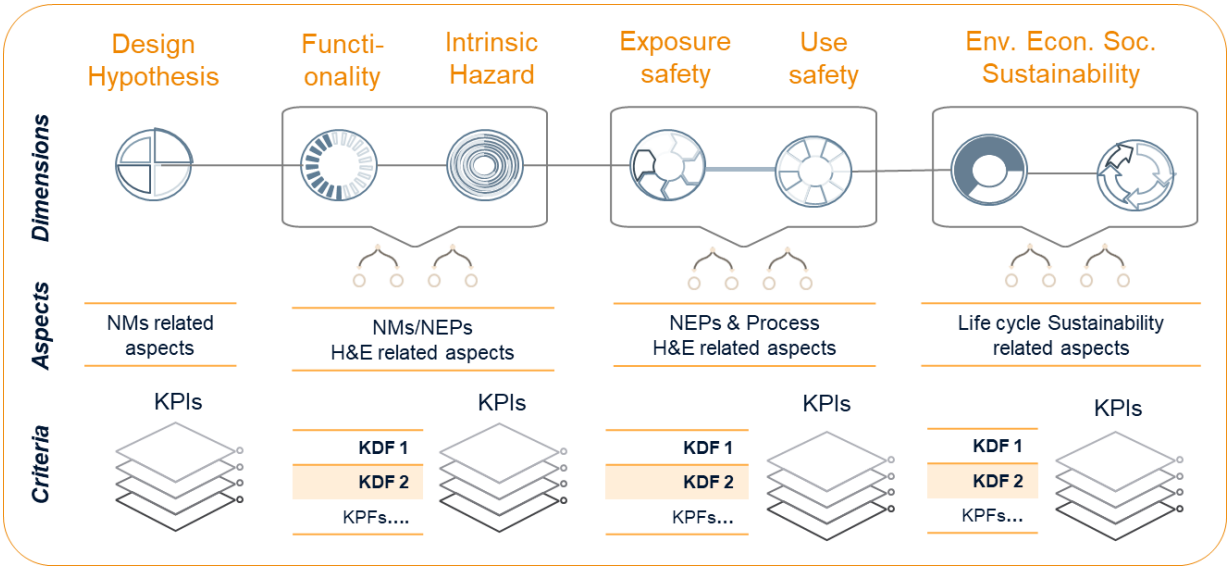

Figure 44. Dimensions, aspects and criteria of the SSbD framework, following a hierarchical approach in which functionality & safety aspects are considered first, followed by process related safety and environmental sustainability and economic aspects, while assuring product functionality. The SSbD approach within ASINA captures Key Performance Indicators (KPIs) in each dimension, Key Decision Factors (KDFs) and Key Performance Factors (KPFs).

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2. ASINA project

ASINA utilizes the structure of the framework in distinct case studies, within the context of nanotechnology. Societal aspects were outside the scope of the project. ASINA supports the re-design of the materials, products and processes by evaluating alternative scenarios within the case studies to improve safety and sustainability of the alternative SSbD solutions. The application of the SSbD concept involves identification of material/product design alternatives at the early stage of the innovation process to reduce the potential for release of hazardous chemicals/materials and/or decrease their hazard, while retaining functionality for their intended uses.

3. The roadmap.

In this presentation we will show the

1. measurable quantitative (either numeric of binary) or qualitative (based on relative comparison) criteria as Key Performance Indicators (KPIs)
   KPIs are based on defined aspects (e.g. health or environmental) measured with an assessment method (experimental, modelling, data-driven) and compared with thresholds or target values when available, based upon the decisions on this comparative SSbD assessment are made.
2. KPIs are strongly depended on Key Decision Factors (KDFs) that allow the differentiation among the final KPIs and thus, the SSbD alternative solutions. Those KDFs can be altered by the designer and allow a degree of freedom in the “re-design” aspect on the SSbD framework.
3. KPIs are depended of Key Performance Factors (KPFs) that differentiate the results but are not manageable by the designer, but are recognised to have a significant effect on KPIs.

In this manner, we are able to provide specific KPIs in each dimension of the frameworks followed by their most important KDFs and KPFs providing future SSbD implementations a scientifically sound basis as a starting point of departure.

4. Conclusions

Being transparent can help ongoing/future projects trying to achieve similar objectives, to get inspired and reach sound scientific approaches. In addition, demonstrating the ASINA cases, might align the efforts towards a common roadmap for executing a SSbD approach, ultimately, promoting the EU ambitious Green Deal goals. Finally, the roadmap acts as an illustrative tool to stakeholders to facilitate engagement and dissemination of results.

Advances and challenges of Safe-and-Sustainable-by-Design: The case of high-entropy alloy coatings

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1. Introduction

In the last few years, the materials research community has seen a great increase in developing multicomponent alloys, known as high entropy alloys (HEAs) with extraordinary properties such as high-temperature and oxidation resistance and structural stability, allowing their use in structural and load-bearing components [1]. Notably, the global high-entropy alloy market size was USD 54.7 million in 2022 and the market is projected to reach USD 202.97 million by 2028, showcasing a compound annual growth rate (CAGR) of 24.42% during the forecast period [2]. The use of HEAs is beneficial in diverse applications in surface protection and engineering, due to their enhanced properties in various environments [3]. It is important to note that each HEA with minor elemental modifications is a new alloy base, therefore limitless combinations could be created [4]. Due to the novelty and the limitless variety of these materials, there is a gap between the research evolution on them and the occupational safety protocols that are required for their proper application. Additionally, the incorporation of sustainability in the design of HEAs not only takes into account the impacts of ores' extraction and metals' processing, but also it sheds light on the environmental concerns of alloys usage and their end-of-life options. The involvement of a large percentage of rare metals in the development of HEAs makes the consideration of sustainability aspects and possibly the inclusion of circular scenarios, imperative, aiming at resource efficiency, tackling the environmental impact of rare metals' mining and processing as well as the reduction of HEA manufacturing costs [5,6]. In order to examine the safety and sustainability level of these advanced materials, the newly developed five-step Safe-and-Sustainable-by-Design framework will be investigated, to support the design and development of safe and sustainable high-entropy alloys [7], as well as reviewing the applicability and limitations of SSbD methodology on the novel HEAs.

2. Framework and Methodology for Materials Safety & Sustainability

Safe-and-Sustainable-by-Design (SSbD) framework is applied as part of the EU funded M2DESCO project (Grant Agreement No. 101138397). M2DESCO is a collaborative, multidisciplinary research project aimed at developing next-generation high-entropy-alloy based multi-component green coatings (free of toxic substances) and sustainable (rare earth free & minimum critical metal elements) with predictable functionalities,

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performances, and life span. Through SSbD, the design criteria and requirements for the relevant coating materials and processes are assessed, while evaluating the models for the calculation of criticality and circularity values and for the selection and development of new coating high-entropy materials (HEMs) and processes (**Figure 45**). The methodology consists of two phases: i) the (re-)design phase that is applied at every stage of development (e.g., research, simulation, lab-scale, pilot-scale), using safety and sustainability design principles, defining the goal, scope and system boundaries of the assessment, and ii) the second phase, where SSbD assessment is applied at each gate or activity and scores feedback to the (re-)design phase, testing alterations to improve safety and sustainability. Reviewing the applicability of the SSbD framework on our case study, we investigate the selection of the materials and the design principles, such as material efficiency, minimization of hazardous chemicals usage, prevention of hazardous emissions etc., and assess the framework's suitability, gaps and limitations for novel advance materials. Within the first steps of the analysis, hazard assessment of the chemicals/materials to be used will take place, followed by the study of occupational risks during production and exposure of hazardous substances, and releases of the final product to the consumer and the environment. To make this possible we will review and employ all available information (e.g. the European Chemicals Agency (ECHA)) and investigate the applicability of ISO standards and publicly available online tools for risk assessment, developed for the chemical industry. In the later steps of SSbD methodology, environmental, social and economic aspects are being investigated based on available information and various tools. The goal is to perform a sustainability assessment that will demonstrate the overall impact of the chemicals and materials which are incorporated into the product's life-cycle.

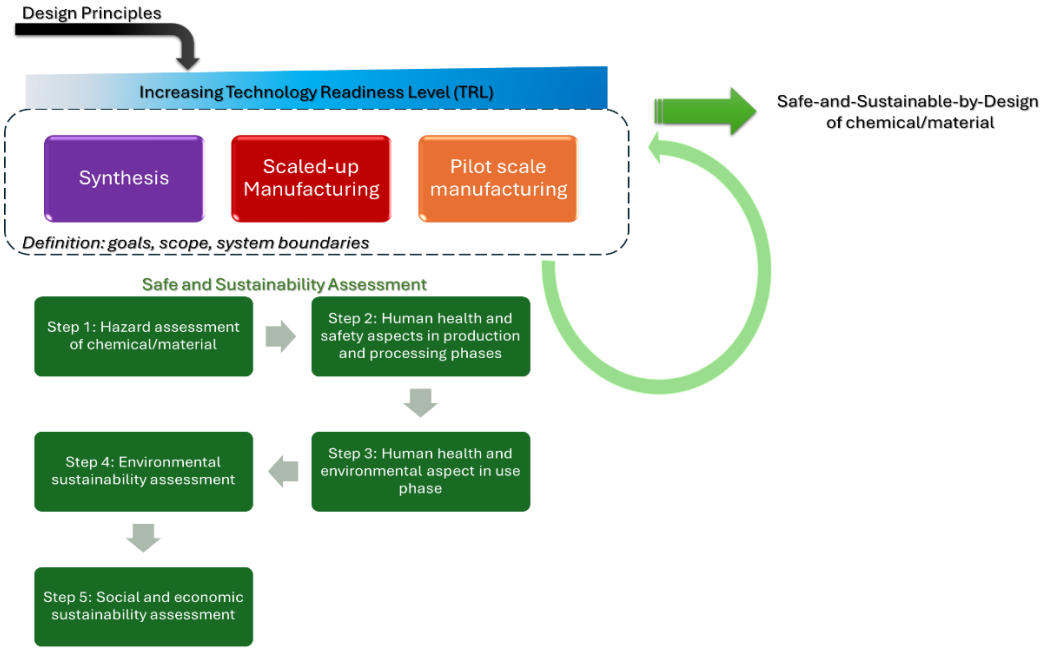

***Figure** 45. Integration of the SSbD framework in the project's innovation cycle.*

3. Conclusions

The outcomes of this study will provide a comprehensive evaluation of the applicability of the SSbD methodology to the production of novel HEMs and identify any gaps and

limitations of the framework, while adding value to the concept of safety and sustainability to the materials industry.

4. Acknowledgements

Funded by the European Union under Grant Agreement No. 101138397. Views and opinions expressed are however those of the author(s) only and not necessarily reflect those of the European Union or HADEA. Neither the European Union nor HADEA can be held responsible for them.

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Towards a nano-specific, quantitative based and human centric-SSbD Approach: Antibacterial nanocoatings case study

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1. Introduction

The need of applying a Safe and sustainable by design (SSbD) strategy to the development of new chemicals and materials finds its main reference guidelines in the EU SSbD Framework[1]. For nano-forms and nano-materials diverse quantitative and semiquantitative SSbD implementation approaches have been investigated within the nano-materials community. However, industrial implementation of the SSbD approach within the engineered nanomaterials arena remains limited and requires support to maximise the advantages of the framework. Towards this, the ASINA[2-10] and INTEGRANO[11] projects aim to support the fast industrial uptake of nanotechnology by providing SSbD solutions and supporting tools.

2. A general SSbD assessment approach based on quantitative evidence

Here, a quantitative, case-specific, and human-centric methodology is proposed supported by the artificial intelligence algorithm implemented within the ASINA and INTEGRANO projects, enabling the selection of SSbD solutions by simultaneously addressing multiple and composite KPIs related to the safety, environmental, economic, and functional dimensions. The methodology requires generating a harmonised data set associated to a specified DoE matrix. The advantage is found in the inherent minimum number of necessary and sufficient specific tox and eco-tox F.A.I.R. primary data required, which implies minimising the experimental burden, while reducing the time and cost for developing each NM design case study. Indeed, a limited amount of experimental samples representing design alternatives needs to be generated, whose number depends on the number of key decision factors (KDFs) that are thought of affecting the addressed key performance indicators (KPIs).

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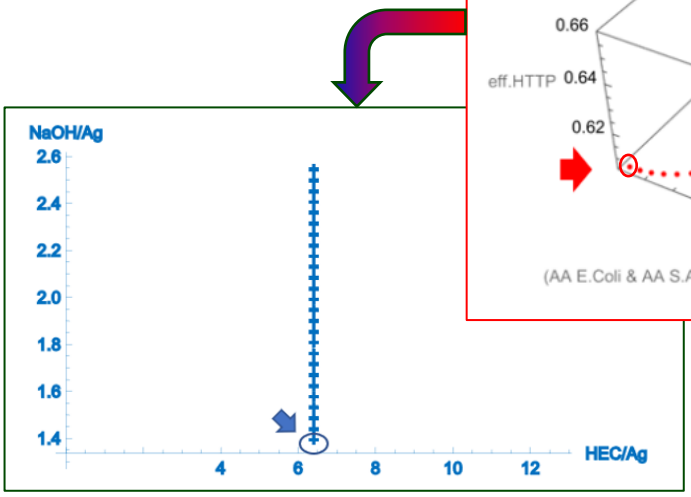
3. Case study – antibacterial nano-coatings

Case studies for the development of antibacterial nano-coatings investigated within the ASINA project through the ASINA-ES decision support system are presented addressing the NMs synthesis and incorporation life cycle stages. The need to integrate the environmental and safety assessments through the development of nano-specific eco-toxicity and human-toxicity indicators addressed in the INTEGRANO project will be presented as an enabling approach for the exploitation of existing international standardised assessment methodologies with defined protocols and metrics such as ISO1040-44 for Life cycle assessment.

Figure 1b: By selecting one point in performance space, ASINA-ES returns the corresponding point in the decision space (blue circled cross), by specifying the values of synthesis Key Decision Factors (KDFs).



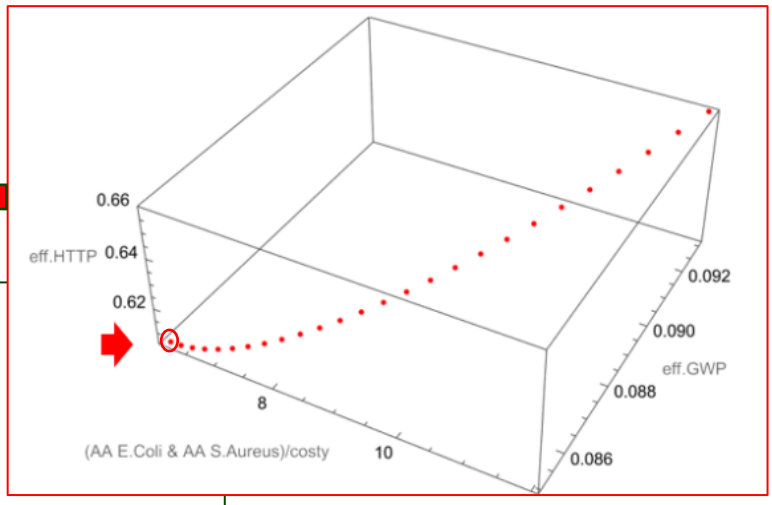


Figure 1a: Set of multi-optimal SSbD cases (red spots) provided by the ASINA-ES in the multi-performance space whose coordinates are the key performance indicators (KPIs) for environmental sustainability (GWP), Human toxicity (HTTP) and composite antibacterial functionality-cost KPI.

4. Conclusions

The methodology presented is a case-specific evidence-based quantitative-approach to SSbD within nanomaterials manufacturing, and which can be extensively applied across materials and chemical development. This approach requires production of a restricted set of experimental samples and generation of a minimum and sufficient number of harmonised related data, leading to enhanced feasibility for implementation in industrial research and development of design cases where minimal prior data is available. This translates into research and technological development cost and time reductions, with >95% reduction in time-to-market. The proposed SSbD methodology corroborated by the MultiOptimal™ decision support system based on artificial intelligence algorithms offers the product designer and decision makers with a refined set of SSbD options on which informed human-centric decisions may be taken within the framework of SSbD nanomaterials and nano-enabled products development. The application of the methodology and the use of MultiOptimal™ for the specific design case study addressed to the development of antibacterial nano-coatings, allowed material designers from CNR to identify the best SSbD synthesis option starting from six

representative design options. Indeed, the selected protocol for the synthesis of the organic-inorganic nano-silver product complies with the lowest environmental impact and the least human toxicity level attainable within the design space defined by the two synthesis key decision factors (NaOH/Ag and HEC/Ag ratios), while the obtained product offers the maximum functionality attainable among the different design options.

5. Acknowledgements

The two-step development of this work has been possible thanks to the ASINA and INTEGRANO projects, ASINA received funding from the European Union's Horizon 2020 research and innovation programme under grant agreement No 862444; INTEGRANO received funding from the European Union's Horizon Europe research and innovation programme under GA No 101138414.

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Poster Presentations: Session 6

From Science to Regulation – The NanoHarmony White Paper on Test Guideline Development

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1. Introduction

International agreement on harmonised and standardised methodologies to test and characterise chemicals and innovative, advanced (nano)materials is essential to protect human health and the environment as well as to ensure sustainability. The OECD Mutual Acceptance of Data (MAD) agreement [1] has clearly demonstrated the benefits of such an international approach. An important cornerstone under the MAD agreement is a set of OECD Test Guidelines for Chemicals (TGs) [2]. These TGs are referred in several legislations (e.g. in Europe [3]).

The European project NanoHarmony (www.nanoharmony.eu) supported the development and adaption of several different OECD TGs to ensure applicability for nanomaterials. The team also analysed processes in TG development to identify hurdles and (unnecessary) delaying factors. This analysis identified issues in OECD TG development in general. The main output is collected in the NanoHarmony White Paper [4].

2. Ensure OECD TGs remain up to date

For the MAD agreement to remain effective, OECD TGs need to remain up to date and fit for purpose. They need to keep pace with new scientific and/or industrial developments and innovations. Also new and future regulatory needs may require new/adapted test guidelines. To allow up-to-date TGs requires an effective strategy for prioritising, initiating, and coordinating TG developments and the funding for these activities.

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[10] UK Health Security Agency (UKHSA)

In a Position Paper [5] the Malta Initiative (MI) identified the need for a formal and continuous structure to accommodate this. They proposed to continue and expand their activities in a so-called 'European Test Methods Strategy'. The MI advocated that such a strategy should include funding of researchers for the development, validation, and harmonisation of test methods. At the same time, it can provide an international (global) platform for collaboration and exchange between stakeholders (researchers, regulators, industry, etc.).

NanoHarmony recommendations to ensure OECD Test Guidelines remain up-to-date

- Establish a formal structure for stakeholder engagement to allow a continuous early identification of required new or adapted OECD Test Guidelines.
- The European Commission, Member States and stakeholders should support the Malta Initiative's European Test Methods Strategy as proposed in its position paper.

3. Engage the scientific community

Many methods developed in the scientific domain will not reach the status of a harmonised and standardised test method. This limits or even prevents their use in regulatory setting.

Awareness of the steps and timing of the OECD process is an obvious benefit for projects aiming to deliver OECD TGs. An educational process is recommended to accommodate this. Such education could also provide broader skills on metrology and documentation.

TG development generally takes 5-7 years, resulting in a substantial risk of scientists moving out of the project and the specific field. Improvement on the FAIRness of research and data (including descriptions of methods used) can mitigate against the potential loss of knowledge and data.

NanoHarmony recommendations to engage the scientific community

- OECD Member Countries should encourage universities, professional societies, industry sector bodies and other relevant stakeholders to include Test Guideline development in their curricula and training to help raise awareness of the role and importance they play in society.
- Funding agencies in OECD Member Countries should encourage and support the scientific community to improve the FAIRness of their research and data.

4. Validation of methods

Validation is key to the successful development of new methods. It enables confidence and trust in the methods and the data generated by using these methods. This requires that once methods are developed, they need extensive validation. OECD Guidance Document No. 34 [6] provides information on these validation aspects. Nevertheless, many stakeholders have difficulties in finding the relevant information.

NanoHarmony recommendations on validation of methods

- OECD and its Member Countries should encourage and support the validation of scientific research, e.g. by providing guidance and tools for researchers over and above that contained in OECD Guidance Document 34.
- The National Coordinators of lead countries for a Test Guideline in development should help ensure effective and efficient communication with all relevant stakeholders during validation and ensure that discussions and decisions are captured and shared.

5. Funding TG development

Obviously, test method development requires funding. While finding funding will remain challenging, investments now can save resources in the future.

Many of the projects on method development finish before (pre-)validation activities or further formalisation into a harmonised TG can actually start. Consequently, many (financial) efforts in method developments may have been in vain.

Apart from funding for validation, additional resources are needed as well. These include reaching agreement with experts and drafting a TG. Such resources may not be immediately available under current financing schemes.

NanoHarmony recommendations on funding TG development

- OECD Member Countries should provide long-term, dedicated additional funding to help ensure that TGs are kept up-to-date and relevant to regulatory requirements, especially for new chemicals and materials, ensuring a prioritised and focussed approach.
- OECD Member Countries should encourage and (financially) support the translation of scientific progress into making Test Guidelines more effective and efficient, including addressing the 3Rs principles.

6. Conclusions

The NanoHarmony project has provided recommendations to ensure engagement of all the relevant stakeholders.

Furthermore, educational material has been developed that aims to help making the process of TG development more effective. This includes the “NanoHarmony OECD TG/GD Process Mentor” (www.testguideline-development.org) that facilitates easy access to the relevant information. This online tool also provides access to the NanoHarmony Training Material (www.testguideline-development.org/useful-resources). This set of slides provides a low-level entry into the topic of standards and harmonised OECD TGs and how science can contribute to this.

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Dustiness testing of high aspect ratio nanomaterials and its use for exposure assessment – towards an OECD Test Guideline

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1. Introduction

High aspect ratio nanomaterials (HARNs) possess exceptional properties that makes them advantageous in different application fields. However, there are concerns regarding their potential harmful effects e.g., carcinogenicity, due to their elongated shape especially when linked to biopersistence and rigidity (Madl and O'Neill 2022, Nagai et al., 2011). WHO (1997) defined a counting rule for fibres which may reach the human lung and even the alveoli with following dimensions: equal or longer than 5 µm, diameter equal or smaller than 3 µm and an aspect ratio equal to or greater than 3. For exposure assessment, the ability of materials to release dust with nanofibers may be determined quantitatively using dustiness test methods, which are already well-established for determination of the respirable mass-fraction and total number-based-dustiness of granular nanomaterials (EN17199).

2. Objectives

The aim of this work was to harmonize and test two dustiness methods for their use on HARNs by means of an inter- and intra-laboratory comparison (ILC) with the final objective to develop an OECD Test Guideline (TG), for both HARN and granular nanomaterials.

3. Methodology

An ILC was conducted with the participation of 7 international partners, which covered two dustiness methods, small rotating drum (EN17199-4) and fluidizer (Broßell et al., 2019). Harmonized SOPs were developed for each method as well as for the analysis of the generated aerosol using scanning electron microscopy (SEM). The two methods

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were tested by two laboratories with 5 different HARNs. The total number-based dustiness index (DI) was calculated based on real-time measurement instruments ($I_{n\text{-}CPC}$) (i.e., condensation particle counter – CPC) as well as on microscopy analysis of collected aerosol samples. In addition, HARN-specific dustiness measurands that take into account the complexity of HARNs and their potential harmful effects were defined and determined based on the microscopy analysis. Outcomes of this analysis include the assessment of the DI in terms of 1) the total number of high aspect ratio objects ($I_{HAR\text{-}object}$) and 2) the WHO criteria-fulfilling objects (I_{WHO}) (L ≥5 µm; D ≥ 3 µm; L:D ≥3).

The agreement of the ILC generated data was assessed by determining the coefficient of variation within and between laboratories. Further assessment of the generated data will include, among others, linear regression and the calculation of the z-score (ISO 13528), which assess the consistency of the data.

4. Results

The coefficient of variation of the calculated number-based DI within each laboratory was <35%. In general, DI calculated with CPC and microscopy analysis were in agreement, which indicates a potential use of CPC data for screening purposes. The coefficient of variation of the CPC number-based DI between different laboratories was <40 and 30% for small rotating drum and fluidizer, respectively. Overall, the DI number-based ranking of the tested materials was similar for all laboratories and methods (Figure 1), with the small rotating drum showing consistently lower DI than the fluidizer. However, some differences were found between the two methods related to the type of objects released by each one with the small rotating drum showing a higher proportion of agglomerates.

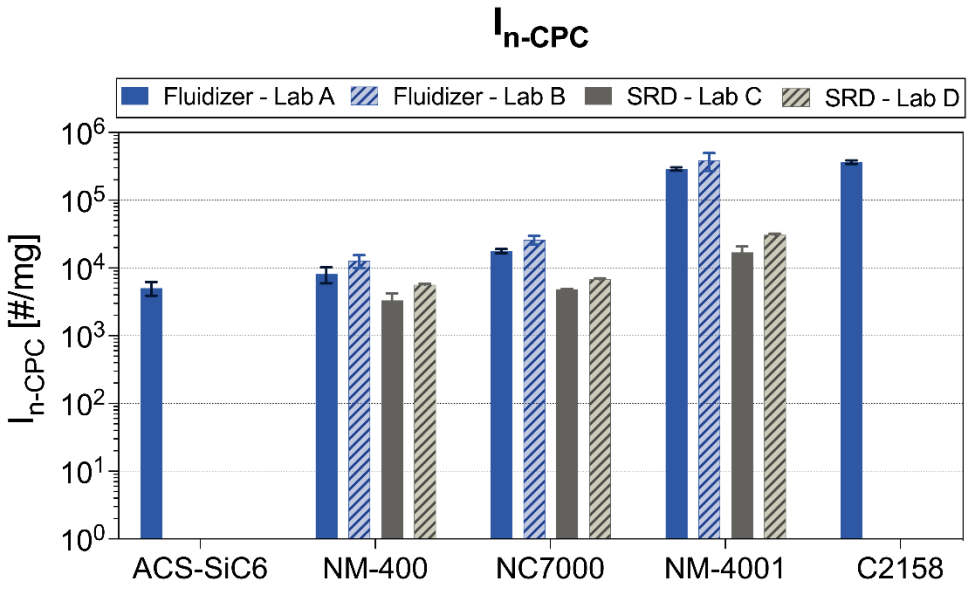

Figure 46: Average and standard deviation of CPC particle number-based dustiness index ($I_{n\text{-}CPC}$) for material, method (Fluidizer and Small Rotating Drum; SRD) and laboratory. Note: logarithmic scale used.

5. Conclusions

With the development of this OECD TG on dustiness of HARN, a harmonized framework for testing and risk assessment of airborne fibrous dust will be built. The long-term goal

is to establish a ranking scheme that enables the comparison of different test methods with the potential to be used for regulatory exposure assessment of HARNs. Reliable test methods for quantifying the potential of HARN release from powders is pivotal to allow informed Safe and Sustainable by Design (SSbD) assessments and decisions.

6. Funding

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Adapting current *in vitro* ecotoxicity standard methods to allow more realistic and environmentally relevant exposure conditions

Alberto Katsumiti[1], Rita Ewela Ojo[1], Mikel Isasi-Vicente[1], Isabel Rodríguez-Llopis[1], Vanesa Benito[1], Felipe Goñi de Cerio[1]

1. Introduction

When assessing the ecotoxicity of Advanced Materials (AdMa), current assays are hampered by a number of issues, including challenges to disperse these materials, as many AdMa are highly hydrophobic, or challenges to expose the test organisms or cells mimicking exposure routes. This work highlights some major issues encountered when setting up *in vitro* ecotoxicity assays for testing poorly water-soluble AdMa. Here, we propose potential solutions that could be explored and developed in order to overcome the existing challenges.

2. Materials and Methods

In this work we tested different dispersion protocols (e.g. low and high energy dispersion methods), dispersion media (e.g. cell culture medium, DMSO, BSA, PVP, conditioned medium, artificial freshwater) and exposure protocols (e.g. submerged, quasi-ALI) to improve the stability of carbon-based AdMa (graphene) and allow more realistic exposure conditions. The OECD TG 249 (Fish Cell Line Acute Toxicity) was then used to evaluate the cytotoxicity of graphene suspensions on RTgill-W1 cells.

3. Results

Results showed that graphene materials disperse poorly in DMSO, artificial freshwater and in cell culture medium, floating away from cells over time. Resulting graphene suspension showed a very low toxicity possibly because they were not accessible to the cells. Graphene dispersed with PVP showed good stability over time, however PVP was cytotoxic to the cells at relatively low concentrations. BSA and conditioned medium slightly improved the stability of graphene in culture medium. Cytotoxicity of graphene dispersed in conditioning medium was higher than that of graphene dispersed in cell culture medium, possibly due to a higher bioavailability to the cells. Cells exposed at quasi-ALI condition showed higher sensitivity to graphene compared to cells exposed at submerged conditions, certainly because quasi-ALI favour a closer contact of cells with the materials. High energy dispersion methods (bath or tip sonication) did not improve the dispersion of the materials. Low energy dispersion (long-term stirring) showed better results than sonication.

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4. Conclusions and future steps

Results indicated that low energy dispersion (long time stirring) of graphene in the presence of mucopolysaccharides and cell culture medium components (conditioning medium) seems to the best suspension protocol. In addition to that, conditioning medium provides protein corona compounds that facilitate the interaction of AdMa with the cells. More realistic exposure conditions are being explored including dispersing graphene in the standard Suwannee River NOM in conditioning medium.

5. Funding

MACRAMÉ has received funding from the European Union's Horizon Europe research and innovation programme under grant agreement No. 101092686.

New approach methodologies (NAMs) for hazard assessment of chemicals and materials at human biological barriers

Beatrice A. Brugger[1]*, Sarah Zehnder[1], Tina Buerki-Thurnherr[1]

1. Introduction

The rapidly increasing development of novel chemicals and materials requires fast, predictive and ethical tools for the assessment of their potential human health hazards. Therefore, we aim to develop, refine and validate new approach methodologies (NAMs) centering on human-based bio-barrier models covering important exposure routes and regulatory relevant endpoints. Specifically, this will include experimental NAMs for next-generation *in vitro* hazard assessment of oral exposure at the intestinal barrier, dermal exposure at the skin barrier and developmental toxicity at the placenta barrier. These tools should contribute to a safe and sustainable design and use of emerging technologies, chemicals and materials.

2. Methods

The intestinal model is based on a combination of epithelial (Caco-2), mucus secreting (HT29-MTX) and immune (Raji-B; induces transdifferentiation of enterocytes into M-cells) cells cultured in inserts. Dermal exposure is studied in a skin model using keratinocytes, the major cell type of human skin. For the placental barrier, a co-culture model of human trophoblasts (BeWo b30) and placental microvascular endothelial cells (HPVEC) is established in microporous inserts.

3. Strategy

We are currently developing and refining three NAMs for skin, intestine and placenta barrier to provide robust and validated models and methods that can address regulatory relevant endpoints such as uptake, translocation, direct toxicity (e.g. cytotoxicity, barrier integrity, inflammation, endocrine function, lipid uptake) and long-term health effects (e.g. sensitization). The performance of the NAMs will be assessed using reference substances with known toxicity. Additionally, an in-project validation and interlaboratory comparison of each NAM will be performed to ensure transferability of the models. In a second phase, other materials, including (nano-pesticides, 2D materials and PFAS will be tested. Furthermore, for the placenta model, the *in vitro* predictions (e.g., for translocation and toxicity) will be compared to the results obtained with *ex vivo* perfusion models of intact human placenta.

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4. Conclusions

The use of advanced human-based *in vitro* methodologies will facilitate the hazard analysis of novel chemicals and materials, reducing reliance on cost-intensive and ethically problematic animal models. Further integration of experimental NAMs with *in silico*/computational NAMs into a next generation SSbD framework for hazard assessment is expected to address industrial and regulatory needs and to fill important knowledge gaps in understanding the interaction of materials with human tissues.

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Testing nanomaterials in complex 3D *in vitro* lung models

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1. Introduction

The potential health and environmental hazards linked to nanomaterials (NMs) present an obstacle to their widespread adoption and impede public perception of the advantages of nanotechnologies. DIAGONAL aims to advance Safe by Design expertise and resources to a stage where they can be integrated into the development process of industries dealing with MultiComponent NanoMaterials (MCNMs) and High-Aspect Ratio Nanoparticles (HARNs). The project relies in part on *in vitro* research to study specific hazard and exposure properties of MCNMs and HARNs. LIST investigates their effects upon inhalation exposure, which is one of the scenarios raising most NM safety-related concerns. To this end, an advanced *in vitro* 3D co-culture alveolar model (Chary et al. 2019) is used where the basolateral side is in submerged conditions while the apical side allows exposure at the air-liquid interface (ALI), resulting in a close replication of the human physiology. Exposure of 3D models to NMs can be performed with multiple exposure strategies, all with advantages and disadvantages which should be considered to ensure its relevance with a high enough throughput and reasonable labour intensiveness. Here, we share tips and tricks on common exposure systems used for *in vitro* testing of NM in the 3D alveolar model.

2. Exposure strategies in 3D *in vitro* lung models

Submerged exposure, where the system is never airlifted during preparation, offers speedy exposure and nominal concentration proximity but lacks human physiology resemblance. Importantly, the sedimentation and diffusion rates of NMs suspended in cell culture media, which is largely dependent upon the effective density and diameter of formed agglomerates in suspension (DeLoid et al. 2014), should be determined. As a compromise, semi-ALI involves airlifting the system but still delivering the NM in limited amounts of medium (65 µL/cm^2). Aerosol-based strategies like Vitrocell Cloud single droplet exposure systems mimic *in vivo* scenario closely but require extensive cleaning between materials to avoid cross contamination, limiting daily usage. Continuous-flow systems allow ALI exposures that closely resemble long-term exposures but obviously, results in a lesser throughput compared to single droplet exposure systems. Albeit being primarily developed for chemicals, high-precision printers like Tecan D300e dispense

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suspended NMs up to 100 nm at ALI (1 µL/cm^2) with minimal setup time and low risk of cross-contamination, yet size restrictions limit its' versatility.

3. Conclusions

Reaching the nominal concentration in the *in vitro* system is crucial to ensure reliable experimental outcomes. Deviating significantly from the intended concentration can introduce errors and impacts the reproducibility of the results. Equally important is to consider the necessity of mimicking the true physiology and its' possible effect on the study outcome. Moreover, understanding the differences between these exposure systems is key to facilitate comparison and extrapolations between studies using different strategies.

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An improved ALI exposure chamber for higher deposition efficiency and optimized operations

Pamina Weber[1], Elisa Moschini[1], Stefania-Delia Isaic[1], Arno C. Gutleb[1], Tommaso Serchi[1]

1. Introduction

In respiratory *in vitro* toxicology, air-liquid interface (ALI) exposure chambers are a promising method for cell culture exposure. However, many ALI exposure systems are characterized by several limitations (e.g. low deposition efficiency - 35-60% for single-droplet deposition systems, risk of chemical carryover, time-consuming operations). The ALI system, on the contrary, should be able to mimic *in vivo* conditions (inhalation) while ensuring high and controlled deposition efficiency, especially when used to deliver valuable compounds (e.g., environmental particles, pharmaceuticals APIs).

2. Objective

To overcome these issues, we have recently developed an ALI exposure system with both housing and casing equipped with an integrated heating mean, thus enabling a non-intrusive heating and temperature monitoring within the housing, and quick temperature rising in the exposure chamber. This innovation allows much higher deposition rates, thanks to the reduced condensation of the aerosol on the casing walls. Additionally, we modified the lower chamber to allow housing of different format of multiwell plates. A disposable pierced lid keeps the hanging wells in place while significantly reducing the risk of chemical carryover and biological contamination. Furthermore, the time needed to set-up and clean the system post-exposure is significantly reduced.

3. Conclusions

To assess the deposition efficiency, sodium fluorescein was aerosolised and quantified after deposition on microporous membrane of hanging inserts. We found out that the deposition was 4-5 times higher in the double heated system compared to the conventional single-droplet deposition system. The use of the disposable lid reduced the operation time by 80%, removing the risk for chemical carryover and biological contamination linked to the exposure operations.

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In Vitro Effect Extrapolation for Human Risk Assessment of Advanced materials

Jimeng Wu[1,2], Co-Authors: Peter Wick[1], Bernd Nowack[2]

1. Introduction

The widespread utilization of advanced materials (AdMas) across various sectors has ignited concerns about potential exposure and risk to human health and ecosystems. Risk Assessment (RA) (McIntosh & Pontius, 2017) is a scientific process to assess a specific stressor's nature and the magnitude of the risk to human health or ecological systems.

Hazard assessment for AdMas has largely shifted from animal testing (Council et al., 2007), which is resource-intensive and raises ethical concerns, to alternative methods such as in-vitro tests (Nel et al., 2013) and in silico (computer-based) (Raies & Bajic, 2016) approaches. In vitro datasets have gone through development to be able to predict more reliably the pulmonary effects observed in vivo. It has been realized that the available in-vitro data sets could be used as alternatives and another source for model evaluation and verification during model development.

To use in-vitro data in risk assessment, quantitative in-vitro to in-vivo extrapolations (QIVIVE) have been developed. QIVIVE approaches for risk assessment have been developed for more than 20 years: researchers simulated realistic physical conditions, using either Physiologically Based pharmacokinetic models (PBPK) ((Lin & Lin, 2020),(Yoon et al., 2012)) or distribution equilibrium principles between cell and serum (Gülden & Seibert, 2003) to extrapolate the in-vivo substance distribution based on in vitro data. The PBPK model was able to describe the experimental data, but there are some limitations and uncertainty as some of the parameters are of high uncertainty (Dong et al., 2017; Wambaugh, 2018).

Besides, the estimations of points of departure (PODs), based on different in vitro studies, are needed to establish causality for the derivation of risk level. Given these differences in the estimation of health-protective exposure values between different studies, a key issue is how to create an integrated approach that can unify different toxicity endpoints from different types of critical studies to support the determination of health-protective exposure values.

To address the abovementioned knowledge gaps, this study developed a Bayesian model to analyse a comprehensive set of toxicity data to determine probabilistic PODs for AdMas. Furthermore, model applications were performed to predict internal dosimetry of relevance to risk assessment for reducing the uncertainty of extrapolation in the derivation of acceptable exposure levels.

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2. Uncertainty space evaluation for toxicity extrapolation

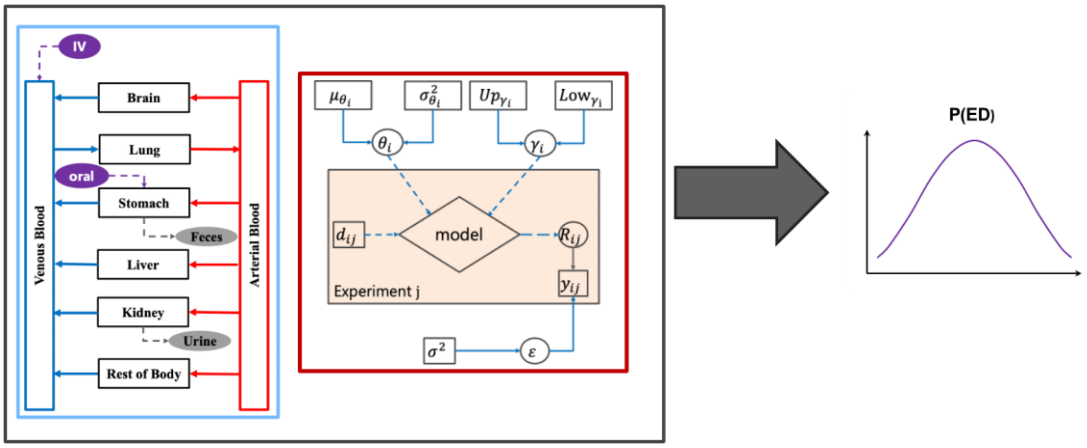

Figure 1: Bayesian Structure to evaluate the parameter and dataset uncertainties.

While some processes inside the PBPK models are well characterized, others are partly or poorly characterized. Information gaps or poor characterization of some physiological processes may cause the PBPK model to not fully capture the kinetics behaviour of particles inside the human body (Khalil & Läer, 2011). Therefore, it is essential to emphasize the uncertainty and variability concerning the PBPK model parameters. Rather than optimizing every possible model parameter, we intend to consider sensitive parameters in the model.

Bayesian analysis with Markov chain Monte Carlo simulation was performed to characterize the uncertainty of parameters and datasets and to further improve the model reliability. A sensitivity analysis of the optimized model parameters was conducted to assess the impact of uncertainty/variability in model parameter values on predictions of output.

Through this analytical approach, we gain insights into the influence of these uncertainties on the extrapolation of safe AdMas concentration levels, a pivotal aspect of risk assessment. It enables the estimation and evaluation of these uncertainties, allowing for a nuanced examination of their impact on the estimation of in vivo effective doses.

3. Conclusions

In conclusion, we are not yet there for a precise calculation of in vitro-based EFs. However, we showed promising methods to evaluate the uncertainties of results.

This collaborative approach allows for a comprehensive assessment of AdMas effects given in-vitro data, including the kinetics process inside the body and toxicological effects, thereby facilitating the development of robust risk assessment strategies.

4. Acknowledgements

This research is part of the project MACRAME, which has received funding from the European Union's Horizon Europe research and innovation programme under grant agreement No. 101092686.

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Boron nitride nanosheets can trigger lipid-mediated autophagy in lung alveolar epithelial cells

Govind Gupta[1], Ziting Wang[1], Vera M Kissling[1], Alexander Gogos[1], Peter Wick[1], Tina Buerki-Thurnherr[1]

Hexagonal boron nitride (*h*-BN) is a newly introduced 2D material gaining wider applications in different sectors from electronics and textiles to biomedical and therapeutics. However, there is a limited understanding of their interaction with lung cells and potential consequences thereafter including the stress response mechanism.

In this study, we investigated the localization of *h*-BN nanosheets at cellular and sub-cellular levels (i.e., in lysosomes) after exposure to alveolar lung epithelial cells (A549 cell line) cultured under air–liquid interface conditions.

Our results showed a significant uptake of *h*-BN nanosheets in cells with a partial co-localization in lysosomes as determined by applying a range of analytical and high-resolution imaging approaches such as flow cytometry, ICP-MS, confocal laser scanning microscopy, RAMAN-confocal microscopy, and STEM-EDX. There was no significant ($p>0.05$) acute toxicity (LDH release), loss of epithelial barrier integrity (TEER), or oxidative damage observed in cells at tested dose ranges (1, 5, and 10 µg/cm^2) for 24 h. However, we observed an imbalance in lipid metabolisms as higher deposits of lipid granules were observed in cells after exposure to *h*-BN as compared to control. To understand further the downstream effect of lipid accumulation in cellular stress, we investigated whether the autophagy pathway was activated. Interestingly, we observed a significant ($p<0.05$) induction of autophagy in cells after exposure to *h*-BN as evidenced by autophagic assay. The immunofluorescence imaging further confirmed enhanced accumulation of LAMP-1 and LC3-B positive vacuoles in *h*-BN exposed cells as compared to control. The observed effects on autophagy could potentially be associated with the downstream processing and breakdown of excess lipid granules to maintain lipid homeostasis. Indeed, we observed lysosomal co-localization of lipid granules supporting this argument. In addition, once the autophagy induction was blocked using wortmannin (a known PI3K inhibitor), the *h*-BN exposure showed a slight improvement in cell death confirming a protective role of autophagy.

Overall, our results suggest that continuous exposure to *h*-BN for the long term may pose autophagic arrest due to insufficiency of autophagic flux that may consequently provoke adverse outcomes (i.e., metabolic disorders or immune diseases) potentially due to imbalanced lipid accumulation in the lungs.

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Form-specific prospective environmental risk assessment of graphene-based materials in European Freshwaters

Hyunjoo Hong[1], Bernd Nowack[1]

1. Introduction

As the application of graphene-based materials (GBMs) in diverse fields escalates, the necessity for environmental risk assessments also grows. Our previous study[1] performed a material flow analysis, identifying GBM release pathways and estimated concentrations in various environmental compartments. Although the importance of considering the different forms of GBM in environmental risk assessments is recognized, e.g. pristine graphene, graphene oxide, and reduced graphene oxide, they have so far not been accounted for.

To bridge this gap, we propose a form-specific environmental risk assessment procedure. This innovative approach combines dynamic probabilistic material flow analysis to obtain predicted environmental concentrations (PECs) with form-specific predicted no-effect concentrations (PNECs) obtained through Probabilistic Species Sensitivity Distributions (PSSD). Finally, the form-specific risk characterization ratios (RCRs) were calculated, aiming for a more accurate understanding of GBMs' environmental impact.

2. Material flow analysis and predicted environmental concentrations

Based on the material flow analysis for GBM, we separated the flows into the three forms pristine graphene, graphene oxide, and reduced graphene oxide and determined their final sinks in technical and environmental compartments. The majority of compartments exhibit distribution patterns of the different forms similar to that of the production compartment positioned in the flow diagram's upper left corner (Figure 1). Here, pristine graphene comprises around 59-66% of the composition, with the remaining portion evenly distributed between graphene oxide and reduced graphene oxide. Based on the environmental release flows and the size of the environmental compartments the PEC values were determined for surface waters: 0.67 ng/L (Q25-Q75 of 0.49-0.81 ng/L) for pristine graphene, 0.32 ng/L (0.25-0.39 ng/L) for graphene oxide, and 0.32 ng/L (0.25-0.39 ng/L) for reduced graphene oxide. These concentrations indicate comparable levels, suggesting similar extents of exposure of the different forms in surface water.

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3. Predicted no-effect concentrations

PNECs for pristine graphene and graphene oxide were derived using the PSSD method. There was a notable scarcity of data available for estimating the PNEC of reduced graphene oxide, both in terms of the number of data points and the diversity of species and taxonomic groups considered (only five data points across five species and taxonomic groups, encompassing algae, plankton, aquatic freshwater plants, and crustaceans). The PNEC for this form was therefore derived from the most sensitive data point and an assessment factor. The PNECs for all GBM forms were found to be within the same order of magnitude. Reduced graphene oxide demonstrated the lowest toxicity, with a mean PNEC of 34 µg/L, followed by pristine graphene at 22 µg/L (13-31 µg/L), and graphene oxide at 14 µg/L (11-17 µg/L).

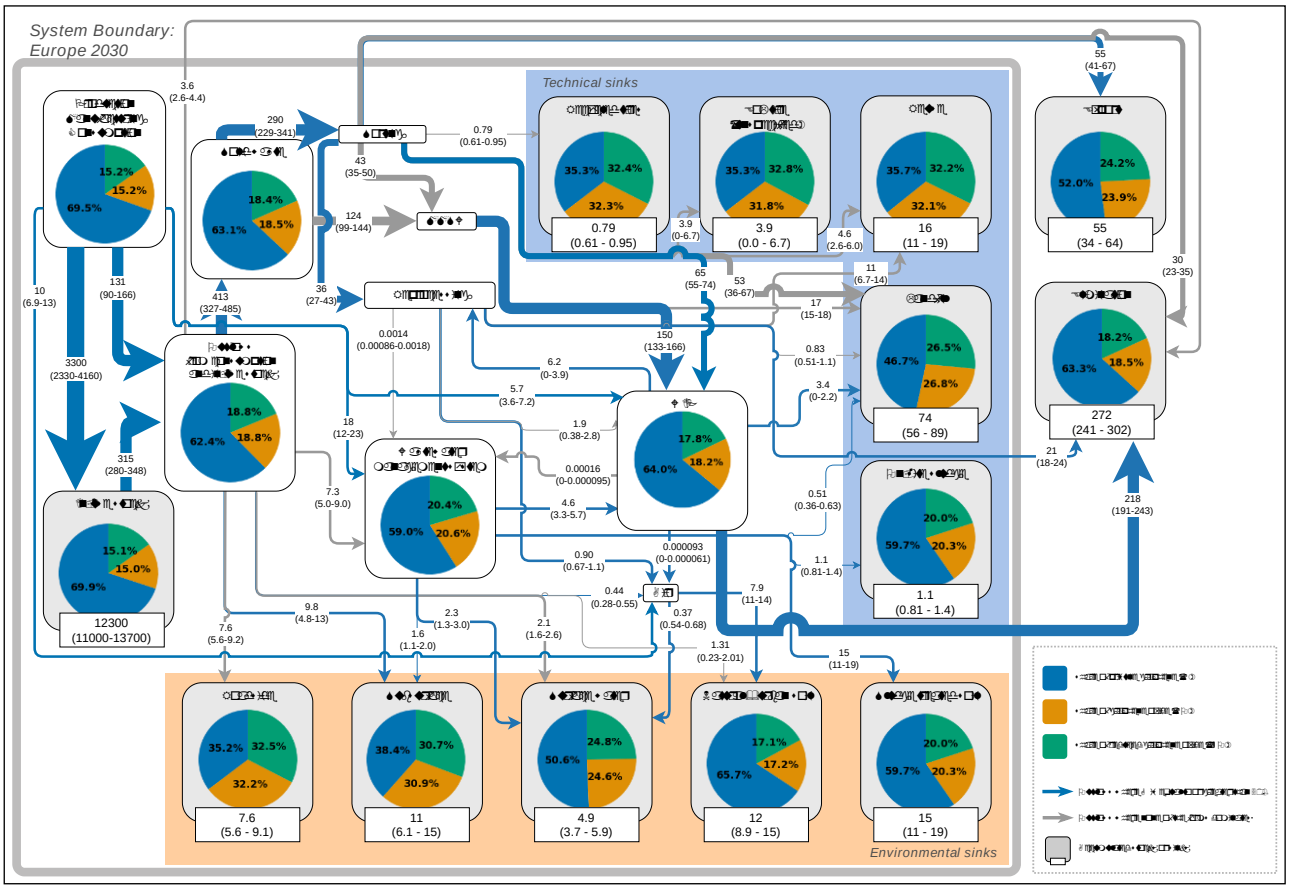

Figure 1: Projected European 2030 GBM flow diagram (in metric tonnes). The arrow thickness reflects the mean flow, and the range between 25th percentile and 75th percentile is stated on each arrow. MMSW: Mixed municipal solid waste; WIP: Waste incineration plant; WWTP: Wastewater treatment plant.

4. From specific risk assessment of GBM

The RCR for various forms of GBM were determined by dividing the PEC by the PNEC. All values were much below 1, signalling a low environmental risk for all forms of GBM. Despite the potential for a significant increase in demand for these materials, our analysis indicates that their environmental impact remains minimal.

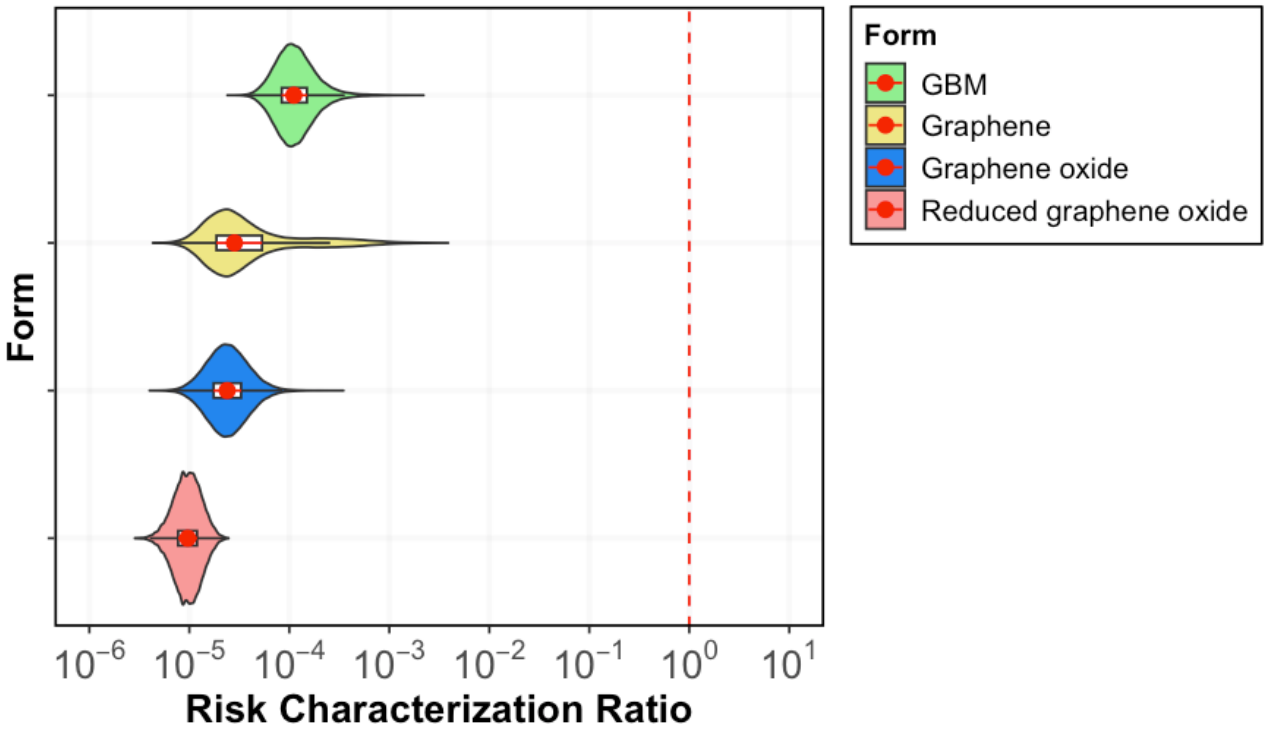

Figure 2: Violin plot of the risk characterization ratio (RCR) of GBM and different forms of GBM. The right side of the dashed line (red) represents the area of potential environmental risks. The red vertical line indicates the RCR of 1. The red dots show the means, and the red lines show the interquartile range of the distributions.

5. Conclusions

The present study effectively assessed the form-specific risk posed by GBM in European freshwaters, yielding valuable insights into the environmental repercussions of these materials. Our results not only aid in comprehending the potential risks associated with GBM but also underscore the significance of considering the distinct properties of each GBM variant in environmental risk evaluations. By elucidating the distinct environmental behaviours and impacts of pristine graphene, graphene oxide, and reduced graphene oxide, our research enhances the precision and comprehensiveness of environmental risk assessments. This comprehensive understanding of GBM's environmental dynamics can inform regulatory decisions, facilitate the development of sustainable material design, and bolster effective management strategies aimed at minimizing environmental impacts.

6. Acknowledgements

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Biological reactivity assessment of graphene oxides

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1. Introduction

Materials, especially advanced materials, are the backbone and source of prosperity of an industrial society (Materials 2030 Manifesto). Graphene Family Materials (GFMs) are considered an advanced material with a wide range of present and potential future applications. GFMs represent a group of carbon-based materials that share the same sheet-like structure as graphene, a single layer of carbon atoms arranged in a hexagonal lattice. GFMs exhibit unique properties such as high strength, conductivity, and flexibility, making them promising for a wide range of applications in electronics, biomedicine, energy sector and for photovoltaics, photocatalysis, biosensors, and functional coatings. The versatility and potential of GFMs have attracted great interest from researchers and industries worldwide, paving the way for innovative advancements in various technologies. Successful commercialization of GFMs requires proper toxicological evaluation to ensure their safe and sustainable use. Although various methods are available to adjust synthesis parameters to refine the morphology and chemistry of the final product and to produce safe by design (SSbD) materials, there is still a lack of practical characterization methods to evaluate the safety and sustainability of GFMs when fine-tuning the synthesis parameters. Within ACCORDs EU Horizon project, we are developing and testing correlative approaches for the physico-chemical characterization of GFMs. Among tests supporting a feedback loop to assure adherence to SSbD criteria during laboratory scale production are acetylcholinesterase (AChE) adsorption and inhibition test and simple cytotoxicity assays. Here we present the initial biological evaluation of 2D graphene oxide (GO) materials synthesized within the Accords EU Horizon project.

2. Initial assessment of biological reactivity

The two GO materials studied have been synthesized using the improved Hummers' method, in which oxidation is guaranteed by the use of $KMnO_4$ as an oxidizing agent (Marcano et al., 2010). In the two cases, different quantities of $KMnO_4$ were used during the synthesis, guaranteeing a different level of oxidation: higher in the case of the GO_2 material. This difference may be one of the parameters to consider when evaluating the functional properties.

An initial assessment of the biological reactivity of GO was performed using an acetylcholinesterase (AChE) adsorption and inhibition assay, and by measuring the cytotoxicity of GO with A549 human lung adenocarcinoma cells.

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Interactions between the enzyme acetylcholinesterase (AChE) and nanomaterials are a reliable high-throughput biological assay that provides information on the adsorption potential of materials by measuring the activity of AChE after adsorption on a material of interest that can potentially interfere with enzyme functionality. The more reactive the surface, the more intense the adsorption and inhibition of enzyme activity. Adsorption of two different graphene oxides (GOs) to AChE and its inhibition were tested using the Ellman's method adapted for microtiter plates as described in Mesaric et al. (2013). The AChE adsorption assay examines how AChE binds to GO by incubating them together, separating GO-enzyme complexes and measuring AChE activity using the Ellman's method. The AChE inhibition assay examines the effects of GO on AChE activity. AChE is incubated with GO and then AChE activity is measured. Together, these assays provide a comprehensive understanding of the interactions between enzyme and nanomaterials, including both adsorption and inhibition effects. The AChE assay is very sensitive for detecting effects of nanomaterials on enzyme function or structure, even at low concentrations of the nanomaterial tested.

The cytotoxicity of GO on A549 cells was tested using the Neutral Red Uptake (NRU) assay, which distinguishes viable cells with functional lysosomes from non-viable cells with unstable lysosomes. Cytotoxicity was measured after a 24-hour exposure to different GOs, according to the protocol described in Kononenko & Drobne (2019).

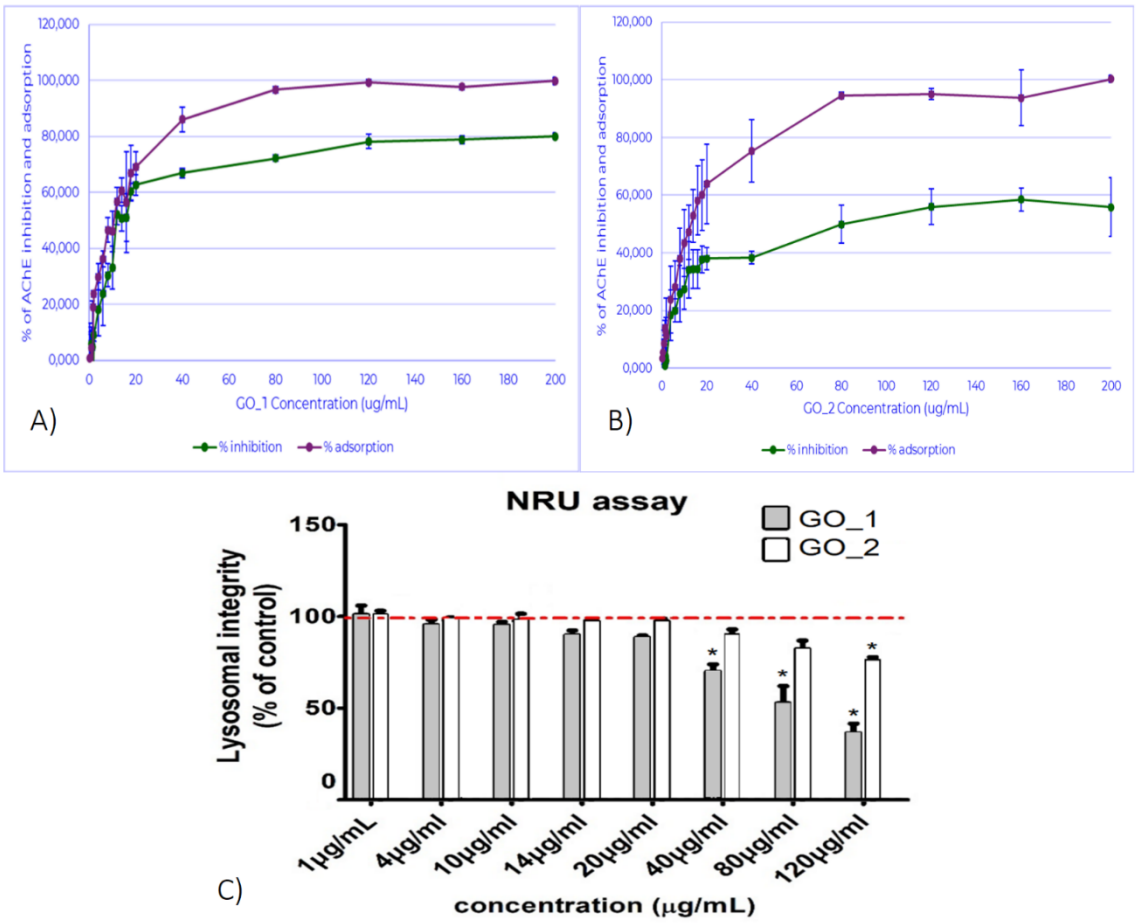

Figure 47: Results of the AChE adsorption and inhibition test (A, B) and evaluation of the cytotoxicity of different graphene oxides (C).

The results of AChE adsorption and inhibition test showed higher reactivity of sample GO_1, which caused about 60% inhibition and 70% adsorption at a concentration of 20

μg/mL (Fig. 1A), while GO_2 caused about 40% inhibition and 60% adsorption (Fig. 1B). The cytotoxicity of GO_1 was also higher compared to GO_2 (Fig. 1C).

3. Conclusions

Here we present the first assessment of the biological reactivity of two types of GOs. The results showed that GO_1 was more reactive than GO_2. GO_1 caused a higher degree of AChE inhibition and adsorption, and it was also more cytotoxic to A549 human lung adenocarcinoma cells. These findings suggest that GO_1 is more biologically reactive compared to GO_2. A possible explanation could be the different oxidation level of the two materials. The presence of functional groups on the surface (higher in GO_2) can play a role in determining reactivity. Further research is needed to fully understand the hazards that GOs pose to humans and the environment, and to develop GO materials for safe and sustainable applications.

4. Acknowledgment

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Risk management tool

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1. Introduction

Within the realm of nanotechnology, Multi-Component Nanomaterials (MCNMs) and High Aspect Ratio Nanoparticles (HARNs) have become increasingly prevalent, presenting unique challenges in terms of safety and risk management. Recognizing the importance of addressing these challenges, a comprehensive effort is underway to define and characterize effective risk management approaches tailored specifically to MCNMs and HARNs.

The use of MCNMs and HARNs has expanded across various sectors including healthcare, pharmaceuticals, and defence, with further anticipated growth in the years ahead. Despite their advantageous properties, research on toxicity has underscored potential adverse health effects. Given the limited understanding of these risks, adherence to the precautionary principle is recommended, advocating for minimizing exposure these materials whenever feasible.

However, quantitative assessment of exposure to MCNMs and HARNs arise difficulties due to lack of adequate equipment for personal sampling, and the scarcity of toxicological and epidemiological studies to set limit values. Despite these limitations, there are other options to monitor the exposure as Control Banding tools, the establishment of internal limit values based on appropriate toxicological studies, or the use of toxicological information of similar substances. These qualitative methods play a crucial role in implementing safe by design strategies, enabling predictions of exposure based on material characteristics and exposure scenarios.

Control Banding tools offer a qualitative approach to assessing exposure to MCNMs and HARNs, facilitating decision-making regarding necessary control measures or the requirement for further risk assessment. These methods categorize situations into different bands, reflecting the likelihood of exposure and potential risks.

To this aim, within the scope of the DIAGONAL project [1], a risk assessment tool has been developed to broaden the application of such tools beyond research facilities to technicians of small and medium-sized enterprises (SMEs), assisting employers and employees in accurately assessing risks associated with exposure to MCNMs and HARNs. This facilitates the implementation of risk mitigation measures based on the priority determined by the risk bands. This interactive Risk Management Tool (RMT) play a key role supporting regulators, industries and other stakeholders on the selection of the best available approaches to reduce risk at source and mitigate the exposure at all stages of MCNMs and HARNs life cycle. .

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2. Applicability

The model and therefore the tool is used for conducting qualitative risk assessment of MCNMs and HARNs, with MCNMs defined as materials comprising multiple components at the nanoscale with a size range lower than 100 nm and HARNs as nanoparticles with a high aspect ratio, typically greater than 3:1. This tool is intended to examine production processes where MCNMs or HARNs are directly used as raw materials; processes where the resulting material intentionally falls within the nanoscale range or exhibits a high aspect ratio; and processes where nanoscale particulate material or high aspect ratio nanoparticles are obtained as by-products at various stages of the production line.

Exposure calculations are carried out based on in-situ data measured by industrial hygiene technicians through continuous monitoring equipment or based on concentration estimation from ITENE's own database, obtained from all nanoparticle exposure monitoring campaigns conducted by the technical staff of the environmental monitoring and safety department under various European projects.

3. The model

The developed risk assessment model implements the control banding qualitative methodology to estimate risk bands. To compute this risk level, the model estimates two different bands for hazard and exposure which result on five possible bands for risk when they are combined.

These bands classification is the outcome of the study of several commercial methods functionality and the experience of ITENE’s technical workers, identifying the best characteristics to give the user a better service, having the hazard bands scheme relying on the COSHH Essentials model widely known on the chemicals risk prevention area, while the exposure bands scheme is based on the combination of several models’ functionalities, such as Cherrie & Schneider model (1999) [2] and other already available platforms, for instance Stoffenmanager [3] nano 1.0 and Nanosafer.

To estimate the exposure band four different factors are considered: the emission source with information about the material and the process; the dispersion which takes into account the distance between the source and the worker; the inmission or personal protective equipment used by the workers; and the intensity, directly related to the task frequency and duration. The hazard band combines information about the material properties and its hazard statements or H-phrases to compute the hazard band.

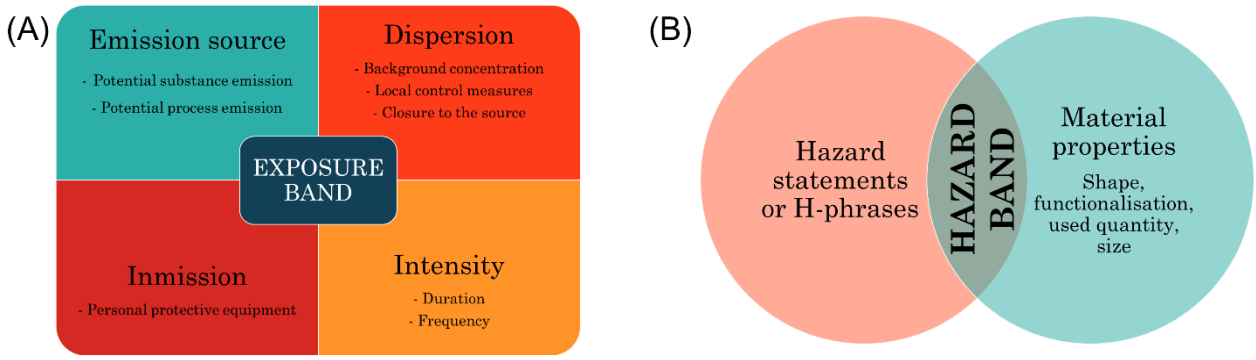

Figure 48: Factors involved in exposure band (A) and hazard band (B) estimation.

For most of the input parameters necessary to run the model, the work consisted of grouping by ranges, assigning a score to each range of the group. This score will be used by the model equations to calculate the respective bands. Once hazard and exposure bands have been set, they are combined to estimate the risk level. For each risk band a set of recommended preventive measures are shown in order to reduce the risk for the workers.

4. The tool

The model roughly described in the previous section has been implemented as a python script and will be included and integrated in the DIAGONAL cloud platform.

As the input parameters are grouped in ranges, the user interface is planned to be a simple form in which the user will select the most suitable option for each of the parameters the model needs. These input parameters will be grouped in three sections to better understanding for the users: working area to provide data about the conditions of the environment, task and the protective equipment used when it is performed, and material to define its specific properties. In this form will be also a question to complete and upload an excel file with the monitoring campaign measures.

Once the form is completed and the file uploaded, it will be shown to the user the computed risk band as well as the recommended preventive measures for that specific risk level.

5. Conclusions

The objective of this control-banding model and therefore of the risk assessment tool is to prioritize the risks related to exposure to nanomaterials, while providing preventive measures, establishing itself as an effective assessment method. Since not all information is currently available for MCNM and HARNs, the DIAGONAL risk assessment model has had to make several assumptions and simplifications. However as more studies are conducted and more information becomes available, both model and tool could be updated.

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Advancing the development of Safe-and-Sustainably-by-Design toolboxes for advanced materials: similarities between the SUNSHINE Tier 1 SSbD approach and Early4AdMa Tier 2

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1. Introduction

The European Chemicals Strategy for Sustainability (CSS) and the Zero Pollution Action Plan have called for a transition to a safe and sustainable-by-design (SSbD) approach to chemicals and materials as part of the policy ambition to achieve a toxic-free environment (EC 2020). Aiming to implement a SSbD approach, the European Commission (EC) adopted a Recommendation for establishing a European assessment framework for SSbD chemicals and materials (EC 2022), which is based on the EC's Joint Research Centre (JRC)'s SSbD framework (C. Caldeira et al. 2022). The recommendation calls for a tiered approach because for newly developed chemicals/materials, the information available can be limited in the early stages of innovation and increases along the product development process (Hristozov et al. 2023). The H2020 SUNSHINE project supports the implementation of the JRC SSbD framework for advanced materials by developing a practical screening approach integrating safety with environmental, economic, and social sustainability assessments to support innovators, and particularly SMEs (Pizzol et al. 2023), in SSbD decision making in the early stages of product development. In parallel, the Early4AdMa early awareness system for regulators and policy makers was developed by RIVM (NL), BfR (DE), BAuA (DE), and UBA (DE) (Oomen et al. 2022) to identify and address potential safety, sustainability, and regulatory concerns. Early4AdMawas later adapted by the OECD Working Party on Manufactured Nanomaterials (WPMN)'s Steering Group on Advanced Materials and subsequently adopted by the OECD WPMN(OECD 2023). This study aims to compare these two approaches in order to understand any possible overlaps and complementarities between them, and to identify potential synergies for application by different stakeholders.

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2. Materials and methods

The SSbD approach developed in the SUNSHINE project is designed to assist industries in evaluating advanced materials and products with the goal to increase their safety and sustainability without compromising their intended functional performance. This qualitative methodology involves a comparative analysis in which the material is compared to a benchmark, which could be an alternative design or a traditional material with similar functions. In parallel, the Early4AdMa system was developed as a systematic approach for early screening of safety, sustainability, and regulatory concerns related to advanced materials. While both methods consist of a series of questions for assessing environmental/health risks and sustainability, they serve different purposes and are intended for different stakeholders. To aid decision-makers from industry, policy and regulation in choosing the appropriate methodology, a comparison between the two approaches was conducted in the frame of the OECD WPMN, focusing on similarities, differences, strengths, weaknesses, and relevance for different users. A classification into common aspect categories such as safety, environmental impact, economic and social sustainability, functionality, and regulatory relevance was used for the comparison. The assessment involved comparing each approach, assigning colours (green, light green, orange, or red) to indicate similarity or variation in questions between the two methodologies, as shown in Figure 1, as well as a comparison in a joint case study. Further comparison of the two approaches has been illustrated through the assessment of a case study, a nanocomposite of graphene oxide (GO) functionalized with chitosan that is used as a substitute for classic flame retardants such as melamine cyanuric acid.

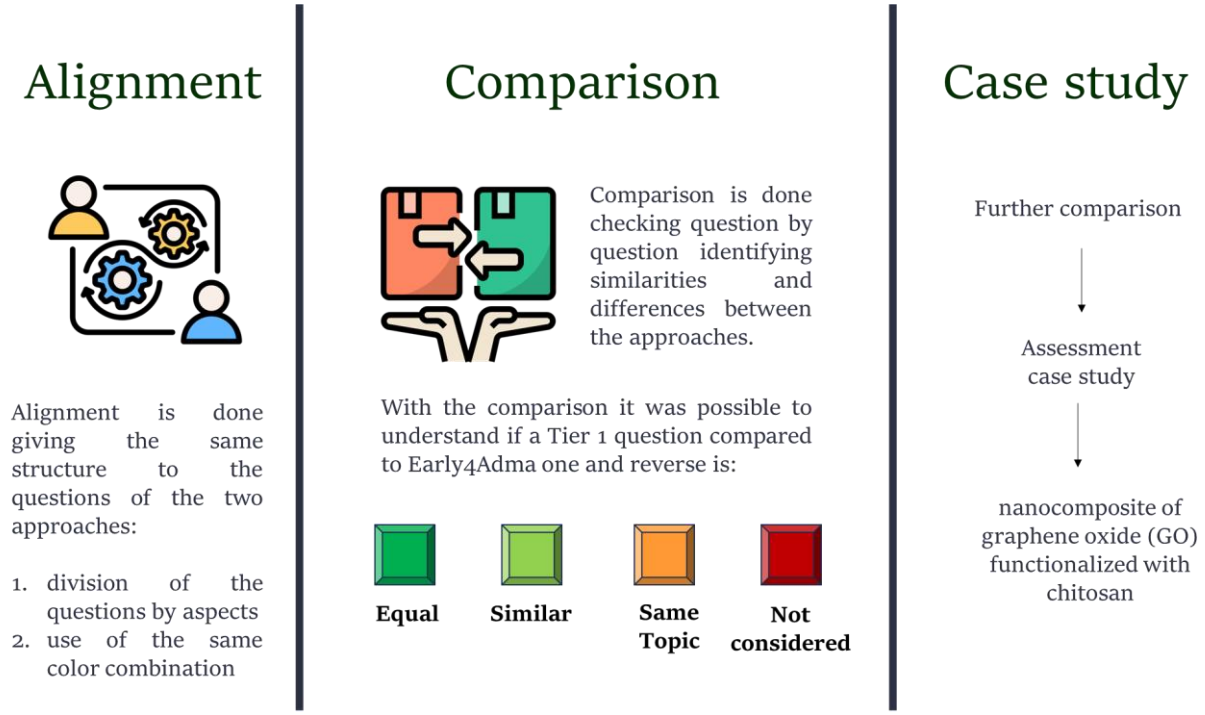

Figure 49: Alignment and comparison method between Early4AdMa and SUNSHINE Tier 1 approach and application to a case study

3. Results

The findings indicated that while both approaches share similarities, they also have distinct differences in the key issues and aspects they address, so we concluded that

both ultimately complement each other. The comparison revealed that Early4AdMa focuses on identifying safety and sustainability concerns and regulatory challenges, while the SUNSHINE approach aims to assess specific impacts on a case-by-case basis to assist companies in creating safer and more sustainable materials or applications. Specifically, SUNSHINE evaluates safety, environmental, social, and economic sustainability, as well as functionality, while Early4AdMa assesses questions about safety, environmental sustainability, and coverage by regulation and regulatory tools. SUNSHINE is designed as a self-assessment tool for industries, especially SMEs, while Early4AdMa assists policy makers in anticipating emerging challenges related to advanced materials, regulators in increasing their preparedness to tackle these challenges, and industrial companies in preparing for regulatory relevant questions when a product is approaching readiness to be placed on the market. Furthermore, SUNSHINE provides a comparative analysis of alternatives, whereas Early4AdMa does not. The comparison of results from applying the approaches to the same case study is challenging due to differences in aspects covered and the way results are presented. However, when comparing safety and environmental sustainability aspects, the results from the two approaches show similar percentages of positive contributions or potential avoided issues.

4. Conclusion

This study compares the Tier 1 SSbD approach from the SUNSHINE project with the Early4AdMa early awareness system within the framework of the OECD WPMN. Both methodologies aim to address early stages of materials development and to support the implementation of the EC's SSbD framework. While similarities and differences were identified between the two approaches, it is clear that Early4AdMa is useful for identifying safety and sustainability issues and regulatory challenges, making it ideal for regulators and policy makers. On the other hand, the SUNSHINE approach focuses on pinpointing safety and sustainability concerns for specific materials/products to aid SSbD decision making by industries, particularly SMEs. We conclude that the two approaches support stakeholders in different ways to apply the SSbD approach described in the EC's SSbD framework.

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Learning from Safe-by-Design for Safe-and-Sustainable-by-Design: Mapping the current landscape of Safe-by-Design reviews, case studies, and frameworks

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With the introduction of the European Commission's "Safe and Sustainable-by-Design" (SSbD) framework, the interest in understanding the implications of safety and sustainability assessments of chemicals, materials, and processes at early-innovation stages has skyrocketed. Our study focuses on the "Safe-by-Design" (SbD) approach from the nanomaterials sector, which predates the SSbD framework.

In this assessment, SbD studies have been compiled and categorized into reviews, case studies, and frameworks. Reviews of SbD tools have been further classified as quantitative, qualitative, or toolboxes and repositories. We assessed the SbD case studies and classified them into three categories: safe(r)-by-modeling, safe(r)-by-selection, or safe(r)-by-redesign. This classification enabled us to understand past SbD work and subsequently use it to define future SSbD work so as to avoid confusion and possibilities of "SSbD-washing" (similar to greenwashing). Finally, the preexisting SbD frameworks have been studied and contextualized against the SSbD framework.

Several key recommendations for SSbD based on our analysis can be made. Knowledge gained from existing approaches such as SbD, green and sustainable chemistry, and benign-by-design approaches needs to be preserved and effectively transferred to SSbD. Better incorporation of chemical and material functionality into the SSbD framework is required. The concept of lifecycle thinking and the stage-gate innovation model need to be reconciled for SSbD. The development of high-throughput screening models is critical for the operationalization of SSbD. We conclude that the rapid pace of both SbD and SSbD development necessitates a regular mapping of the newly published literature that is relevant to this field.

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Applying the SSbD framework for the development of bio-based PFAS-free alternatives for textile and packaging sectors – The ZeroF case study

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1. Introduction

The Chemical Strategy for Sustainability (EC, 2020) has introduced several ambitions in the innovation environment, through the introduction in 2022 of the "Safe and Sustainable by Design" (SSbD) framework (Caldeira et al., 2022 / EC, 2022), for chemicals and advanced materials. The framework is intended to support research and innovation (R&I) activities for the development of alternatives that are designed and produced with the use of available resources in a more ethical and sustainable way.

The SSbD framework has been developed by the Joint Research Centre (JRC) and is currently being tested in various, wide industrial applications and research projects for refinement and further development. The framework defines the general approach, provides guidance for the definition of safety and sustainability criteria, and describes the related evaluation procedures.

Within the ZeroF project (http://zerof.eu/), the application of the framework performed to support the development of the per- and polyfluoroalkyl substances (PFAS) alternatives for the packaging and textile coating applications and ensure their safety and sustainability. The project consortium aims at guiding the design of the new materials and verify their compliance with safety and sustainability criteria through the two main components of the framework: i) the (re)design phase, and ii) the safety and sustainability assessment phase. In this study we present in detail how the re(design) principles have been iteratively applied and how the safety and sustainability has been implemented in parallel with the innovation processes. Preliminary information of the safety and environmental sustainability assessments are presented, related to steps 1&2 (safety assessment) and step 4 (environmental sustainability assessment) of the SSbD framework. Initial plans related to the socio-economic assessment (step 5) of the ZeroF case studies are discussed. The application of the SSbD framework to real life innovation processes comes along with specific advantages but also with sets of challenges faced, mainly related to data availability and complex laboratory scale or industrial setups.

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Respiratory deposition estimates of airborne per- and poly-fluoroalkyl acids (PFAS) powered by Enalos Cloud Platform

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1. Introduction

Exposure to per- and poly-fluoroalkyl acids (PFAS), present in particulate matter such as soils and dust, or in the gaseous phase as vapor, has been observed to yield potential detrimental effects on both the environment and human health.[1] Several studies have addressed waste streams as critical sources of PFAS in the environment.[2, 3] Lin et al.[4] conducted a study wherein they sampled air and size segregated particulate matter from the largest landfill and three Waste Water Treatment Plants (WWTPs) in Hong Kong. These samples were then compared to those obtained from coastal and natural reserve sites to assess any differences.

The objective of the present study is to use the particulate size data of PFAS collected by Lin et al.[4] from various WMIs, as well as coastal and natural reserve sites, to assess the deposition rates of PFAS in different regions of the human respiratory tract when individuals inhale PFAS in these outdoor environments.

2. Methodology

To assess the deposition efficiency and flux of inhaled PFAS within the human respiratory tract, the simplified equations derived from the International Commission on Radiological Protection (ICRP) model are utilized.[5] This model provides calculations for the deposition flux and efficiency of inhaled particles across three distinct regions of the respiratory tract: the head airways (HA), the tracheobronchial region (TB), and the alveolar region (AR). The deposition efficiency of particles across these three distinct regions is calculated as follows:

$$DE_{HA} = IF \times \left[\frac{1}{1+\exp\left(6.84+1.183\ln D_P\right)} + \frac{1}{1+\exp\left(0.924-1.885\ln D_P\right)} \right] \quad (1)$$

$$DE_{TB} = \left(\frac{0.00352}{D_P} \right) \left[\exp\left(-0.234\left(\ln D_P + 3.40\right)^2\right) + 63.9\exp\left(-0.819\left(\ln D_P - 1.61\right)^2\right) \right] \quad (2)$$

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$$DE_{AL} = \left(\frac{0.0155}{D_P}\right)\left[\exp\left(-0.415\left(\ln D_P + 2.84\right)^2\right) + 19.11\exp\left(-0.482\left(\ln D_P - 1.362\right)^2\right)\right] \quad (3)$$

$$IF = 1 - 0.5\left[1 - \frac{1}{1 + 0.00076 \times D_P^{2.8}}\right] \quad (4)$$

Where D_P (μm) is the diameter of the particle and *IF* is the inhalable fraction of all particles. The D_P in the above equations is the mass median aerodynamic diameter (MMAD) of each PFAS compound. The deposition flux (*DF*, pg h^{-1}) of particle-bound PFAS in the respiratory tract is estimated by:

$$DF_i = \sum\left(DE_i \times C_i\right) \times V \quad (5)$$

Where DF_i is the particle deposition efficiency in each region for DP_i (the average diameter of each particle size fraction), C_i is the concentration of PFAS in each size fraction, and *V* is the human breathing rate under normal conditions (0.45 m^3 h^{-1}).[6]

The equations discussed above, which are used to predict lung deposition in the HA, TB, and AL regions/compartments using the ICRP model, have been incorporated into the Enalos Cloud Platform.[7, 8] This integration has been achieved through the development of a web application: https://enaloscloud.novamechanics.com/proplanet/lungdeposition/, which was created as part of the PROPLANET project (Funded by the European Union under the GA no 101091842).

3. Results and Discussion

The deposition flux of inhaled PFAS (pg h^{-1}) and its relative abundance (%) is calculated using the ICRP model, as implemented in the Enalos Cloud Platform[7, 8] (https://enaloscloud.novamechanics.com/proplanet/lungdeposition/). This can be seen in the figure provided below. The deposition flux at the landfill is found to be higher, as expected, owing to the elevated concentration levels of total PFAS. This is followed by the two wastewater treatment plant (WWTP) locations and the natural sites, encompassing the coast and rivers regions. In general, the deposition flux of inhaled PFAS associated with coarse particles was found to be higher in the HA (76% - 92%) and TB regions (46% - 67%), while fine particles were the primary contributors in the AL region (34% - 64%). The relative abundance of inhaled particulate PFAS in the ultrafine fraction increased in the alveolar region, aligning with prior investigations on halogenated and organophosphate flame retardants.[9, 10]

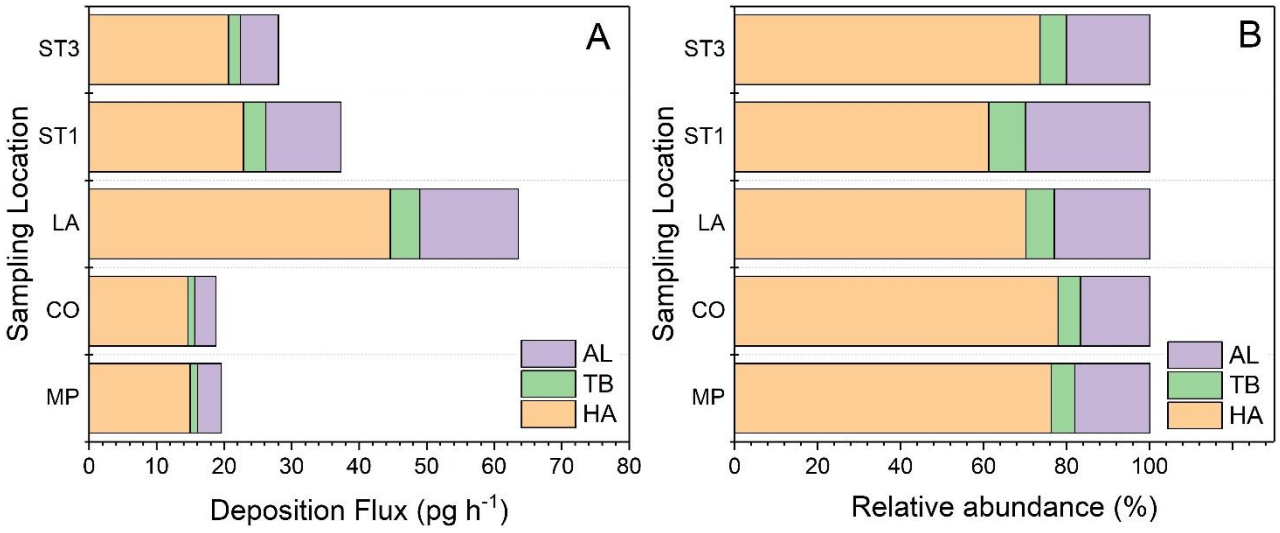

Figure 50: (A) Deposition flux of inhaled PFAS (pg h^{-1}). (B) Relative abundance (%) of inhaled PFAS at different sampling locations.

4. Conclusions

To summarize, in this study the ICRP model is utilized through the Enalos Cloud Platform[7, 8] to assess the deposition of inhaled PFAS particles in the human respiratory tracts. The findings revealed that larger particles are predominantly deposited in the HA region, whereas ultrafine PFAS particles are significantly present in the AL region. It is noteworthy that coarse particles (>0.5 μm) are more prevalent in natural environments such as rivers and coasts, while finer particles (<0.5 μm) are more abundant in landfill and wastewater treatment plant (WWTP) sites (LA, ST1, ST3). These deposition patterns raise concerns regarding inhalation exposure risks and potential implications for human health. The higher concentrations of PFAS in landfill and WWTP areas contributed to an increased deposition flux of PFAS in the human lungs.

In future endeavors, there are plans to carry out epidemiological investigations aimed at establishing a direct link between PFAS exposure through inhalation and specific health effects. These studies will contribute to a better understanding of the risks associated with particles of different sizes that are contaminated with PFAS. Additionally, it is intended to utilize alternative models, such as the National Committee on Radiation Protection (NCRP) model[11] and the Multiple-Path Particle Dosimetry (MPPD) model.[12]

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Investigating the influence of nanomaterials metal composite ratios on the toxicity and intracellular uptake in epithelial cell lines

Kailen Boodhia[1,2], Charlene Andraos[1,2], Mary Gulumian[1]

1. Introduction

The ratio of metals in nano-composite materials significantly influences their efficacy in intended applications as nanoparticle systems. Two such composites, Cobalt-Iron Oxide ($Co_xFe_xO_4$) and Cerium-Zirconium Oxide ($Ce_xZr_xO_2$), have gained attention for their unique properties. Cobalt-Iron Oxide nanomaterials (NMs) are highly attractive due to their moderate magnetization, high coercivity, chemical and thermal stability, catalytic potential, and applications in biomedicine and sensors. In contrast, one of the main properties of Cerium-Zirconium Oxide nanomaterials is their oxygen storage capacity, making them effective environmental catalysts for pollutant removal. They also exhibit high activity, selectivity, and stability, being crucial materials in three-way catalysts.

2. Problem Statement

While intentional modifications to nanomaterials may enhance their function, it may also inadvertently influence their toxicity and interactions with cells. This study investigated the toxicity and intracellular uptake of Metal Oxide NMs: Cobalt (II, III) Oxide (Co_3O_4), Iron Oxide (Fe_3O_4), Cerium (IV) Dioxide (CeO_2), and Zirconium (IV) Dioxide (ZrO_2) as well as nanocomposites Cobalt-Iron oxide ($Co_xFe_xO_4$) and Cerium-Zirconium oxide ($Ce_xZr_xO_2$), with varying metal ratios.

3. Methods

Human bronchial epithelial (BEAS-2B) and human alveolar basal epithelial (A549) cells were exposed to the different NMs, with toxicity assessed using xCELLigence RTCA impedance-based technology system. The BEAS-2B and A549 cells were seeded in 96-well E-plates in 100 µl dispersion medium (i.e., cell culture medium). The cells were incubated for 24 h to allow the cells to adhere and proliferate before treatment. The medium was then replaced with fresh dispersion medium containing NMs at concentrations of 1, 10, 25, 50 and 100 µg/cm^2, with control cells receiving dispersion medium only. Data points collected every 15 minutes for 24 hours and every 30 minutes for an additional 24 hours. Data was normalized at the point of treatment.

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The intracellular uptake was investigated using the CytoViva dark-field hyperspectral imaging system. Microscope slides were prepared as follows: BEAS-2B and A549 cells were seeded on 8-well EZ-slides in 500 µl dispersion medium. The cells were incubated for 24 h to allow the cells to adhere and proliferate before treatment. The medium was then replaced with fresh dispersion medium containing NMs at sub-lethal concentrations (as determined from the xCELLigence RTCA viability studies) for treatment periods of 12 and 24 h. Control cells received dispersion medium only.

4. Results and Discussion

Results indicated that Metal Oxide NMs increased cytotoxicity with increased concentration, except for Cerium (IV) Dioxide in both cell lines. A549 cells showed greater sensitivity, although interestingly, BEAS-2B cells was more sensitive with Iron Oxide NM in, however recovery of the cell index was seen in the latter part of the experiment. The Cobalt-Iron Oxide composite NMs displayed increased toxicity over the concentration range, with the $Co_{1.5}Fe_{1.5}O_4$ only displaying toxicity at 100 µg/cm^2 in the BEAS-2B cells and from 25 µg/cm^2 in the A549 cells. The Cerium-Zirconium Oxide composite NMs showed relatively little to no toxicity in the BEAS-2B cells, whereas with the A549 cells an increased sensitivity was seen. The increased toxicity could be attributed to the increase in Zirconium ratio in the nanocomposite.

When assessing the intracellular uptake of the Metal Oxide NMs, internalization of the Cobalt Oxide, Iron Oxide and Cerium Dioxide was observed in both cell lines, while Zirconium (IV) Dioxide showed a lack thereof. The Cobalt-Iron Oxide composite NMs were internalized in both BEAS-2B and A549 cell lines and in all cases, internalization of particles appeared to increase from 12 h to 24 h. On the contrary, the only Cerium-Zirconium composite NMs that showed internalization was the Cerium Zirconium Oxide ($Ce_{0.9}Zr_{0.1}O_2$), which interestingly has the lowest Zirconium ratio.

5. Conclusions

In conclusion, Metal Oxide NMs can induce toxicity and when combined to form nanocomposites can decrease the observed toxicity, although this appears to be cell line specific. The effects of metal composite ratio, particularly with Zirconium-based NMs, demonstrate how variations can influence cell response and internalization. Metal composite ratio may therefore be another factor to consider when implementing safe-by-design principles at the synthesis and manufacturing stages of NMs.

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Establishing the methodological basis for environmental, health and safety (EHS) impacts assessment- The SUNRISE approach

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1. Context

The SUNRISE project endeavours to formulate a comprehensive Integrated Impact Assessment Framework (IIAF), grounded in lifecycle perspective, aimed at supporting Safe and Sustainable by Design (SSbD) decision-making across the supply chains of advanced materials (AdMa) and their related products. This framework, structured into three tiers, will incorporate integrated methodologies supported by toolboxes for assessing health, environmental, social, and economic impacts. Tailored to diverse user groups and innovation stages, each tier will demand varying levels of data and expertise.

2. The SUNRISE EHS impact assessment

The SUNRISE approach for defining methodologies for environmental, health, and safety (EHS) impact assessment will include hazard and exposure considerations across the 3 tiers of the IIAF. In pursuit of this goal, we have identified potential EHS-related building blocks: tools, models, databases, and methodologies, including NAMs based on non-animal methods such as *in vitro*, *in chemico*, and *in silico* methods. These building blocks are evaluated for their suitability across the different tiers and are aligned with Steps 1, 2, and 3 of the EC-JRC SSbD framework. The identified building blocks encompass existing

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methods/tools for measuring indicators related to intrinsic physicochemical identity ('what they are'), lifecycle release, environmental fate, biodistribution, transformation by-products exposure ('where they go'), and human health and environmental effects ('what they do'). Additionally, the need to adapt existing NAMs for hazard assessment of AdMa or develop new ones in accordance with the principles of the three Rs (Replacement, Reduction, Refinement) for regulatory purposes has been identified.

3. Expected outcomes

In the upcoming months, SUNRISE aims to be able to identify the most appropriate methodologies for assessing EHS impacts across the 3 tiers of the IIAF, ultimately culminating in the development and utilization of Integrated Approaches to Testing and Assessment (IATA) built upon New Approach Methods (NAMs). These endeavours seek to facilitate the generation of reliable non-animal data for next-generation risk assessments (NGRA).

4. Funding

SUNRISE has received funding from the European Union's Horizon Europe research and innovation programme under grant agreement No. 101137324.

Implementation of Safe-by-Design (SbD) and Safer and Sustainable by Design (SSbD) within the Health, Safety and Environment (HSE) Platform in South Africa

Victor Wepener[1], Richard Harris[2], Yolanda Tancu[3], Tarryn Botha[4], Nonhlangabezo Mabuba[4], Mary Gulumian[1]

The focus of the HSE Platform is to ensure the safety of those who encounter or apply nanomaterials (NMs) in occupational, and environmental settings and also from consumer products to mitigate its risks.

1. Safe by Design (SbD)

The aim is to conduct the risk assessment of the nanomaterials by assessing occupational, consumer and environmental exposures as well as the development of predictive tools to ensure safer innovation of nanotechnology in South Africa with safe by design (SbD) approach (Figure 1).

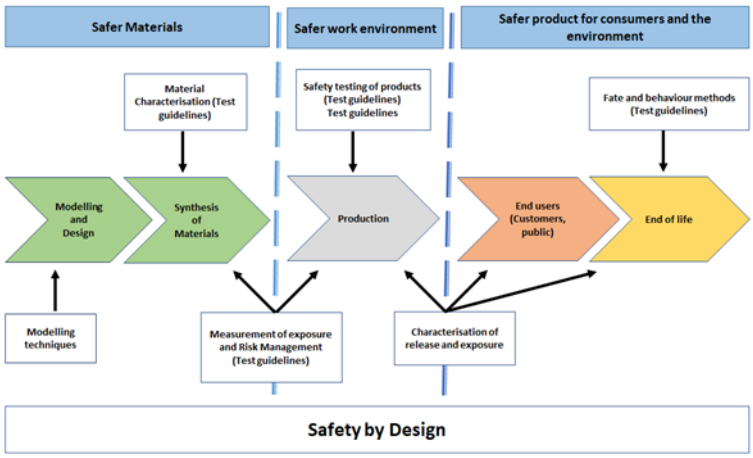

Figure 1: Safety by design

2. Safer Materials:

For Heman Health: For the early development and design phases of a new nanomaterial or nano-enabled product it is essential to identify the hazards of the nanomaterials synthesized. This involves the basic toxicological information to establish the relationship between designed nanomaterial properties, their interactions with biological systems and environmental systems, and effects at the cellular and molecular

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level. The development and use of validated assays is therefore a critical issue that needs to be addressed prior to their implementation to confirm or negate the toxicity of nanomaterials in this initial stage of SbD. Within this part of the SbD, in silico models computational modelling and were implemented since nanoparticles of various shapes, sizes, materials (elements) chemical properties etc. can be designed in a virtual environment and tested without any detrimental consequences (Ngake et al., 2022; Nqayi et al., 2022). Moreover, nanoQSAR modelling was developed to tailor metal oxides is the success of various synthetic methods in influencing the formation of desired faceted surfaces for toxicity prediction (Thwala et al., 2022; Nqayi et al., 2022). For safety testing, dissolution of nanoparticles as a measure of biodurability and persistence was assessed to provide an insight on the behaviour of these particles in biological and environmental surroundings (Mbanga et a., 2021; 2022a; 2022b; 2023). Participation in Round Robin on OECD Test guidelines on dissolution was also conducted. Moreover, the assessment of lysosomal membrane permeabilization (LMP) as a prediction of the long-term toxic effects of nanoparticles is established as well as a new work item proposal was made to ISO. Within this project, the methodologies the methodology to assess free radicals using cyclic voltammetry is also established. Finally, culturing and characterizing representative alveolar- and bronchial-barrier co-culture models, at the ALI to investigate systemic translocation was also established.

For Environmental health: Nanomaterials synthesised in research laboratories and in industrial settings were tested for their environmental exposure (aqueous and diet) using aquatic model organisms (macroinvertebrates and fish). Bioassays are conducted in the National Bioassay Facility at NWU using zebrafish and daphnia as model organisms.

3. Safer Work Environment:

The important of exposure assessments has been influenced by a rapid increase in the mass production of nanomaterials and their application in various fields of work including water treatment, food technology, pharmaceutical applications and human care products. This development has also evoked increasing societal and industrial concerns regarding incidental release of nanoparticles which may threaten employee's safety. Exposure assessment was therefore conducted in South African research laboratories and also in industrial settings during the synthesis and handling of nanomaterials.

Safer product for consumer and the environment:

The section above has demonstrated that applications of nanoparticles can improve the efficiency of a wide range of consumer and industrial products. However, unlocking this potential requires a responsible and co-ordinated approach to ensure that potential challenges are being addressed in parallel with the development and use of nanotechnology. Safety assessment of nanomaterials should be incorporated in the early developmental stages of nano-enabled products rather than later where a nanomaterial has reached the market.

4. Safer and Sustainable by Design (SSbD)

The SSbD approach addresses the safety and sustainability of the material/product and associated processes through the whole life cycle.

Figure 2: Safe and Sustainable by Design

The SSbD concept refers to identifying and minimising the risks and uncertainties concerning humans and the environment an early phase of the innovation process: Hazard, Exposure. And End of life

Stakeholder Engagement Plan:

A plan to guide the engagement process between the project team with various stakeholders/parties throughout the life of the DSI Nano HSE Risk project. This is to assist in developing safer nanotechnology and enable the risk assessment of nanomaterials synthesized in South Africa to facilitate their exports internationally and support government in areas requiring regulatory solutions for nanotechnology. A case in point, SabinanoTubesTM was chosen to implement the SSbD approach. This industry said to be supplying carbon nanotubes (CNTs) and graphene and graphene oxide. In addition, they seem to produce a large list of nanomaterials including different metal based nanoparticles. Sabinano indicated that they recognise the importance of research and innovation for the sustainability of the company. They also indicate that the founder and partners of the company have solid experience in nanotechnology research and its applications. They also mention the importance of sustainable development with the application of green chemistry and engineering principles to nanotechnology (green nanotechnology) and to use a renewable energy source (e.g. solar, wind, biomass).

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ChemPharos: a comprehensive database of plastic-degrading enzymes, powered by Enalos Tools

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1. Introduction

The use of plastics, in everyday life, has contributed significantly to environmental pollution. In response to the escalating issue of plastic waste, natural degradation methods have emerged as potential waste management protocols. Notably, biodegradation by microorganisms has gained prominence as a preferred approach among environmentally conscious societies [1]. To address this environmental issue, we present ChemPharos, a database tailored for modelling-reading chemical datasets powered by the Enalos Cloud Platform [2] and demonstrate its use for rapid prediction of plastic degrading enzymes.

ChemPharos is a computational framework designed to store various data regarding chemicals, their properties and their functionalities, illustrated here via a dataset of enzymes that can degrade plastic polymers. The scope of the specific modelling-ready dataset is to harness cutting-edge Artificial Intelligence (AI) and Machine Learning (ML) tools for Micro and Nano-Plastics (MnNP) risk assessment as part of the EU-funded Marie Curie Training Network, Plastic Underground. The ultimate goal of the Plastic Underground instance of ChemPharos is to serve as a robust platform facilitating the seamless integration and automation of Molecular Dynamics (MD) simulations, enabling in-depth investigations into the impact of MnNP in soil and groundwater environments.

One of the key objectives of Plastic Underground is to fundamentally reshape MnNP risk assessment methodologies by integrating a comprehensive cloud-based platform with advanced data analytics and simulation functionalities. The deployment of ChemPharos aims to catalyse understanding of methods for remediation of plastic pollution in terrestrial and subterranean aquatic ecosystems. This platform is specifically designed to yield innovative insights into the behavioural dynamics of MnNPs and their subsequent environmental ramifications, thereby augmenting current strategies in environmental sustainability management.

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[4] School of Geography, Earth and Environmental Sciences, University of Birmingham, Birmingham B15 2TT, United Kingdom

2. Data Collection

MySQL was selected as the Relational Database Management System (RDBMS) for ChemPharos due its known fast performance, scalability, reliability, and robust security features. MySQL, being open source, offers cost-effective management of large datasets and facilitates seamless integration with server-side java scripting [3]. Moreover, its compatibility with cloud environments ensures seamless integration for deployment and scaling within the cloud infrastructure. Additionally, MySQL provides tools for administration, monitoring, and optimization, aiding in efficient database management and performance monitoring [4].

Integrating data from ChEMBL, an existing open-source bioactivity database that is regularly updated [5], enriches ChemPharos by providing valuable insights for Micro and Nano Plastic (MnNP) risk assessment. By integrating ChEMBL into ChemPharos, the Plastic Underground project aims to enhance automated molecular simulations and enable explicit data insertion and modification with well-defined authorization mechanisms.

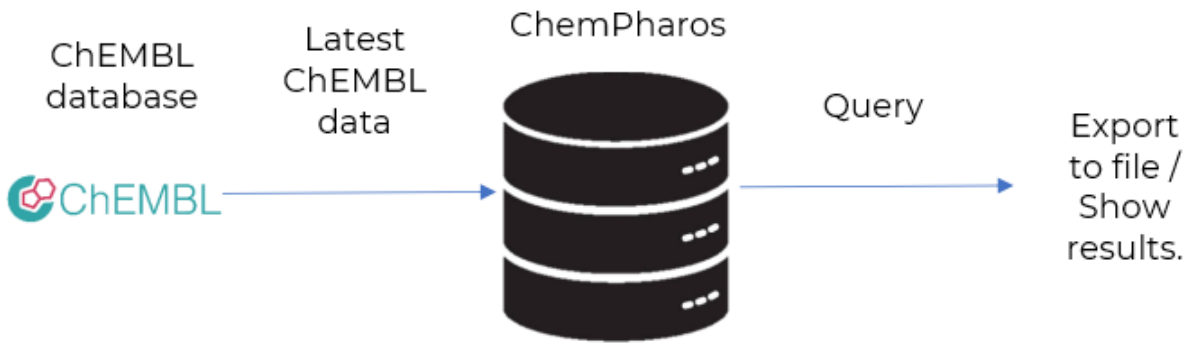

Figure 51: Proposed data workflow of ChEMBL and ChemPharos.

3. Tools

Java (https://www.java.com/en/) has been chosen as the backend server-side programming language of ChemPharos for its versatility, portability and robust ecosystem [6].

Javascript (https://www.javascript.com/) is used as the scripting language for visualisations, empowering the user interface with dynamic and interactive content. [7].

ZK Framework (https://www.zkoss.org/product/zk) and the ZK User Interface Markup Language (ZUL) has been selected for developing the front end due to its component-based architecture which facilitates modular development of the graphical user interface [8].

Keycloak (https://www.keycloak.org/) has been employed as the Identity and Access Management System for ChemPharos to ensure that only authorised individuals (curators) have access to sensitive data and functionalities. [9].

Wildfly (https://www.wildfly.org/) has been selected as the runtime server for deploying and running the Java based backend of ChemPharos.

4. User Interface (UI)

Figures 2 and 3 provide a shapshot of the user interface, and how the user selects the features of interest.

4.1 Search Configuration

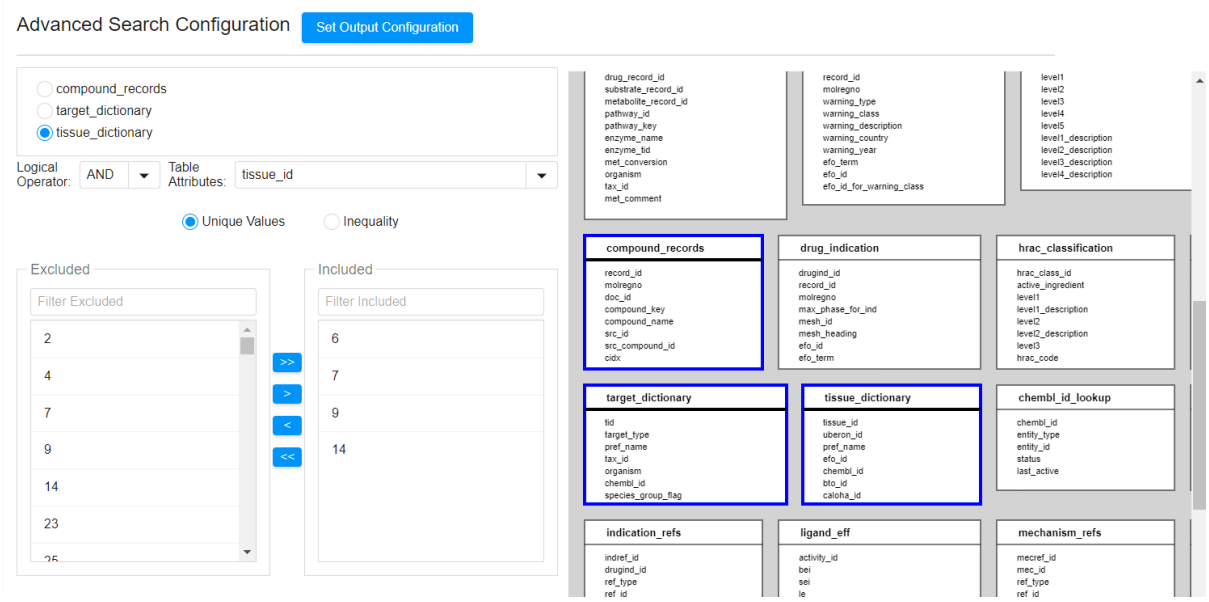

Figure 2: Advanced Search Configuration Page of ChemPharos.

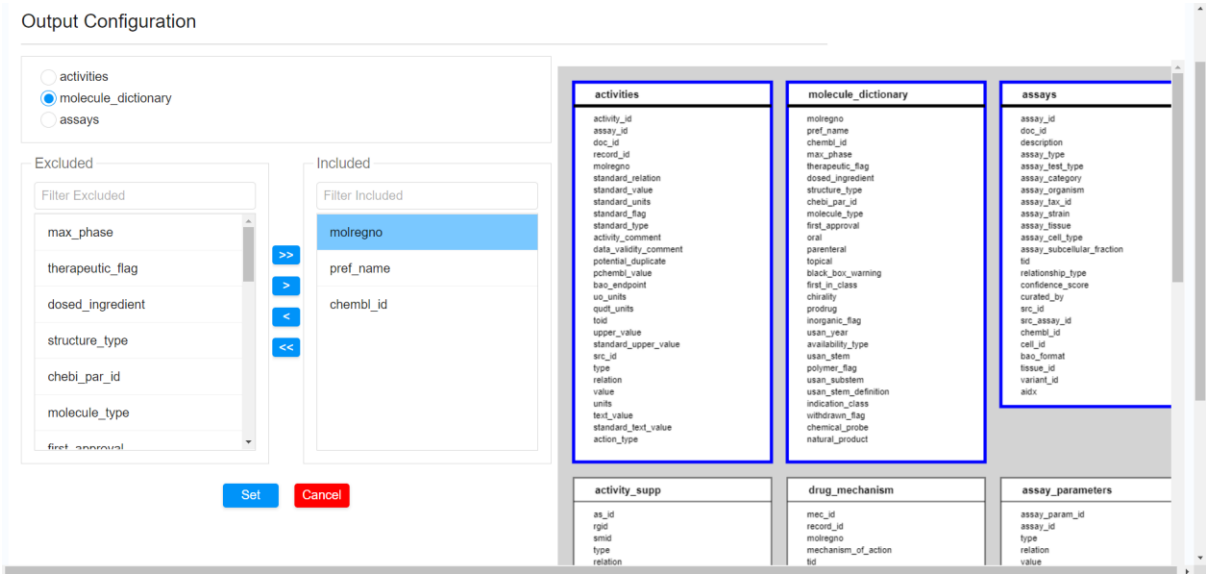

Figure 3: Output Configuration Page of ChemPharos.

5. Future Work

While ChemPharos is set for beta deployment on the Enalos Cloud Platform, upcoming enhancements are in the pipeline to elevate its capabilities, including:

- Optimisation of querying and export functionalities
- Paging of results
- AI and ML tools for MnNP risk assessments
- Automation of molecular dynamics simulations

These envisioned developments showcase ChemPharos' dedication to provide an adaptable, user-friendly platform that remains at the forefront of molecular data analysis and visualisation.

6. Conclusions

The ChemPharos platform provides an integrated and user-centric solution for molecular simulations and MnNP risk assessments. Fundamentally, the Plastic Underground instance of ChemPharos is designed not only to refine the process of MnNP risk evaluation but also to exemplify the progressive and collaborative ethos inherent in software development. This approach ensures that the platform remains adaptive and responsive, effectively addressing the dynamic needs and challenges faced by researchers and decision-makers in the scientific domain.

7. Acknowledgments

This work received funding from the European Union's Horizon Europe research and innovation program under the Marie Sklodowska-Curie Doctoral Network PLASTICUNDERGROUND (Grant Agreement No. 101072777)

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Integrated computational methods for the development of Safe and Sustainable-by-Design Innovative Advanced Materials: the case of surface modified nanophotocatalyst

Tomasz Puzyn[1,2], Alicja Mikolajczyk[1,2]

1. Introduction

The rapid development of Innovative Advanced Nanomaterials (IAMs) inevitably exposes organisms to multiple types and combinations of nanoparticles (NPs) at varying levels. Understanding the combined impacts of IAMs and their individual components, as well as predicting the toxicity of IAMs mixtures, is crucial.

The innovative design of IAMs, which considers environmental health and safety concerns alongside functionality, has become an integral part of the Safe and Sustainable by Design (SSbD) approach that has gained prominence in recent EU Commission policies. Accelerating the implementation of SSbD can be achieved through the application of artificial intelligence (AI) and digital tools, including Molecular Modeling (MM), Machine Learning (ML) algorithms, and Quantitative NanoStructure–Activity Relationship (Nano-QSAR) models, enabling early consideration of safety aspects in product design in a cost-effective and policy-compliant manner. However, due to the complex structure of Innovative Advanced Materials computational methods such as predictive ML-based models or Nano-QSAR methods to forecast specific properties and risk of more complex systems, remain limited. In our work, we propose for the first time an approach to support the characterization of IAMs at the theoretical level by developing additive descriptors of nanostructure. The development concept of additive nanostructure descriptors is motivated by the increased need for answering the question: How the structure and the structure modifications influence the functionality and activity of more complex systems such as IAMs? The proposed computational approaches that integrate additive descriptors for IAMs and Nano-QSAR models are the first step for the development of safe and sustainable by designing innovative advanced chemicals and materials.

2. Case study

The case study was developed for photocatalytic properties and *in vitro* cytotoxicity of 29 TiO_2-based IAMs (i.e., hybrids of more than two composition types of nanoparticles). They were evaluated using a combination of the experimental testing and supervised machine learning modeling. TiO_2-based nanoparticles combined with metal clusters of silver, and their mixtures with gold, palladium, and platinum were successfully synthesized. Two types of the activity, photocatalytic activity and cytotoxicity, were studied. A novel cheminformatic approach was developed and applied for the

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computational representation of the photocatalytic activity and cytotoxicity effect. In this approach, features of investigated TiO_2-based hybrid nanomaterials were reflected by a series of novel additive descriptors for IAMs (denoted as “additive descriptors for IAMs”) based on quantum chemical calculations. The obtained experimental data and calculated nanostructure descriptors were used to develop novel predictive Quantitative Structure-Activity Relationship computational models. The proposed modeling approach is an initial step in understanding the relationships between the physicochemical properties of IAMs, their toxicity, and photochemical activity under UV-vis irradiation.

3. Conclusions

We believe that knowledge based on theoretical evidence is critical for developing efficient SSbD strategies and Innovative Advanced Materials to assess hazards induced by combined exposure to multiple components of IAMs and to facilitate their modification with non-animal alternative methods at the earliest possible stage. Moreover, it helps considering properties of much more theoretically possible structures (virtual twins) at the virtual screening stage to select the most optimal ones to be synthesized and then experimentally tested.

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Session 7: Sustainability & Circularity driven by Advanced Materials

This Session is focussed on the contributions that materials R&I can make to improving the sustainability and circularity of products and processes containing or involving materials. The relevant improvement of sustainability and/or circularity may pertain to the functionality of a material (e.g. enhanced durability, energy efficiency) or of the product or process containing the material (e.g. improvement of the barrier or containment of a material within a product or process). Use of materials in delivery of the SDGs is also targeted.

Demonstration of improved sustainability (including safety) / circularity of processes through inclusion or use of advanced materials is encouraged.

Presentations (oral and poster) will also cover the following topics:

- materials R&I for the substitution of incumbent materials with greener, more abundant, safer alternatives,
- materials R&I for the improvement of the safety, sustainability and/or circularity of a material, product, or process (e.g., innovation of barrier materials),
- process innovation to improve the safety, sustainability and/or circularity of materials (e.g. innovation of containment, handling, or processing)
- structural or compositional changes improving the functionality of a material, product or process,
- Materials Optimization based on AI/computational studies, from screening to market, and
- demonstrations of improved sustainability/circularity of materials/processes/ products through application of the SSbD framework.

Detailed Programme

Start	End	Title	Presenter
11:10	11:30	Sustainability & Circularity driven by 2D-materials	Sofia Öiseth
11:30	11:45	Circularity of MAX phases: from worn parts and broken samples to 2D functional materials	Grzegorz Kubicki
11:45	12:00	The Safe and Sustainable by Design Framework applied to Graphene-based Materials	Fiorella Pitaro
12:00	12:15	The reproducibility of green synthesized nanomaterials: a study comparing the antimicrobial effectiveness of green-produced ZnO vs. fossil-based particles	Benjamin Punz
12:15	12:30	Safe-and-Sustainable-by-Design for Advanced Materials – A case study on the agricultural use of imogolites	Veronique Adam
12:30	12:45	Sustainable value chains in an emergent context: The case of BIO-SUSHY coatings	Jesse de Pagter

12:45 13:00 24/7 Poster Presentations

Posters

S07_P01	Cradle-to-Gate Life Cycle Assessment of Nano-enabled All-Carbon Recyclable Electronic (ACRE) Materials for Flat-panel Displays	Arianna Livieri
S07_P02	Life Cycle Assessment of Advanced Materials – The case study of graphene oxide in drinking water filters	Veronique Adam
S07_P03	Safe and Sustainable by Design framework for advanced materials: the HARMLESS approach	Veronique Adam
S07_P04	Life Cycle Assessment Applied to Antimicrobial Materials – Review of Studies	Beatriz Beccari Barreto
S07_P05	Application of the SSbD framework to biocidal nanocoatings: gaps and steps towards its implementation	Merve Tunali
S07_P06	Managing the complexity: tailored IATA for safe by design MCNMs	Elisa Moschini
S07_P07	Exposure of an alveolar model to aerosolised dry materials at the Air-Liquid Interface (ALI)	Aline Chary
S07_P08	Prospective dynamic probabilistic material flow analysis of advanced (nano)materials in Europe: moving forward to a Circular Economy scenario	Luis Mauricio Ortiz Galvez
S07_P09	Geopolymers: Highly Efficient Green Materials for Energy Storage Applications	Ioanna Giannopoulou

Oral Presentations: Session 7

Sustainability & Circularity driven by 2D-materials

Sofia Kihlman Öiseth[1]

The transformation into a sustainable society requires new thinking on many levels. We need to use less resources and reuse materials and products that are already in use. 2D-materials offer possibilities for more sustainable alternatives in many areas e.g. less material use due to additional strength, substitution of rare metals with more sustainable alternatives, reduced energy use, improved recyclability and longer product lives by increased wear resistance.

The Graphene Flagship was funded to ensure that Europe would maintain its lead in graphene research and innovation following the scientific breakthrough of graphene's isolation at the University of Manchester in 2004. This presentation will showcase some of the advances developed through the Graphene Flagship that will contribute to a sustainable future and circular material flow.

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Circularity of MAX phases: from worn parts and broken samples to 2D functional materials

Grzegorz Kubicki[1], Jakub Wiśniewski[1], Albert Kania[1], Dariusz Garbiec[1]

1. Introduction

MAX phases are a group of ternary compounds with the general formula $M_{n+1}AX_n$, where M stands for early transition metal, A – group 13 or 14 element and X – carbon or nitrogen atoms. Due to their unique mechanical properties, these materials has been extensively researched for over 20 years and have been proposed for multiple demanding applications [1], where high temperature oxidation and corrosion might occur [2]. By selective etching the A element of MAX phase, 2D structures – MXenes might be crated [3]. Those nanomaterials exhibit excellent functional properties making them promising materials for energy storage, EMI shielding, lubrication and many more applications [4]. As the M transition metals require energy-consuming refinement processes, and the MAX phases synthesis is also conducted by high-temperature synthesis, employing the circularity of MAX phase parts and samples will provide a cost-efficient MAX phase precursor source.

2. MAX phase synthesis

Synthesis of MAX phases is most commonly based on elementary powders mixing and high temperature sintering of said mixture[5]. While different mixing and sintering techniques may be applied, the reaction synthesis between the substrate materials results in crystallization of MAX phase ternary compounds, with some degree of secondary phases, like MX carbides or M-A intermetallic phases. Currently, numerous research papers report work on increasing the synthesis process yield, productivity as well as purity of the MAX phases.

3. Turning bulk sintered parts and worn elements back into powder

In order to create a bulk body, pressure is applied to promote the bonding between powder particles during sintering process. The exerted load upon the sintering tools tend to wear them down, increasing the possibility of their failure and loss of large quantities of costly material (Figure 1).

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Figure 52 Result of a failed sintering densification of MAX phase (about 600g of material)

Turning bulk bodies into powder is mainly conducted using a high temperature atomization process, that melts the material and quickly cools it by means of gas or liquid cooling agent. In the case of MAX phases, melting the material would result in the MAX phase decomposition to MX carbides, due to outward A element diffusion [6]. Such process is also energy-intense, as it requires to heat the substrate material to extreme temperatures in a short period of time. In order to avoid using a high temperature process, crushing may be applied using jaw crusher (Figure 2) in order to turn bulk bodies back into a powder form, ready for further processing.

Figure 2 Laboratory-grade jaw crusher with tungsten carbide crushing jaws

This process may be applied to failed sinters, electrical discharge (ED) machining leftovers (Figure 3), machining scraps as well as worn elements after surface cleaning process. This allows the implementation of fully circular approach that will result in increased cost-efficiency and eco-friendliness of MAX phase products and limit the usage of Critical Raw Materials such as titanium and chromium transition metals.

Figure 3 Leftover sintered preform after ED machining

4. MXene etching

In order to ensure the sustainability of the entire MXene supply chain it is necessary to provide an acid-free A element etching route, that ensures good quality of etched products as well as increased yield of the process. The SAFARI project aims to develop safe and sustainable by design ways to provide MXenes and their hybrid systems with aim to improve various end user applications, such as biodetectors with increased sensitivity, coating with improved EMI shielding performance and more [7].

5. Conclusions

The authors have proposed a cost-efficient route for fabrication of MAX phase precursor powders out of worn parts, failed sinters and process leftovers to be used for 2D MXene etching, reducing the cost of the final products. The crushing process has not affected the purity of the feedstocks in a significant way, confirming that recycled MAX phases may be employed without diminishing the functional properties of the products.

6. Funding

The research was funded by the European Union under GA number 101135965. Views and opinions expressed are however those of the author(s) only and do not necessarily reflect those of the European Union. Neither the European Union nor the granting authority can be held responsible for them.

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The Safe and Sustainable by Design Framework applied to Graphene-based Materials

Fiorella Pitaro[1,2], Stefan Seeger[2], Bernd Nowack[1]

1. Introduction

In 2022, the proposal for a framework that connects safety and sustainability aspects was disclosed by the European Commission with the main objective to boost innovation towards a toxic-free environment and retain the position as a frontrunner in this regard.[1] This safe and sustainable by design (SSbD) framework aims to identify and substitute the chemicals of high concern as well as point out safe and sustainable chemicals and materials to continue developing them. The years 2023 and 2024 are the periods of testing the framework and submitting feedback to improve and further develop the framework.[1] In this context, we performed a case study involving graphene-based materials (pristine graphene, graphene oxide, and reduced graphene oxide). Graphene and its relatives have gained interest after their discovery in 2004 thanks to their enhanced properties counting exceptional thermal and electrical conductivity, flexibility, and mechanical strength that are very desirable in the electronics and energy sectors.[2]

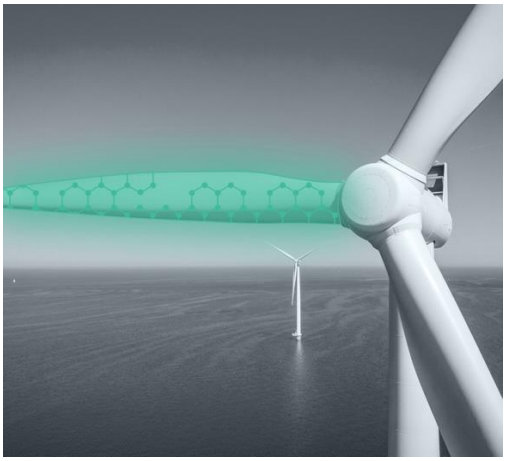

Figure 53: graphene-based additives in wind turbine blades are beneficial especially in harsh environments as they increase the strength and durability of coatings. Picture retrieved from sparctechnologies.com.au.

2. Methodology

To assess the operability of the framework applied to materials instead of conventional chemicals, the proposed approach was followed in this case study of graphene-based materials (GBM). The primary focus was placed on the evaluation of the applicability of

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the suggested models and tools to novel materials. Secondly, the framework was applied to the materials as the final product instead of predefining an application to evaluate to what extent the framework can be used if it is independent of a final application.

In Step 1 of the SSbD framework, a hazard assessment was conducted for each of the three GBM forms. The primary classifications were collected from the ECHA database and the missing hazard classes were evaluated and justified by data obtained from published papers and studies. For the occupational safety and health (OSH) assessment in Step 2, the Stoffenmanager Nano Module was used to perform an inhalation risk assessment of six different techniques to produce GBM. In Step 3 of the framework, the risk assessment during the final application phase, GBM in wind turbine blades was chosen as specific application. To conduct a complete environmental risk assessment, a published prospective material flow analysis (MFA) of graphene-based materials was used.[3] The MFA considers all flows along the life cycle and from all expected uses and allocates them into different compartments. To evaluate the impact of GBMs coming solely from the application in wind turbine blades, all other flows were set to 0. This approach allows us to estimate the exposure to humans and the environment by deducting the information from the overall consumption data and put in relation. Lastly, in Step 4, the environmental sustainability assessment was done by a function-based life cycle assessment where the reference product was a wind turbine blade without the addition of GBM. Finally, the scores of each step (1-4) are summed up to get an SSbD score.

3. Discussion and Results

Starting with the hazard assessment, graphene-based materials have not been fully classified under CLP. Based on the classifications available, all three forms pass the cut-off criteria suggested in Step 1. Nonetheless, the classification of respiratory sensitization and endocrine disruption (environment) was not possible due to a lack of data. These potential hazard classifications could change the final scoring of the GBM, and they wouldn't pass the cut-off criteria. While the hazard assessment step is resource- and time-demanding, it provides an overview of (eco)toxicological properties of the material and identifies data gaps and needs to allow a more accurate assessment.

The results obtained with the Stoffenmanager Nano Module show a risk priority level for the six production techniques. The chemical vapor deposition route resulted in the least risky one. Information requirements for this step are very extensive and data concerning the production of a material is often not given due to confidentiality reasons. Additionally, exposure estimation models for materials are not as developed as for conventional chemicals.

Continuing to Step 3, the environmental exposure of graphene-based materials present in wind turbine blades was estimated starting from a prospective MFA by Hong *et al*. To get the relevant PEC and PNEC values, all data from flows other than into wind turbine blades was removed. Compared to the overall exposure of all combined uses the environmental release is a very small amount since the majority of the GMB remains in in-use stock. From the human health perspective, the GBM are considered not to be hazardous since they are embedded into a polymer and hence lose the hazardous properties that come from the dusty nature of the material. On the other hand, the exposition is set to be zero since no clear information about possible abrasion of the graphene content is known. Additionally, there is no direct contact between consumers and the final application. The availability of a MFA is beneficial to conduct a risk

assessment that considers various uses and life cycle stages because it shows not only an absolute score but also relative amounts.

The LCA conducted in Step 4 show the changes in environmental impacts that come from the addition of GBMs in wind turbine blades respective to the blades that are GBM-free. This assessment requires a lot of different information and is not accurate until a certain degree of data certainty is achieved.

4. Conclusion

Overall, the SSbD assessment incorporates many safety and sustainability aspects that provide an overview of challenges, data gaps and other features of the GBM throughout their life cycle. Until there is no planetary boundary for novel entities to use the absolute sustainability concept, to evaluate the safety and sustainability of the GBMs, one specific application needs to be selected. Hence, the effort in terms of time, knowledge, and other resources for a single application is very high. To increase the efficiency of the framework especially when applied to non-conventional chemicals, models and tools need to be further developed.

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The reproducibility of green synthesized nanomaterials: a study comparing the antimicrobial effectiveness of green-produced ZnO *vs*. fossil-based particles

Benjamin Punz[1], Lisa Kleon[1], Vanessa Auer[1], Magdalena Weiß[1], Constantin Christ[1], Flora Boekhout[1], Patricia M.A. Farias[2,3], Olavo Cardozo[2,3], Andreas Stingl[2], and Martin Himly[1]

1. Abstract

The production of the annually required thousands, if not millions of tons of metallic nanoparticles typically involves the usage of fossil-based reagents and significant energy input. More and more different types of raw materials touch upon the planetary boundaries, and extensive energy consumption and high temperature requirements, as often applied during the production of nanomaterials, provide a long-lasting, negative influence on the environment. Driven by the goals of the European Green Deal, new concepts and approaches for green synthesis of nano- and advanced materials, therefore, attempt to combat these issues by reducing the generated environmental footprint, utilizing more sustainable and renewable products in the process. In this work, three different batches of zinc oxide (ZnO) nanoparticles were synthesized following the VERDEQUANT [1] green production process by Phornano. These batches were compared to fossil-based commercially available ZnO nanoparticles in respect to their antimicrobial effectiveness for generation of advanced surfaces, which has recently been defined as a priority research area in materials for the health and medical market by the Advanced Materials Initiative 2030 [2]. A number of physicochemical properties, like primary particle size, polydispersity and surface charge were investigated and compared. The dissolution rate & integrity of the nanoparticles and, thus, the potential toxic ion release was quantified by Inductively Coupled Plasma - Mass Spectrometry (ICP-MS) over time. Further, human safety concerns were taken into consideration by assessing the cytotoxic effects of the various ZnO nanoparticles on the identified two main areas of exposure, *i.e.* inhalation during the intended use as coating in face masks and dermal exposure during use on various surfaces, Hence, human lung epithelial cells (represented by A549 cell line) & primary human epidermal cells (keratinocytes) were used as models. In order to quantify functional performance, as ZnO nanomaterials have been well reported for their antimicrobial effectiveness, the different candidates (production batches) were assessed for several criteria and compared against bacterial, fungal and pseudoviral representatives. In line with the recently proposed holistic concept of evaluating safety and sustainability aspects well in relation with functional performance, we developed a novel antimicrobial scoring system to allow the direct comparison of results between unrelated assays and readout-methods and enable

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quantitative approaches that can be adopted by the Safety-and-Sustainability-by-Design (SSbD) [3] approaches. Results showed a comparable, if not better antimicrobial effectiveness, whilst posing minimized toxic effects to the investigated human cells. Similar and comparable results between green and fossil-based materials already represent vast improvements, since the significant reduction of energy and investment of renewable resources by green synthesized materials pose a tremendous advantage compared to conventionally produced materials.

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3. Acknowledgements

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Safe-and-Sustainable-by-Design for Advanced Materials - A case study on the agricultural use of imogolites

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1. Introduction

Following the European Commission Recommendation for a European assessment framework for 'safe and sustainable by Design' (SSbD) chemicals and materials (European Commission 2022), the HARMLESS project built a SSbD framework tailored to Advanced Materials (AdMa). Based on this framework, an online Decision Support System, directed towards innovators, is being created.

2. Materials and method

In this study, functionalised imogolites developed for agricultural purposes (imogolite_OH, imogolite_CH_3, Cu-doped imogolite_CH_3) are taken through a flexible stage-gate innovation process and used to test the HARMLESS framework and decision support system. At the ideation and business case stage, the HARMLESS WASP module, composed of 14 questions to the user, raises potential concerns on safety and sustainability aspects of the different imogolites versions. At the second innovation stage (i.e. lab phase), key physchem, exposure, hazard and sustainability descriptors are measured to further define potential issues on the aspects that raised red flags.

3. Results

Differences among imogolite versions mainly come from increasing the complexity in terms of multi-component composition. Hazards could arise from components issued from the pristine materials such as gibbsite, alumina, silica, methyltrihydroxysilane and copper. Nevertheless, these AdMa show benefits towards sustainability as compared to benchmark materials (such as Cu salts), as they require less use of Cu. The contribution to several Sustainable Development Goals (SDGs) as defined by the United Nations, such as sustainable food production (SDG 2), efficient use of resources (SDG 12) or clean water

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and sanitation (SDG 6) will be discussed regarding their composition and potential functionalities.

4. Outlook

The quantitative SSbD assessment currently taking place at lab phase on physchem characteristics (e.g. size, composition, dissolution rate), toxicity (e.g. inflammation potential, cytotoxicity) and sustainability descriptors (e.g. use of critical raw materials, release of hazardous chemicals) feeds the discussion on the balance between risks, benefits, costs and performance of each imogolite version and helps the selection of the most appropriate version to take to pilot phase.

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Sustainable value chains in an emergent context: The case of BIO-SUSHY coatings

Jesse de Pagter[1], Stefan Philipp[1]

1. Introduction

Advancing insights into the impacts of polyfluorinated alkyl substances (PFAS) on the environment and human health have brought about a mix of increasing public pressure, strengthened activism, and new regulatory developments.[1] In this emergent but insecure context, the search for sustainable PFAS-replacements is becoming increasingly prominent. As this issue has gained momentum, R&I funding on the topic is currently on the rise. Furthermore, this also fits into a wider trend of different sustainability transitions, which has led to a general increase in attention for biobased, sustainable materials that are to be developed on the basis of Safe and Sustainable by Design (SSbD) approaches.

The Horizon Europe-funded BIO-SUSHY project can be seen as part of this development as it targets to develop three PFAS-free novel coatings that are envisioned to be applied in textile, food packaging, and cosmetic glass. The goal is to create high-quality, durable, sustainable composite coating solutions that can replace PFAS-based coatings. This contribution reports on important aspect of the project's strategy: the focus on promoting the resilience, sustainability, responsibility of the value chains in each of the different coating solutions. This contribution is meant to discuss the ways in which these value chains can be strengthened in the volatile context that we operate.

2. The volatile context of alternatives to PFAS coatings

There are a few specific developments that spur the insecurity that characterizes the establishment of sustainable value chains. First, especially in its commitment to include a wide group of stakeholders, it is pivotal to engage with current regulatory developments when it comes to new PFAS regulation under REACH. Crucially, there is an important role that the availability of alternatives play in the proposal. [2] While such a ban can on the one hand create demand for biobased coatings, the insecurity around its approval and implementation makes for a high level of insecurity. Second, PFAS awareness is currently rising, leading to a rather high level of controversy around the topic.[3] This is generally often driven by pollution scandals, while also a rising number of consumers and consumer organizations are becoming engaged with PFAS in consumer products. PFAS, in this regard is becoming an increasingly widespread household term with negative associations. While this is generally creating an opening for alternative solutions, it also creates a situation where different stakeholder groups can subscribe to different realities that increase tension, thus makes it difficult to come to a consensus on establishing progress towards new equilibria. Third, the development process of PFAS alternatives needs a continuous range of new impulses in order to become properly established. This particularly concerns investments that can push the technology readiness level of the coatings, in order to accelerate a convincing substitution of PFAS-

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based coatings. Fourth, in a global context there is a rising need for elevating the resilience of value chains. While on the one hand the challenges in this regard (e.g. energy insecurity, pressures on global trade, worries over international competitiveness) help to establish the conviction that there is a need for broader change in the coatings industry, it also contributes to a more volatile context.

3. Towards durable value chains

Important to note here is that was never going to be easy to establish an innovation framework that aims to include different elements towards more just, safe, socially robust, resilient, and sustainable value chains. In general, the aim to include such elements in the early stages of R&I processes, contains a certain commitment to grapple with highly contingent and controversial issues. Instead of discrediting this volatility, our aim is to mobilize it in order to help building visions towards stronger, more sustainable value chains.[4]

Therefore, in the BIO-SUSHY project we try to anticipate on the abovementioned insecurities in different ways. First, it is done by building in different kinds of analysis and methods that are explicitly meant to include a wide variety of stakeholders and keep an eye on a range of issues. This helps to maintain a strong focus on the resilience and sustainability of the value chains, early on in the process. In the BIO-SUSHY project we do this by combining the overarching goals of SSbD development with a quadruple helix approach to the understanding of the innovation ecosystem. Second, a useful way to anticipate uncertainties is to gain a clear and neutral overview of the controversies that play a role for the relevant value chains. Not only does this help to understand the context, but it also is useful way of anticipating the possibility of change in the different value chains. Third, a good way to embed different insecurities in their wider context is by clear understanding of the broader trends in which the innovation ecosystem is embedded. In BIO-SUSHY we focus on understanding environmental issues and public health around PFAS to gain a better insight into the potential of biobased coatings. Furthermore, in direct relation to that we have studied the social setting and issues around public trust. Combined with that we also closely monitor regulatory developments as well as general trends in the chemicals industry when it comes to biobased materials and the potential for large scale transformative innovation. Fifth and final, we focus on the concept of interdisciplinarity as a basis for innovative approaches. This is mainly manifested through looking at different methods that can be combined to come to actionable solutions. Prominent examples from the BIO-SUSHY project include combining (Social) Life Cycle Assessment (SLCA & LCA) with co-design approaches and issues around social acceptance in the different value chains. Another example can be found in the way computational tools for SSbD can be combined with approaches focused on stakeholder involvement.

4. Conclusions

Finding replacements for PFAS-based coatings is inevitably linked to a range of challenges. From challenges in terms of quality of the coatings, to regulatory developments, to industry trends, to consumer preferences. Nevertheless, with the right focus it is possible to contribute to the right mix of innovations and measures in order to come to more sustainable solutions that increase the well-being of many.

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Poster Presentations: Session 7

Cradle-to-Gate Life Cycle Assessment of Nano-enabled All-Carbon Recyclable Electronic (ACRE) Materials for Flat-panel Displays

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1. Introduction

The production of semiconductor components causes the usage of various acid/base solutions, organic solvents, and toxic gases releasing highly polluting toxins, wastewater, and waste gas (Lin, Lin, e Lu 2019). Additionally, the manufacturing processes of silicon- or metal oxide-based semiconductor materials for devices like flat-panel displays are known to release high levels of greenhouse gases (GHGs) into the atmosphere. Indeed, the semiconductor industry makes up 1.3–2.0% of the overall electricity usage in the manufacturing sector in the US. (Kuo, Kuo, e Chen 2022). In response to this problem, the *LEAP-HI: All-Carbon Recyclable Electronics (ACRE) Realizing a Sustainable Electronics Lifecycle* project, awarded by the National Science Foundation, aims to develop all-carbon recyclable electronic (ACRE) materials as a more environmentally friendly alternative to traditional semiconductor materials. A transistor typically consists of various components constructed using silicon- or metal oxide-based semiconductor materials. In the case of an ACRE transistor, these components are replaced with materials in the form of ink such as crystalline nano-cellulose (CNC), carbon nanotubes (CNT), and graphene. By using carbon-based materials, the expectation is to significantly reduce the emissions associated with electronic manufacturing processes. This study aims to conduct a comparative cradle-to-gate life cycle assessment (LCA) between ACRE thin-film transistors (TFTs) and classic TFTs. A classic transistor is considered as a transistor already available on the market, modelled thanks to ecoinvent database. By comparing the environmental impacts of these products, it is possible to better understand the potential benefits of switching to ACRE materials in terms of such factors as reducing GHG emissions to mitigate climate change.

2. Materials and methods

LCA is a methodology used to assess the environmental impacts associated with a product, process, or activity throughout its entire life cycle, from raw material extraction to end-of-life disposal. The LCA results provide valuable insights into the environmental performance of different products and can help identify areas for improvement. In this

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study ACRE TFTs are compared with two classic TFTs. The functional unit of the assessment, which is a quantified performance measure used to define the function of a product or system, was defined as “the production of 4 transistors”. The production of 4 transistors, rather than just 1 transistor, has been chosen with the aim of encompassing all relevant data collected for the ACRE TFTs within the LEAP-HI project. Any alteration to this unit would necessitate making assumptions that would bring additional uncertainty to the assessment. The two selected benchmarks are represented by “the production of 4 classic transistors”, and “the production of 4 classic transistors with the same weight of the 4 ACRE TFTs”. The latter was chosen to balance the weight of the ink used to print the 4 ACRE TFTs, which, due to technical issues encountered in the initial development phases, leads to an overestimation of the overall weight of the 4 TFTs. Therefore, four classic transistors, each weighing the same as four ACRE TFTs, were selected as a secondary benchmark to a more appropriate comparison scenario than the significantly lighter primary benchmark. In the next paragraph, the results of the comparative cradle-to-gate LCA are reported.

3. Results

In this section, the comparative LCA between the production of 4 ACRE TFTs, the production of 4 classic transistors and the production of 4 classic transistors with the same weight of the 4 ACRE TFTs is presented. Figure 1 displays the characterized endpoints across the various examined categories. The characterized endpoints included human health impacts such as respiratory diseases, cancer, and neurological disorders. Environmental impacts were also assessed, including climate change, acidification, eutrophication, and ozone depletion. Additionally, resource depletion and ecosystem quality were considered in the LCA analysis. Overall, the characterized endpoints highlighted the potential negative impacts of the product throughout its life cycle. For each impact category, the higher impacts are related to the production of 4 classic transistors with the same weight of the 4 ACRE TFTs. Additionally, the lower impacts are related to the production of 4 ACRE TFT for all the impact categories except for one. Indeed, the least relevant contribution to the “fossil resource scarcity” impact category is provided by the production of 4 classic transistors.

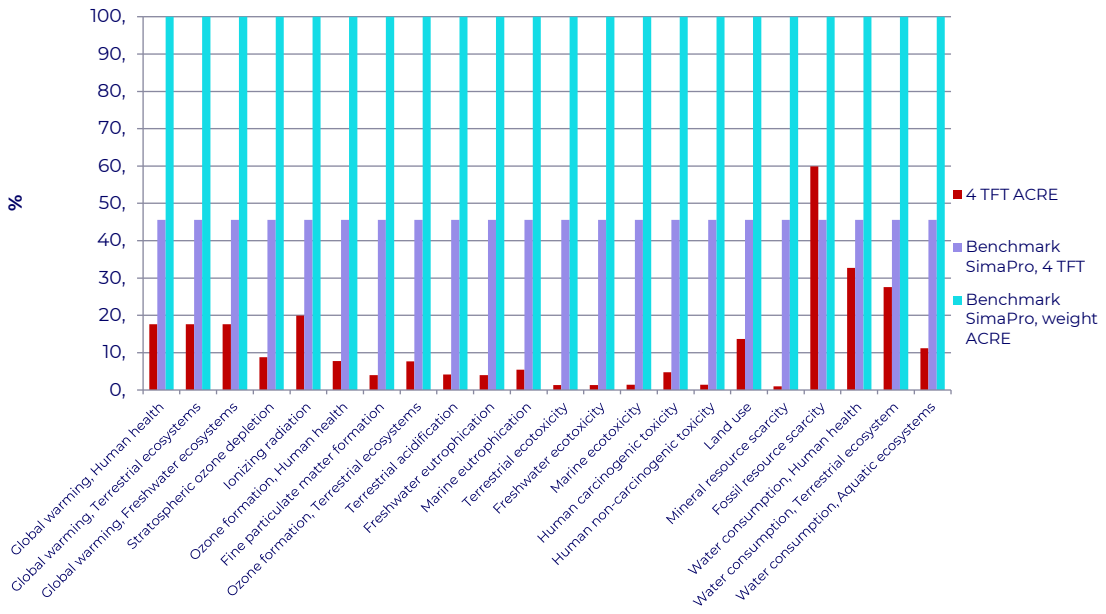

Figure 54: characterized endpoints for "4 ACRE TFT" compared to "4 classic transistors" and "4 classic transistors with the same weight of the 4 ACRE TFTs"

4. Conclusions

This study showed a comparative cradle-to-gate life cycle assessment (LCA) between the production of 4 ACRE TFTs, the production of 4 classic transistors and the production of 4 classic transistors with the same weight of the 4 ACRE TFTs. By comparing the environmental impacts of these materials, it was possible to understand the potential benefits of switching to ACRE materials in terms of reducing the environmental impacts, specifically reducing GHG emissions thus to mitigate the climate change. Indeed, it is important to consider these endpoints when making decisions about the product's design, production to minimize its environmental and human health impacts. Further research is needed to explore potential improvements and alternatives that could reduce these negative endpoints and promote sustainability in product life cycles.

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Life Cycle Assessment of Advanced Materials – The case study of graphene oxide in drinking water filters

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1. Introduction

The European Commission, in its Recommendation for the implementation of a framework for safe and sustainable by design (European Commission 2022), advises to use Life Cycle Assessment (LCA) to evaluate the environmental sustainability of chemicals and materials. LCA is a standardised methodology (ISO 2006a, 2006b) to assess the environmental impacts of a product lifecycle across various impact categories. However, its applicability to Advanced Materials (AdMa) can be challenging due to lack of data, pertaining to the novelty of these materials and the products in which they are embedded.

2. Case study

Graphene oxide (GO) is used in drinking water filters to enhance their functionality and enable the removal of molecular-level emerging contaminants such as PFAS, metal ions and antibiotics. This case study is investigated within the MACRAME project with a contribution analysis of the flows and unit processes of the filters production to various environmental impacts, including climate change, resource use and ecotoxicity.

The lifecycle inventory was built on exchanges of information with the filters producer, enabling the use of first-hand foreground data, but several data gaps still needed to be covered. The Lifecycle Impact Assessment shows the contributions of different flows and unit processes to environmental impacts; the need for a GO-specific characterisation factor is discussed. The potential implications of these results on the design of the industrial process and on the environment are discussed.

3. Outlook

The filter use and end-of-life will be investigated in continuation of this work to obtain a cradle-to-gate LCA, and the lifecycle impacts of these filters will be compared to the benchmark product (i.e. same filter without GO). This work contributes to the sustainability assessment of AdMa; it will be considered in the GO drinking filter production in the aim of making it as sustainable as possible.

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Safe and Sustainable by Design framework for advanced materials: The HARMLESS approach

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1. Introduction

The European Framework for 'safe and sustainable by design' chemicals and materials (Caldeira et al. 2022) represents an important step towards the production of safer and more sustainable products. Yet, it requires resources not compatible with the expected commercial value at early innovation stages and recommends methods that are not applicable to emerging materials. To address such issues the HARMLESS project developed a SSbD framework that considers data availability and resources along the innovation process, is applicable to Advanced Materials (AdMa) and is cost-effective. It is aligned with the EU framework, complemented with a flexible stage-gate model and implements New Approach Methodologies (NAMs) tailored to AdMa.

2. SSbD framework

The HARMLESS SSbD framework includes three innovation stages (Figure 1): ideation and business phase, laboratory phase and pilot phase. It starts with the categorization module of AMEA (Advanced Material Earliest Assessment) at the first innovation stage, testing the applicability of the Framework to the business case. At each innovation stage, five different modules enable the assessment of 1) intrinsic safety, 2) occupational and environmental safety at production, manufacturing and end-of-life, 3) consumer and environmental safety at use, 4) environmental sustainability at production and manufacturing and 5) environmental sustainability at use and end-of-life.

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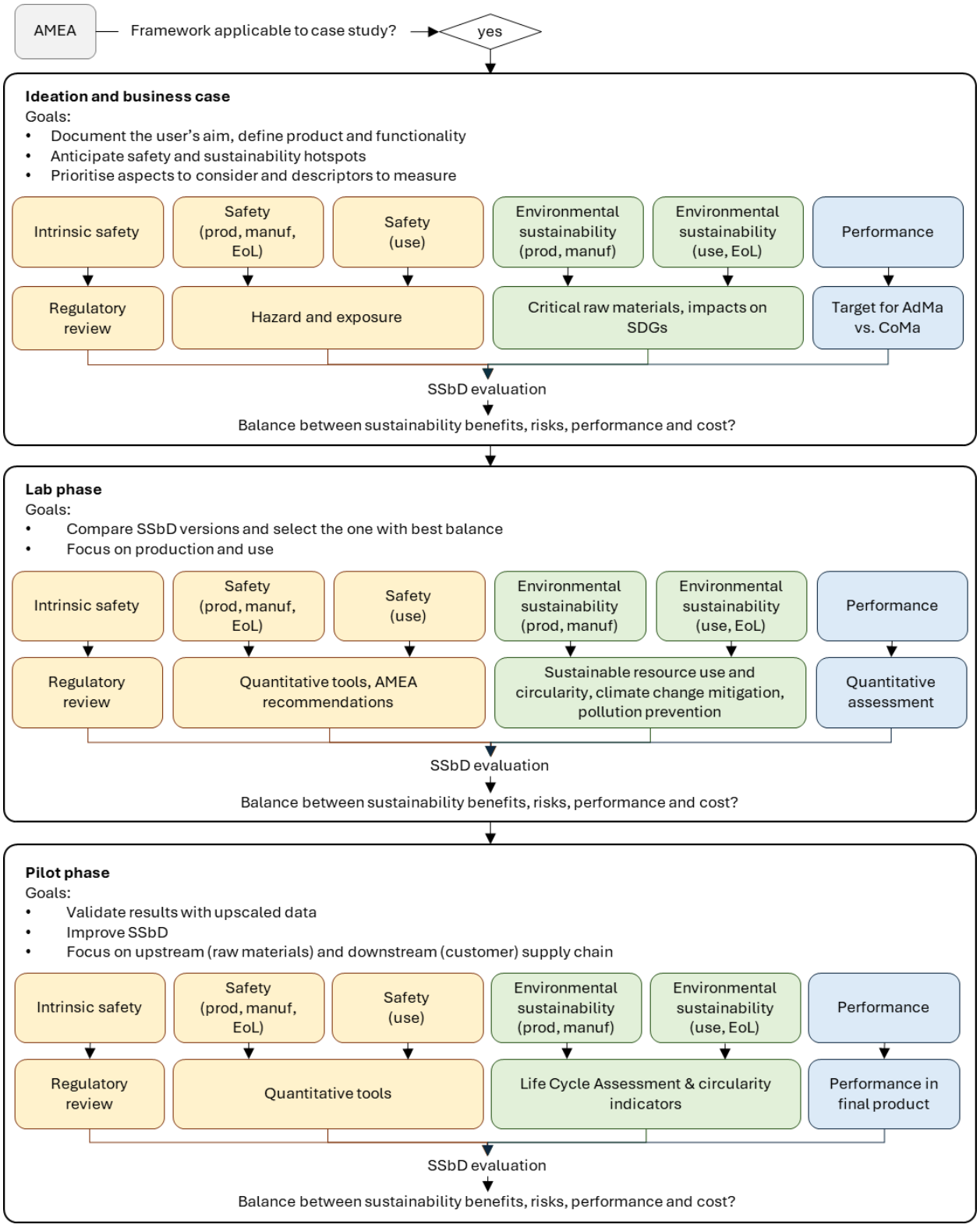

Figure 55: Overview of the HARMLESS SSbD framework

Within each module, design principles are given to guide the user in making a product as safe and sustainable as possible, and methods and tools are suggested to facilitate the SSbD assessment. NAMs are prioritized to make the SSbD assessment as cost-effective as possible. After all modules are completed, a gate enables the user to balance the safety and sustainability of their product with cost and performance, assessing the

relevance of going to the next innovation stage. This framework guides the creation of an online decision support system, which will be publicly available. The framework has been further tested with industrial case studies from the HARMLESS project.

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Life Cycle Assessment Applied to Antimicrobial Materials – Review of Studies

Beatriz Beccari Barreto[1], Tommasso Serchi[1], Enrico Benetto[1]

1. Introduction

The European Union Green Deal has set the ambitious goals of (i) zero net emissions for greenhouse gases by 2050, (ii) economic growth decoupled from resources use, and (iii) no person nor place left behind (European Commission, 2020). One of the corner stone of this ambitious plan is the full implementation of the safe and sustainable by design (SSbD) framework, which is necessary to address the changes and challenges of modern society and makes the EU a step closer to the Green Deal objectives and to tackle the problem of toxicity and sustainability as early as possible.

However, lack of stakeholders' coordination, limited access to relevant data, and absence of standardised methods have thus far hampered the emergence of a comprehensive approach to SSbD. The project INSIGHT - Integrated Models for the Development and Assessment of High Impact Chemicals and Material[2] aims to overcome these challenges by developing an innovative framework for mechanistic impact assessment of chemicals/materials.

The INSIGHT's framework will be applied to case-studies covering different industrial segments and including antimicrobial materials (metal-oxide based UV-C-upconverters in novel coatings). The main materials used for antimicrobial coatings are graphene materials, graphene-like two-dimensional materials, polycationic hydrogel, silver nanoparticles, dendrimers, copper and its alloys, and polymer brushes. These features can be applied to a wide range of materials, including metals, plastics, textiles, and ceramics, making them suitable for diverse applications, e.g., medical, textile, and food and beverage. Despite their benefits, antimicrobial coatings can rise the potential environmental impacts of a product. As a result, environmental assessment in the form of life cycle assessments (LCA) have been conducted to understand the full extent of the potential impacts.

A literature review of the LCAs for antimicrobial materials is necessary to comprehend the data available, the method used, and how far this topic has advanced so far. Thus, the aim of this study is to provide a review of the LCAs produced for antimicrobial materials.

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Application of the SSbD framework to biocidal nanocoatings: gaps and steps towards its implementation

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1. Introduction

The Safe and Sustainable by Design (SSbD) Framework has the aim to facilitate the design and development of chemicals and materials to be safe and sustainable through research and innovation initiatives. The framework considers the intrinsic hazards of a chemical or material, environmental and human safety during production, use and disposal as well as environmental sustainability through life cycle assessments. The result of the assessments provides a score that indicates the level of SSbD [1]. The SSbD framework is currently in the development and testing phase, and presently, there are no specific approaches available for specific groups of chemicals or materials. In particular it is unclear how functional and societal benefits can be included within the SSbD Framework. Biocides, for instance, are being used for the protection of living organisms against infectious diseases. Nevertheless, their impact may extend beyond controlling the intended harmful organisms, potentially affecting humans and non-target organisms in the environment. Biocides are also being promoted to achieve several United Nations Sustainable Development Goals, however, it is so far not possible to consider this within the SSbD [2]. Thus, due to the dual nature of biocides—offering benefits and carrying negative effects caused by their nature as being toxic to target organisms— a specific SSbD approach considering their functionality is crucial for evaluating their safety and sustainability alongside societal benefits. Sudheshwar et al. (2023) also suggested SSbD should place greater emphasis on the material and chemical functionality and their practical advantages [3]. An approach therefore needs to be developed to incorporate the benefits derived from the use of biocidal products into the general SSbD framework.

2. Materials and Methods

First, the data and methodological challenges to apply the current SSbD framework to biocidal products was assessed considering hazard assessment, environmental and human safety during production, use and disposal as well as environmental life cycle assessment in this phase. Secondly, to examine the benefits of using biocides, we considered methodological approaches that can be integrated into the SSbD framework, along with a discussion. The overview of the study can be seen in Figure 1.

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Figure 1: Overview of the study

3. Results

Some of the gaps observed were based on data requirements. To give some examples from Step 1, for instance, certain hazard classes identified in SSbD Step 1 are not currently recognized as hazard classes under CLP, indicating a misalignment between the two classification systems. Not having clear classifications, along with missing data and difficulty in figuring out classifications, creates significant obstacles. Our analysis underscores the demand for a high level of expertise in both the assessment and conclusive determination of hazard classes. The study also emphasizes the need for a good understanding of data generation due to the complex information involved. Problems also arise in getting and assessing literature data because of a lack of tools and the complicated nature of the information. The prevalence of technical and lengthy reports further adds to the intricacies encountered in navigating these classification challenges. Our discussion also includes the possible methodological differences that can be followed in Step 2, and 3. The second important point is that, even though the benefits of biocides are considered in The Biocidal Products Regulation [4], the benefits for society are not yet considered in SSbD. This may not only be applicable to biocides but also to other chemicals/materials. Thus, the functionality of the assessed chemical/material plays an important role within the SSbD Framework. We developed several criteria to be considered within the SSbD framework to account for functionality and follow a holistic approach. While a more comprehensive approach is needed for the biocides that are already on the market, a more simplified approach is needed for the early design stage of biocidal coatings due to limitation of the data. As many data are required to complete an SSbD assessment, this is obviously not possible for the materials at an early state of innovation.

4. Conclusion

In summary, our investigation addresses data limitations, complexity, and various methodological approaches for Biocidal-Spesific SSbD Framework. Moreover, the oversight of societal benefits in SSbD has led us to develop criteria for a holistic approach through the integration of benefit assessment.

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Managing the complexity: tailored IATA for safe by design MCNMs

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1. Introduction

The fast development of a variety of new materials with enhanced properties and heterogeneous composition is introducing new challenges in terms of their (eco)toxicological hazard evaluation. Different approaches to replace a complete case-by-case experimental assessment are currently under development. Within the SUNSHINE project, an integrated approach for testing and assessment (IATA) to guide users in the decision-making process for the prioritization of testing and the implementation of safe by design (SbD) strategies during the early innovation stages of multicomponent nanomaterials (MCNMs) has been proposed, based on a previous work (Murphy et al., 2021). The tool is based on a framework combining both experimentally and *in silico* generated data, with existing information retrieved from literature. The framework has been applied to different case studies to evaluate the suitability for its implementation at the industrial level.

2. Methodology

The first step for the application of the framework is setting the boundaries of the specific *case study* through i) the selection of the target MCNMs and the single components, ii) the identification of a specific hotspot of exposure (posing concerns either for human or

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environmental health) by analysing the life cycle of the MCNMs and iii) the formulation of a potential mode of action (MoA).

Then, a stepwise approach aiming at the formulation and verification of hypothesis, linking one-by-one, the relevant physicochemical properties of the MCNMs and the enhanced properties (*what they are*), to the fate (*where they go*) and the potential hazard (*what they do*) is suggested. Previously identified putative source materials (e.g., precursors, single components) undergo to the same evaluation. The verification or rejection of the hypothesis through the application of the similarity concept allows to justify or to exclude the possibility of grouping the MCNMs (prior or after SbD modifications) with their single components or with arbitrary chosen data-rich materials used as benchmarks. This process is iterative and allows the continuous modification and verification of the grouping hypotheses.

This specific work wants to show how the framework has been applied to selected industrially relevant MCNMs to guide their further improvement in term of safety. First and second generation (*Tier1 and Tier2*) MCNMs (prior and after SbD modifications) have been assessed.

Case study 1: *Tier1* SiC@TiO_2 MCNM represents a promising replacement of PTFE for the coating of aluminium trays used in the baking industry, because of their anti-stick properties. Concerns have been raised about potential occupational exposure by inhalation of workers involved in the handling of the MCNM in powder form during the tray production process. SiC@SiO_2 has been proposed as *Tier2* MCNM with comparable functionality and lower safety concerns. Internally generated hazard data obtained by *in vitro* testing using a model relevant for the specific MoA has been combined with existing data on the MCNMs an as well on their single components. Each of the tailored hypothesis has been evaluated based on similarity assessment.

Case study 2: bentonite-clove oil (*Tier1*) has been proposed as effective anti-pest MCNM to be embedded in LDPE food packaging. Concerns have been raised about potential release in the environment of the MCNM and its single components in the water compartment. A modified formulation of the *Tier1* MCNM obtained through the addition of stabilisers has been evaluated. Internally generated hazard data obtained from the application of acute and chronic toxicity test on ecotoxicologically relevant organisms has been combined with literature data on the same MCNMs and the related single components.

3. Results

For each case study, a matrix highlighting the minor/major impact of the different hypotheses has been drafted and, depending on the evidence of similarity, grouping of the MCMNs with single components or benchmark materials has been suggested. All together, these outputs were used for the prioritisation of additional testing (Case study 1), or to justify the implementation of SbD strategies at the initial stages of product development helping the user in the choice of safer alternatives (Case study 2).

4. Conclusion

The SUNSHINE framework proved to be a flexible tool for information gathering especially at the early stages of product development. However, the integration of

computational tools helping in streamlining data extraction and performing a targeted and systematic review might help to make it a more powerful tool for faster screening and comparison of different SbD alternatives.

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6. Acknowledgements

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Exposure of an alveolar model to aerosolised dry materials at the Air-Liquid Interface (ALI)

Aline Chary[1], Charlotte B. A. Stoffels[1], Carla Ribalta[2], Dirk Brossell[2], Rob Vandebriel[3], Tommaso Serchi[1]

1. Introduction

The MACRAMÉ project (for Advanced Characterisation Methodologies to assess and predict the Health and Environmental Risks) is dedicated to creating a structured approach for studying in vitro inhalation toxicology through a series of in vitro and ex vivo models that mimic the biological complexity of the human respiratory system, including both the upper and lower airways. This project will conduct rigorous testing, validation, and implementation of various biological models that reflect the human respiratory system, focusing on the bronchial region (upper airways) and the alveolar region (lower airways). Currently, there exists a noticeable data gap concerning the suitability of these models for nanomaterials and advanced materials. MACRAMÉ seeks to validate the efficacy of these proposed methodologies in assessing such inhalable pollutants. In this context, it is essential to assess various exposure devices to establish a decision tree for selecting the most suitable device and biological system depending on the nature of the material and biological endpoint of interest.

2. Method

In this study, a monoculture of A549 cells grown on the membrane of transwell inserts at the Air Liquid Interface (ALI) was used as a model for the alveolar barrier. Given the technical challenges and reduced relevance to in vivo conditions associated with dispersing advanced materials in liquid such as cell culture medium, the PowderX device (Vitrocell®), which allows aerosolization of dry powders, was evaluated.

The cells were exposed to varying doses of reference materials (Quartz DQ12, Corundum nanoparticles, and multi-walled carbon nanotubes (NM-401 from JRC)) at the ALI using the PowderX device, which was then compared to semi-ALI exposure. Semi-ALI exposure utilizes a reduced volume of medium, unlike the traditional submerged exposure, ensuring that it just covers the entire surface of the membrane insert, which then evaporates to restore ALI conditions.

The metabolic activity of the A549 cells was evaluated using the Alamar Blue assay, while the production of reactive oxygen species was quantified via flow cytometry. The production of key cytokines was evaluated by Luminex in both the apical wash and in the basolateral compartment. The cellular localization of the particles was determined using light microscopy on Richardson-stained cell sections.

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3. Conclusion

The use of the PowderX facilitates the exposure to dry materials, eliminating the need for a dispersion protocol and allows to obtain dose-response curves for each tested material. However, since PowderX can only accommodate exposure to four wells simultaneously, it does not support high-throughput screening. In contrast, the semi-ALI exposure method is more cost-effective for such applications.

Prospective dynamic probabilistic material flow analysis of advanced (nano)materials in Europe: moving forward to a Circular Economy scenario

Luis Mauricio Ortiz-Galvez[1], Lora Dameska[1,2], Roland Hischier[1], Bernd Nowack[1]

1. Introduction

Climate change, chemical pollution, and circular economy are currently key points in the European policy agenda, for instance, in the EU Green Deal [1], the Circular Economy Action Plan [2], the Chemicals Strategy for Sustainability [3], and the Zero Pollution Action Plan [4]. Therefore, industry needs to ensure that the production and consumption of innovative materials are safe and sustainable along the value chain.

"Advanced materials" (AdMa) is a term broadly used by many researchers since years [5]. The term AdMa usually refers to innovative materials that are rationally designed through the control of their composition and structure or materials that are produced or transformed through advanced manufacturing techniques, in order to fulfil new functional requirements [5-9]. Implementing AdMa in different industrial sectors can be an alternative to achieve the European policy goals [9]. For example, in aeronautics, making lightweight airplanes; in construction, implementing technologies to improve energy efficiency and increase circularity; and, in semiconductor manufacturing, producing smaller and faster integrated circuits [6]. Additionally, advances in science and technology are leading to complex materials [10], such as hybrid materials. One group of such advanced materials are multicomponent nanomaterials (MCNMs), a subgroup of engineered nanomaterials (ENM), which will be referred to as "advanced nanomaterials".

New materials not only present great opportunities but could also have unintended consequences, for example they could disturb the recycling process or lead to the accumulation of problematic substances [9]. This could become more challenging in the future if European countries move forward a circular economy, because a circular economy requires pollutant-free material flows [9]. Although the Circular Economy Action Plan mentions sectors where ENM are applied (or intended to be) [11], only linear life cycles have been studied, from production to the End-of-Life (EoL) of the products.

For instance, nowadays, the recycling techniques are usually not used intentionally to recover ENM but other materials from the nano-enabled products [12, 13]. However, ENM can also enter into recycling and reprocessing processes when there are available techniques to treat products in the geographical boundary [12, 14]. Thus, it is essential to evaluate what could happen in the future due to the long-lasting products involved (in-use stocks), the intention to close the loops, and if advanced (nano)materials can impede

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the recycling process of economically interesting parts of the product (secondary materials).

The goal of this study is to evaluate possible flows of advanced (nano)materials in the context of a circular economy, principally during the EoL stage of solid mixed waste, considering the outflows of the recycling compartment. Thus, in this study, we used prospective scenario formation and dynamic probabilistic material flow analysis (DPMFA) to explore the potential releases of advanced (nano)materials in a future circular economy context in Europe.

2. Methods

First, we created a tool to guide what could happen with the advanced (nano)material and where it could go during different recycling processes, based on the matrix in which the advanced (nano)material could be embedded, the recycling conditions (e.g., temperature, presence of water, mechanical forces), and the advanced (nano)material's properties (size, surface functionalization, melting point, etc.).

Second, we created three prospective scenarios which represent the dynamics of the system over the years, such as the production development, solid waste collection and sorting, recycling capacity, and circularity. We used DPMFA [15] of ENM to model the flows of advanced (nano)materials across the European Union (EU-27), Norway, Switzerland, and the United Kingdom (referred as EU) from 2025 to 2050 (Figure 1). The code was written in Python and will be publicly available in Zenodo.

The technosphere includes the production of the material under study, manufacturing of the products in which the material is embedded, consumption stage, wastewater treatment systems, and the EoL of the municipal solid mixed waste compartment. While the ecosphere includes environmental compartments, such as the atmosphere, natural and urban soil, sludge-treated soil, subsurface, and surface water. It is important to highlight, that in case the secondary material goes to a product not allocated in the product categories, this flow goes out of the system, mentioned as products "out of the loop" in Fig. 1 (red arrow).

We then evaluated what could happen in Europe according to the EU waste-policy targets, i.e., reducing landfilling and improving recyclability, promoting circular life cycles, and closing-the-loop (red- dashed arrow in Fig. 1, from reprocessing to manufacturing).

The end-of-life (EoL) scenarios are:

- S1 - "Business-As-Usual (BAU)": solid waste collection, recycling, landfilling, and incineration are constant according to the current situation, and linear life cycles are mostly studied;
- S2 - "Exploring circularity": represents the development of recycling techniques, the reduction of landfilling, and the implementation of circular product life cycles within the system;

- S3 - "Closing-the-loop": represents an ideal scenario in which EU waste-policy targets are reached by 2050 and circularity is implemented in most of the product life cycles.

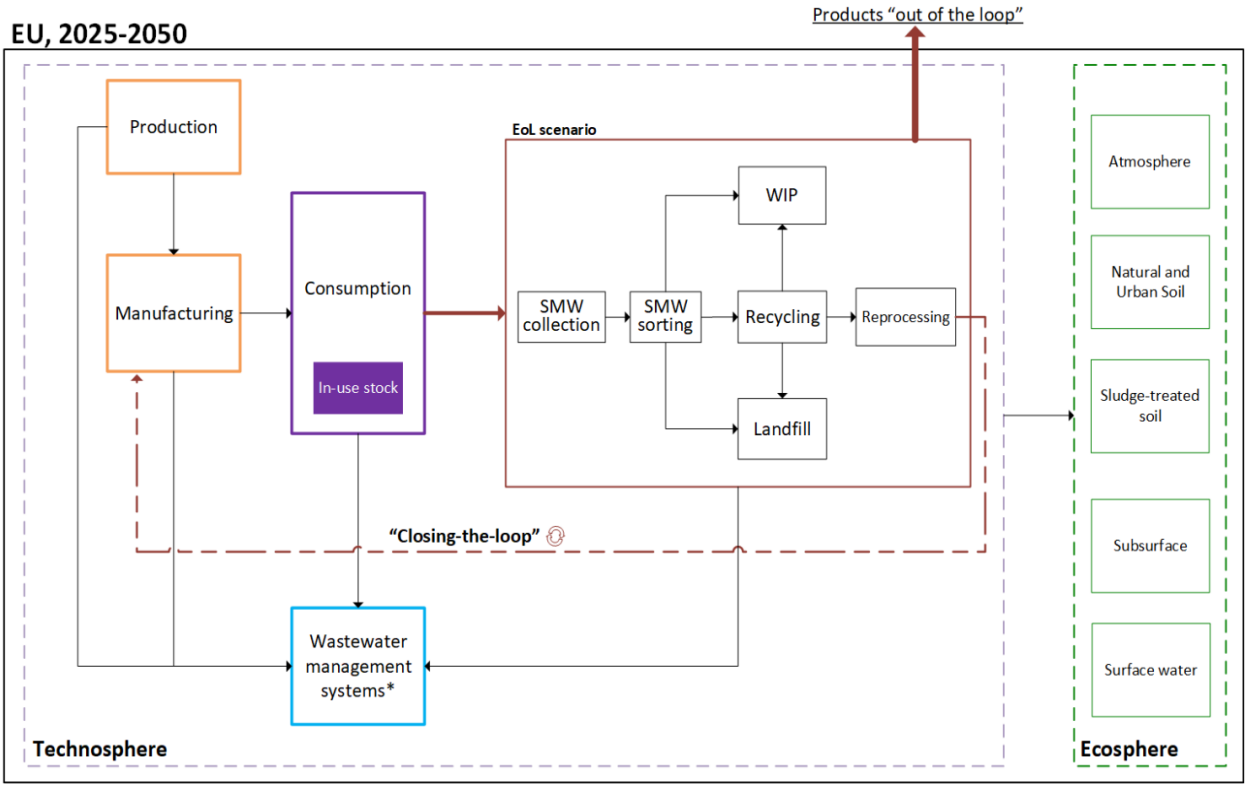

Figure 56. Representation of the material flows. The technosphere, purple-dashed rectangle, includes the technical compartments, such as production, manufacturing, consumption, wastewater management systems, and the EoL management of municipal solid mixed waste, this last section (red rectangle) serves to emphasize that the scenarios consider the SMW collection, sorting, and subsequent compartments where the material could go. The ecosphere, green-dashed rectangle, includes the environmental compartments, such as the atmosphere, natural and urban soil, sludge-treated soil, subsurface, and surface water. Arrows represent flows. EoL stands for End-of-Life, SMW for Solid Mixed Waste.

3. Results and discussion

The scenario are depicted in Figure 2 serve as the possible outflow from the collection and sorting stage of solid mixed waste, which can represent potential circularity of one of the product categories where the advanced (nano)material is embedded, and show the last dynamic layer of the model in which one of more of these pathways might apply depending on the product, matrix, material, recycling technique(s), and so on.

We investigated the available recycling techniques to recover economically interesting parts of the products, in order to analyze if the advanced (nano)material might "pollute" secondary materials and re-enter the life cycle of the product (scenario 3 in Fig. 2). Advanded (nano)materials might therefore end up in other products unintentionally, mainly when there are no industrial techniques to recover those materials, such as in the case of ENM.

The procedure will be first applied in a case study of products containing graphene-based materials [16] with the possible recycling processes from the corresponding products, such as wind turbines, electronics, batteries, among others.

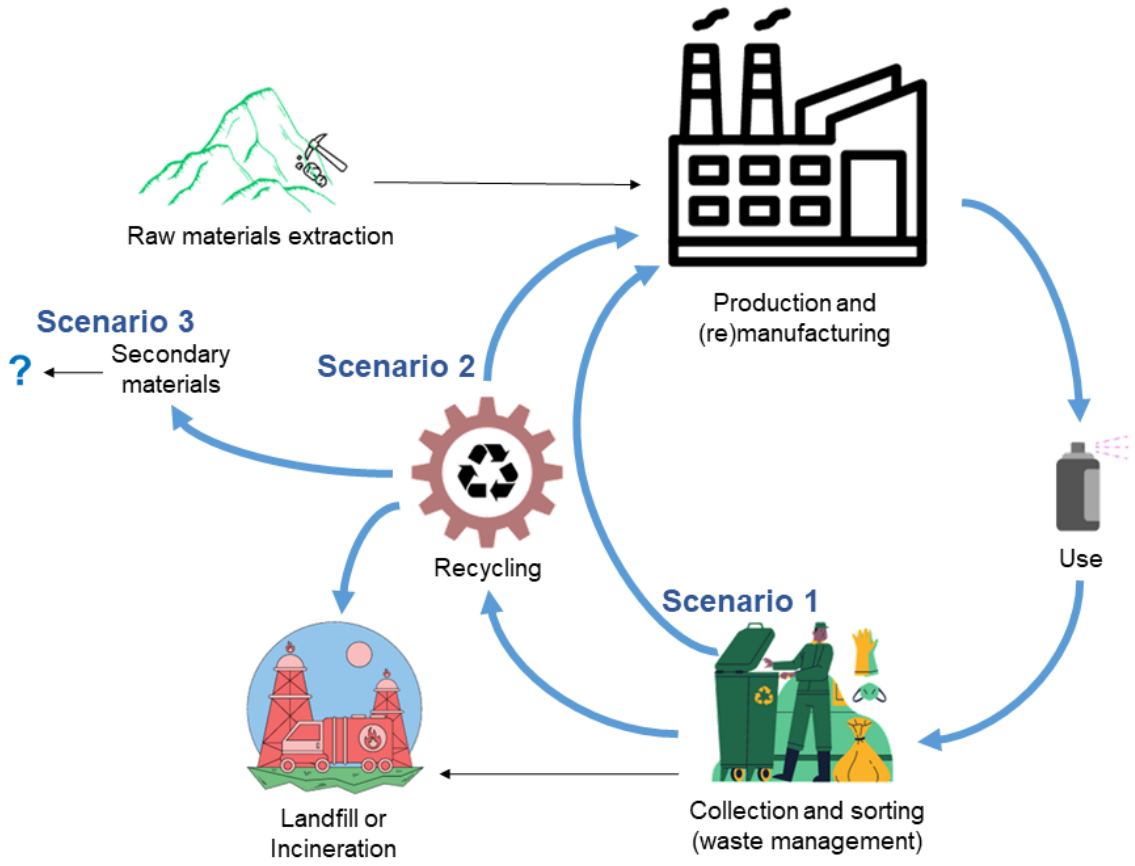

Figure 2. Scenarios to study the flows of the releases of the advanced (nano)materials in the context a circular economy. Life cycle stages under study are represented as blue arrows. Scenario in this figure means possible outflows from the collection and sorting stage of solid waste, as part of the last layer of the model. Created on Canva.

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Geopolymers: Highly Efficient Green Materials for Energy Storage Applications

Giannopoulou Ioanna[1], Georgiou Loizos[2], Michaelides Alexandros[3], Nicolaides Demetris[4]

1. Introduction

In recent decades, renewable energy sources such as the wind, geothermal and solar power, have gradually assumed a more substantial role in the European Union's (EU) energy landscape. However, the transition from the existing fossil fuel-based energy systems to green and sustainable systems that will be based almost entirely on renewables is associated with important challenges, like the operational variability, the grid stabilization and the balancing, management and responding to high loads demand.

The thermal energy storage systems capture and store the excess thermal energy (heat) produced during periods of low demand for later utilization, in the peaks of energy demand. These systems can have both small and large scale applications, such as heating/cooling of houses and power generation in industries and are considered as flexible systems that can be designed according to the requirements of the application area. TES systems can be divided into three main categories, as sensible heat, latent heat and thermochemical.

Sensible heat TES systems are able to store energy by increasing the temperature of a material, such as water, rocks, ceramics and concrete. In these systems, temperature and energy remain proportional, so the more energy is stored in a material, the higher its temperature [1]. For large scale and high temperature applications, sensible TES are based on solid materials as they are more stable in the long term, cost-effective and avoid problems such as freezing, evaporation or leakage. A suitable solid material for sensible TES should have specific thermal properties at high temperatures, such as high heat capacity and thermal conductivity, low density, and chemical stability [1].

Ordinary Portland Cement (OPC)-based concrete is a widely used construction material that gains increasing attention as a TES medium, due to the low cost and the advantageous properties, like as thermal stability, high storage performance and durability for a large number of thermal cycles [2]. Indeed, the applicability and performance of OPC-based concrete as TES have been largely investigated at research centers and validated in solar thermal applications [2-5]. However, the durability and thermal stability of concrete is largely controlled by the formed C-S-H gel, the most important hydration product of OPC, which degrades at temperatures between 400 and 600 °C. This fact prohibits the use of the OPC-based concrete TES modules in

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Concentrated Solar Plants (CSP) and the Solar Process Heat (SPH) applications that necessitate high temperatures, up to about 1000 °C.

Geopolymers are innovative and pioneering materials with great potential to be used in sensible TES applications. They are formed through the alkali activation of solid materials rich in silicate and aluminosilicate reactive phases, under a temperature below 100 °C. Alkali activation involves a sequence of chemical reactions that give rise to the development of a partially or fully amorphous polymeric structure (network), consisting of the molecular units (or chemical groups) Si–O–Si and/or Si–O–Al. The resulted materials possess excellent physicochemical, mechanical and thermal properties, such as micro- or nano-porosity, low water absorption and permeability, thermal stability, chemical and fire resistance, high mechanical strength, negligible shrinkage and low thermal expansion at high temperatures (up to 800 °C). Due to the unique structure of the geopolymeric network, these materials present thermal and mechanical stability at temperatures much higher than those that OPC-based concrete can withstand.

This paper aims at exploring the potential use of geopolymers as TES modules, alternative to the OPC-based concrete, since they can withstand running temperatures higher than 500 °C. To this end, the thermal and mechanical behavior of geopolymers based on Construction and Demolition Waste (CDW), Fly Ash (FA) and Blast Furnace Slag (BFS) is investigated at temperatures higher than 500 °C. Moreover, a comparison between geopolymers and the conventional solid materials used currently as sensible TES devices is performed, in order to better quantify the potential use of geopolymers in this engineering application.

2. Geopolymers in Sensible TES Applications

As raw materials, four different industrial wastes were used for the preparation of geopolymers, specifically waste bricks (WB) and waste ceramic tiles (WCT) provided by a Cyprus CDW recycling plant and fly ash (FA) and blast furnace slag (BFS) imported in Cyprus for the cement industry. All these materials were ground to a particle size below 150 μm. The chemical and mineralogical composition of raw materials was fully determined in a previous paper [6], where the experimental procedure followed for the preparation of the geopolymers is also described in details, along with the analyses and tests performed for the evaluation of the final materials. The performance of geopolymers at high temperatures was assessed trough their thermal stability and compressive strength after 2 hours residence time to temperatures up to 1050 °C, using a muffle furnace (Fig. 1).

According to the experimental results, all studied geopolymers presented excellent thermal stability at the temperature of 600 °C. After their exposure to 800°C, only a few intensive surface cracks, without any other sign of spalling or deformation, were visible on the specimens of the CDW-based geopolymers. It is important to note that these cracks disappeared after the exposure of geopolymers to 1050 °C, due to the sintering of the viscous geopolymeric gel phase occurred at this temperature.

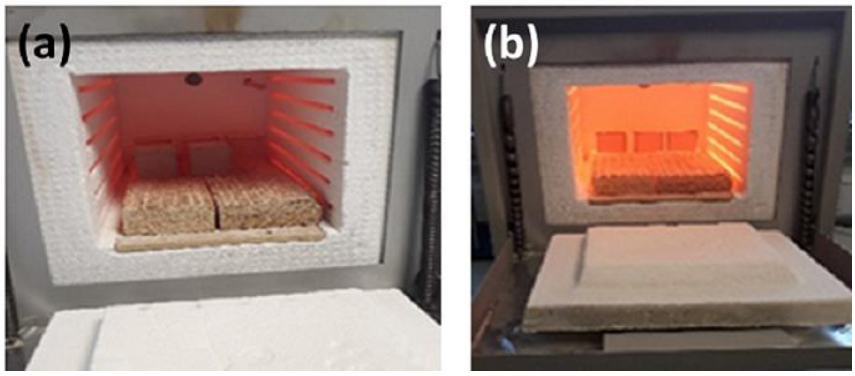

Figure 57: The used laboratory electric furnace in operation, at (a) 800 °C and (b) 1050 °C

The mechanical behavior of geopolymers varied, depending on the raw material. The BW-based geopolymers kept an almost constant compressive strength after their thermal treatment, while the compressive strength of the FA- and BFS-based geopolymers was increased after their exposure to the selected high temperatures. Finally, the compressive strength of the CTW-based geopolymers was drastically decreased after their exposure to 600 and 800 °C. Regarding the high temperature compressive deformation of materials, the BW-, FA- and BFS-based geopolymers behaved as ceramic materials up to 1000 °C, while the CTW-based geopolymer exhibited plastic behavior at temperatures higher than 600 °C, undergoing permanent deformation.

Overall, this work demonstrated that geopolymers are promising materials to be used as TES systems, and especially in CSP and SPH industries, providing sustainability and high efficiency. An intensive study, including measurements of different thermal properties of geopolymers, like the specific heat, thermal diffusivity and thermal conductivity in the studied temperature range is necessary, as well as the design of prototypes to scale up the obtained values to real operating conditions.

3. Conclusions

This work explored the possible use of geopolymers in sensible TES applications and specifically at high temperature ranges, as alternative to the OPC-based concrete. The investigated geopolymers presented excellent thermal stability and good compressive strength to temperatures between 600 and 800 °C.

According to the results, the geopolymer-based TES systems are very promising and should be considered as alternatives in energy sector, providing both sustainability and high performance.

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Session 8: Materials Innovation & collaborative Approaches for Resilience

This Session focuses on the contributions that materials R&I can provide to meeting the resilience targets of Europe, such as those stipulated in the Critical Raw Materials Act, and the need to develop climate resilience.

Giving a focus to the resulting socio-economic improvements, the presentations in this session will highlight innovative strategies or business plans for the sourcing of materials, including the (re-)use of hitherto unused by-products, or the re- or up-cycling of materials from waste processes.

- Presentations (oral and poster) will also cover the following topics:
- Innovation of materials, their products and/or processes to substitute or avoid CRMs,
- Novel materials sourcing strategies that improve the resilience of the application of materials in their relevant value chains,
- New business models regarding the (re-)use of byproducts, or the re- or up-cycling of materials from waste processes,
- Economic considerations of re- or up-cycling processes, or measures to implement circularity, and
- Material R&I initiatives under the scope of resilience targets.

Detailed Programme

Start	End	Title	Presenter
14:30	14:45	Safe by design assessment of a multi-component nanomaterial as anti-pest in food packaging	Andrea Brunelli
14:45	15:00	Approaches to Accelerating Materials Discovery: International Ecosystem Building	Anjuli Szawiola
15:00	15:15	Accelerating the development of new battery materials	Maha Ismail
15:15	15:30	Material Acceleration Platforms (MAPs), Standards and Workflows for reference data	Bastian Rühle
15:30	15:40	24/7 Poster Presentations	

Posters

S08_P01	EMMC: Communities and governance of models and digital representations of materials	Gerhard Goldbeck
S08_P02	Computational Multi-Models Enabled Design of Safe & Sustainable Multi-Component HighEntropy Coatings – M2DESCO	Gonzalo García Fuentes

S08_P03	Molecular Dynamics Investigation into the binding mechanisms of PET polymer – enzyme PETase Complex	Athina Karaoli
S08_P04	Developing advanced biological models to anticipate possible side effects in next-generation antimicrobial coatings	Philipp Meier
S08_P05	Application of Ionic Liquids (ILs) for the preparation of nanostructured carbons as oxygen reduction reaction catalysts	Fotios Katsaros
S08_P06	ZnO nanoparticles supported on mesoporous silica hosts as efficient antibacterial agents for nanocoating applications	Zili Sideratou
S08_P07	Advances in combating antimicrobial resistance of materials via laser based techniques	Albena Daskalova
S08_P08	New Products from Waste PVC Flooring and Safe End-of-Life Treatment of Plasticizers	Marcus Süß
S08_P09	Fraunhofer flagship project »ORCHESTER«: Digital ecosystem for a resilient and sustainable supply of functionally reliable materials	Madalina Rabung

Oral Presentations: Session 8

Safe by design assessment of a multi-component nanomaterial as anti-pest in food packaging

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1. Introduction

Insect pests can infest each year as much as 40% of the world's crop yield, resulting in substantial resource losses. Plant diseases alone incur an economic toll exceeding $220 billion annually on a global scale (FAO 2024). Addressing this challenge calls for innovative, eco-friendly solutions, as advocated by the European Green Deal. In this context, a safe and sustainable assessment of a multi-component nanomaterial (MCNM) (i.e., bentonite nanoclays encapsulating clove essential oil) embedded into a low-density polyethylene (LDPE) film food packaging as anti-pest was carried out. This work is part of the industry-oriented H2020 SUNSHINE project, which aims to create materials in accordance with the Safe-and-Sustainable-by-Design (SSbD) framework recently proposed by the European Commission (Caldeira et al., 2022).

2. Methodology

According to the SSbD framework, the first step concerned the material safety by merging information from the literature and from experimental work performed within SUNSHINE, on: i) physico-chemical characterization of both individual components and MCNM; ii) hazard characteristics of the precursors for the MCNM synthesis; iii) (eco)toxicological data. Afterwards, in line with step 2 of the SSbD framework, an

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industrial hygiene survey to identify potential hotspots of particles emissions from MCNM production, handling, processing or maintenance and cleaning phases was developed to then design a tailored monitoring campaign for occupational exposure assessment. Moreover, as indicated in the final application/use phase of step 3 of the SSbD framework and according to Regulation (EU) N°10/2011, the potential migration of the active ingredients and of the inorganic elements constituting the MCNM was investigated from both pristine LDPE films and those after accelerated aging.

3. Results

Physico-chemical characterization showed that the thermal stability of clove essential oil encapsulated into the nanoclays was significantly increased over time with respect to the clove oil alone. This improvement was also observed in both toxicological and ecotoxicological assays. Data revealed that that the encapsulation of clove essential oil lowers the overall toxicity of eugenol (i.e., the main organic compound of the essential oil). With regards to the materials safety during production/processing phases, corresponding to step 2 of the SSbD framework, three different exposure scenarios (ES) were identified from the results of the survey: ES1) extrusion of micronized mixture; ES2) pellet drying; ES3) film production on a blower. A first workplace air-monitoring campaign to monitor the extrusion step showed the first ES as the one that needs most attention regarding to the nano-sized particles release. However, awareness should be also dedicated to the other two ES with respect to the release of micrometric-sized particles. A further campaign is underway for the scale-up of the process. As far as the investigation of the potential migration of chemicals/materials from both pristine and accelerated aged MCNM-nanobased LDPE film, did not raised concerns. In details, the overall data generated on the i) overall migration, ii) specific migration and iii) inorganic elements constituting the MCNM, never exceeded the thresholds established by the Regulation N°10/2011 on plastic materials and articles intended to come into contact with food and by its amendment n°1245/2020.

4. Conclusions

Following the first steps of the SSbD framework, a safety assessment of the MCNM embedded into an LDPE film for food packaging was performed. This approach showed its usefulness for gathering information and for highlighting potential issues at an early stage of the product development. The results from this safety assessment are going to be then integrated with the application of sustainability assessment methodologies to finally achieve the Green Deal ambitions of phasing out harmful substances from the EU market.

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6. Funding

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Approaches to Accelerating Materials Discovery: International Ecosystem Building

Anjuli Szawiola[1], Mark Kozdras[1]

1. Introduction

To achieve net-zero goals by 2050, Natural Resources Canada (NRCan) has supported the uptake of the accelerated materials discovery (AMD) approach for clean energy technologies in research facilities within Canada and around the world, since 2018. This approach couples advanced simulation and modeling on high performance computing with closed loop automation of materials synthesis and characterization, all accelerated by artificial intelligence.

2. International Ecosystem Building

Beyond providing research funding and capital and infrastructure investments [1], NRCan's approach is three-fold, including research excellence, strategic partnerships, and capacity building. This talk will highlight NRCan's work over the last five years toward international network building for training & knowledge mobilization.

To that end, NRCan has led numerous initiatives such as Mission Innovation: Materials for Energy (formerly Innovation Challenge 6: Clean Energy Materials) and the German Canadian Materials Acceleration Centre (GCMAC) [2], in part focused on educating on the AMD approach. This talk will present a case study in NRCan's approach to addressing technology specific challenges in the clean energy technology space for scale-up across the research and innovation continuum via training & knowledge mobilization, as well as connecting in with the broader ecosystem.

3. References

[1] Public Services and Procurement Canada. "Government of Canada Invests in Laboratories to Support Science and Research in Canada." Canada.Ca, Government of Canada, 15 Apr. 2021, www.canada.ca/en/public-services-procurement/news/2021/04/government-of-canada-invests-in-laboratories-to-support-science-and-research-in-canada.html.
[2] Natural Resources Canada. "Government of Canada Announces New German-Canadian Materials Acceleration Centre." Cision Canada, 7 May 2021, www.newswire.ca/news-releases/government-of-canada-announces-new-german-canadian-materials-acceleration-centre-808761841.html.

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Accelerating the development of new battery materials

Ainhoa Bustinza[1], Maha Ismail[1,2], Iciar Monterrubio[1,2], Oier Arcelus[1], Nebil Katcho[1], Javier García[1], Evaristo Castillo[1], Javier Carrasco[1], Montse Casas-Cabanas[1,3], Marine Reynaud[1]

1. Introduction

Battery innovation relies on developing new electroactive materials. To timely respond to the increasing demand for energy storage solutions, the European Battery 2030+ Initiative targets accelerating by 5-to-10 fold the current rate of battery materials discovery within the next 5-10 years [1]. Taking up this challenge requires disruptive approaches that allow rethinking the traditional experimentation process (based on researcher's chemical intuition and trial-error scheme), which is inherently slow and economically expensive. Indeed, the crystal-chemical space offered by the periodic table for the search for new battery materials is huge and still far from being exhaustively explored.

2. Experimental screening of electrode materials

To accelerate the exploration of broad chemical spaces, our group is developing an autonomous Materials Development Platform, capable of making effective modelling-based predictions, self-driving inorganic synthesis and performing high-throughput characterization experiments. This requires a mind change in our approach to materials research, but also building new lab infrastructures and analytical tools, which include automated high-throughput synthesis modules, automated data analysis programs able to handle large amounts of data, as well as AI-aided experimental planners.

In this presentation, we will present several strategies explored at CIC energiGUNE to speed up the different stages of the development of new materials for Li-ion and Na-ion batteries. Such approaches include:

(i) the use of automated machine-learning-aided screenings of materials databases in search for new families of compounds that can be converted into electroactive materials [2, 3];
(ii) the development of solutions to automatize inorganic syntheses (e.g. co-precipitation, solvothermal, sol-gel; Figure 1) and characterization techniques (e.g. XRD, electrochemistry) [4];
(iii) the development of analysis tools for automated data treatment and analysis, including a Machine-Learning experimental planner, chemometrics

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approaches for data analysis of large XAS data sets, or the new FullProfAPP that enables automated Rietveld refinements of large series of data, in particular those generated from operando experiments [4, 5].

Figure 58: Photo of one of the experimental modules for inorganic syntheses developed at CIC energiGUNE

3. Acknowledgments

This work was in particular supported by the Spanish MCIN/AEI/10.13039/501100011033 and ERDF/EU (project ref. PID2019-106519RB-I00, PID2022-140823OB-I00, PhD grant PRE2020-092978), the Basque Government (PhD grants ref. PRE-2021-2-011) and the European Commission (G.A. No 957189).

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4. https://cicenergigune.com/en/fullprof-app
5. Fehse et al. Chemistry of Materials, 2022, 34(14), pp. 6529-6540. 10.1021/acs.chemmater.2c01360

The potential of Material Acceleration Platforms (MAPs) for creating resilient and sustainable technology value chains

Bastian Rühle[1] and Ozlem Ozcan[1]

Material Acceleration Platforms (MAPs) represent a transformative approach to the development of resilient and sustainable technology value chains. These platforms can identify candidate chemistries and structures via simulations, and database searches and leverage machine learning-based rapid screening to accelerate the discovery and deployment of novel materials, thereby addressing critical challenges in modern technology sectors.

Incorporating high-fidelity advanced characterization in the early phases of material development is crucial for early de-risking. Advanced characterization techniques, such as X-ray diffraction, advanced electrochemical and spectroscopic techniques provide comprehensive insights into the structural, chemical, and physical properties of materials. Long-term testing further contributes to the de-risking process by evaluating the durability and stability of materials under various environmental and operational conditions. Early identification of potential degradation mechanisms enables the refinement of material compositions and processing methods, ultimately leading to the development of more resilient materials.

Early upscaling attempts are integral to assessing the feasibility of material leads generated through machine learning-based rapid screening to evaluate the scalability of synthesis and processing techniques. This step is critical for identifying potential challenges in manufacturing, such as issues related to reproducibility, yield, and cost-effectiveness. Process design has to be a major part of the MAP-based material design to cope with the increasing share of secondary raw materials in supply chains.

This presentation will briefly summarize possible strategies to address these issues and provide deep-dives on best practices. As the demand for advanced materials continues to grow, MAPs will play an increasingly vital role in driving technological advancements and addressing global challenges.

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Poster Presentations: Session 8

EMMC: Communities and governance of models and digital representations of materials

Gerhard Goldbeck[1], Alexandra Simperler[1]

1. Introduction

EMMC (European Materials Modelling Council) [1] supports all aspects of modelling and digital representations of materials. It brings together all stakeholders including modellers, data scientists, software owners, translators and manufacturers in Europe. EMMC supports wide collaboration and industrial uptake of a digital and model-based approach to the whole materials life cycle. Key activities of EMMC are in data- and physics-based multiscale modelling and in harmonisation and standardisation of terminologies and ontologies to support data management and AI.

2. Materials modelling communities

EMMC has arisen as a bottom-up community starting in 2014 to address the diversity and confusion about the wide range of materials models and to support their industrial uptake. To date, EMMC represents hundreds of individual members and tens of European organisations covering all types of models, including physics-based, empirical and ML/AI. The MODA CWA [2] represented a unified representation of all types of materials modelling for the first time.

3. EMMO: model of the material world

Based on the need for a human-centred, science-based, machine actionable representation of the material world (including all physical objects, materials, processes, models, data etc), the EMMC-CSA project initiated the development of the EMMO ontology, with further development in a large number of Horizon projects. EMMC ASBL provide the overarching governance required to support collaboration and ensure alignment of efforts. This is achieved via EMMC Task Groups in the Focus Area Digitalisation and Interoperability. EMMO is already widely used in the battery field [3] and provides the framework for documentation of characterisation [4]. It is ready for uptake across all types of materials applications and can provide a basis for FAIR data documentation required e.g. in materials passports. EMMO is a foundational ontology that is ready to support FAIR data in a Materials Commons (see Figure 1).

4. Digital transformation of Materials Life Cycles.

A model-based approach is at the heart of a digital transformation of materials life cycles from design to re-use. It relies on a virtuous cycle of innovation as shown in Figure 2. For further details, see the EMMC Roadmap [5], elaborated in collaboration with AMI2030.

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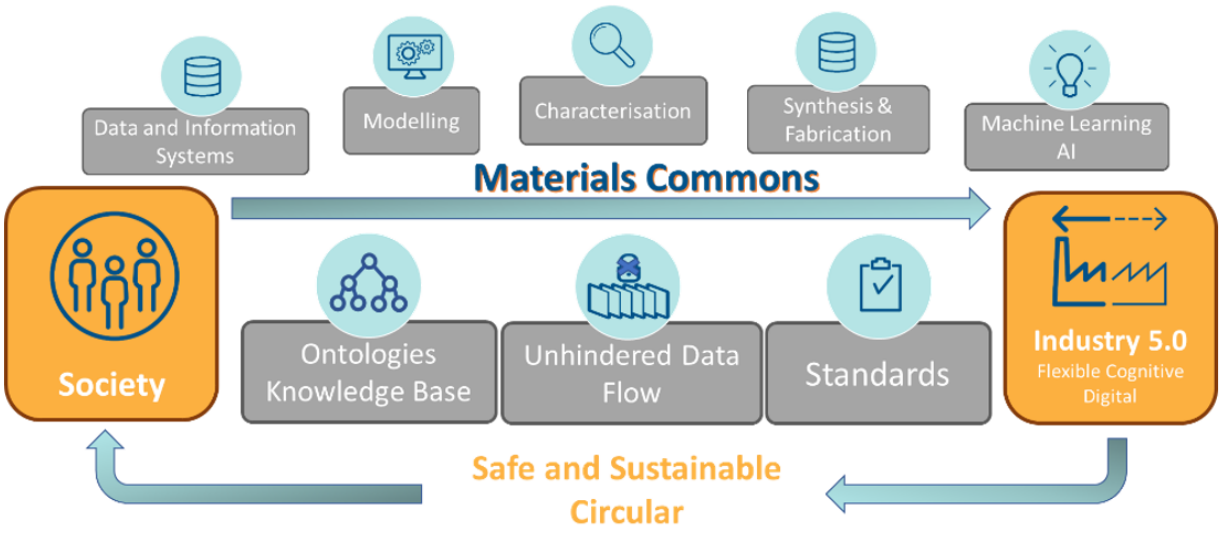

Figure 59: EMMC supports the creation of a Materials Commons in an Industry 5.0 context.

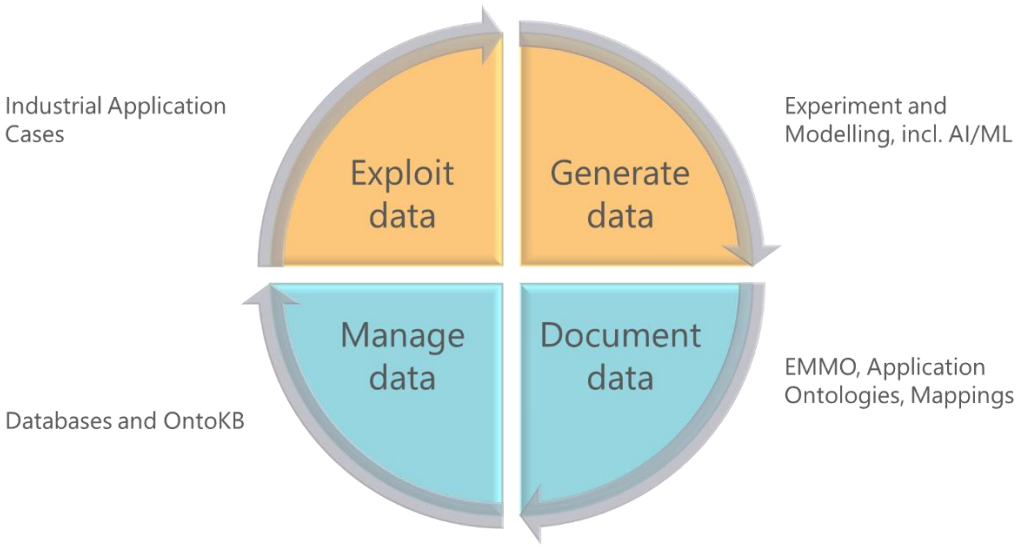

Figure 60: EMMC communities collaborate to support a virtuous cycle of innovation based strongly on models and digital representations of materials

5. Conclusions

EMMC and its stakeholders have been spearheading a harmonised, model-based approach to materials innovation for more than 10 years. The combination of advanced materials models and ontological models of the material world are instrumental to achieving a Materials Commons which is built on shared knowledge (rather than confidential data) and fosters cooperation and exchange.

6. References

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[5] EMMC Roadmap: https://emmc.eu/emmc-roadmaps/

Computational Multi-Models Enabled Design of Safe & Sustainable Multi-Component HighEntropy Coatings – M2DESCO

Gonzalo García Fuentes[1], Yi Qin[2], Hanshan Dong[3]

1. Introduction

M2DESCO - HORIZON-CL4-2023-RESILIENCE-01 [1] is a collaborative, multidisciplinary research project aimed at developing next-generation high-entropy-alloy based multicomponent green coatings (free of toxic substances) and sustainable (rare earth free & minimum critical metal elements) with predictable functionalities, performances, and life span. The purpose of the project is to increase wear resistance by 100%, corrosion/oxidation resistance by 50~60%, of metal components, while effectively reducing the criticality of coating materials by at least 70%. The project counts on the participation of AIN as coordinator, the Universities of Strathclyde (UK) and Birmingham (UK), the Politecnico di Torino (IT), the National Technical University of Athens (HE), the National Research & Development Institute for Non-ferrous and Rare Metals (RO) and the SMEs: Anter Ltd (HE), Durante Space Tech (ES), PVT GmbH (D), Innovation in Research & Engineering Solutions (BE), Laneko S.A.L. (ES) and Innovative Coating Solutions (BE).

To achieve these goals, the project shall to integrate AI/ML underpinned, highly effective and highly efficient Computational Modelling that is guided by a novel Safe and Sustainability by Design Framework and facilitated by high-throughput characterisations and evaluations, to speed up material-design and coating-product development process (reducing the development cycle-time by 400~500%), and concomitantly the overall product manufacturing cost by 20% due to use of the new tooling developed.

The advancement of M2DESCO will contribute significantly to combating the loss in EU region caused by corrosion and wear, to the enhancement of the global profile and leadership of the EU material modelling/research community, to strengthening of the innovation capability of the EU coating industry/business, and ultimately to reinforce the PVD EU sector which leads a world-wide market projected to reach 40.97 billion in 2028, thus, rendering great benefit to the wider advanced manufacturing chain, and effectively enhancement of the global competitiveness and the resilience of the EU industry.

The project will spin around the knowledge enhancement of 5 different THEMEs, as depicted schematically in Figure 1:

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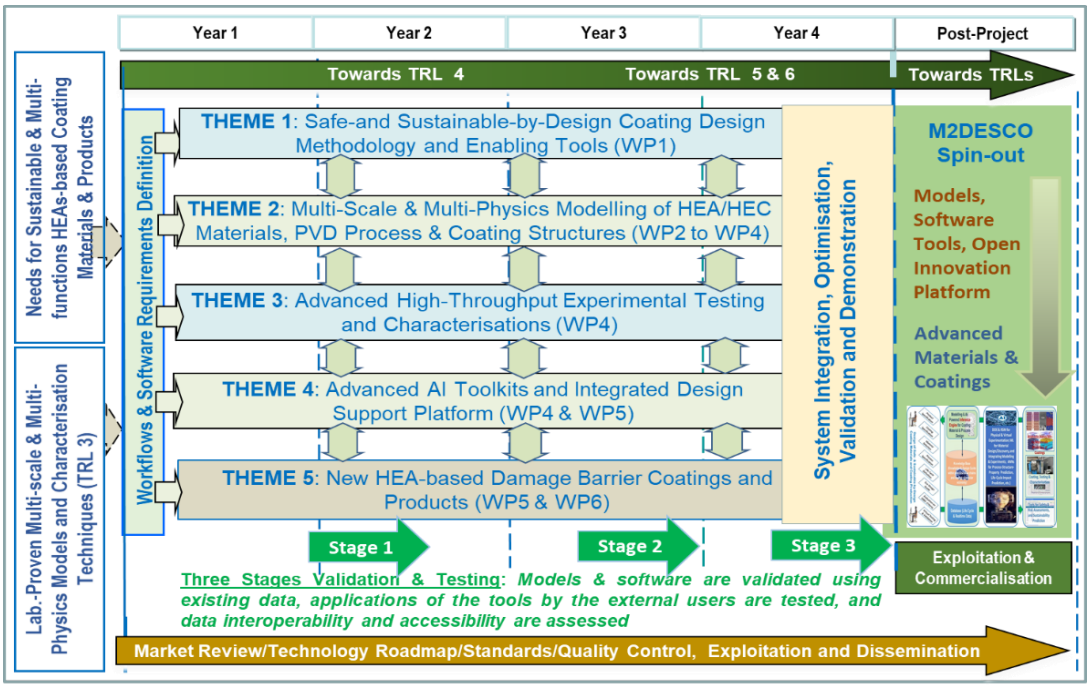

Figure 1: M2DESCO project development pipeline

(i) Safe-and Sustainable-by-Design Coating Design Methodology and Enabling Tools. This topic intends to adopt a "Seven-Steps Approach" for SSbD coating materials and production processes and includes the development of Combinatorial Safety and Risk Assessment (SRA), and Hybrid Life-Cycle Assessment and prediction.

(ii) Modelling of the Coating Processes and Film Growths encompasses the calculation of phase diagrams and thermodynamics of HEA configurations for low criticality combinations of coating materials. It will make use of Density functional theory (DFT), molecular dynamics (MD) and finite element (FE) cohesive-zone calculations, all interacting at different atomic-cluster-continuum scales. Theme 2 also includes calculations of coating processes and film growth by the development of kinetic Monte-Carlo non-equilibrium approaches. This topic is framed in a multiscale model framework, so the models and approaches cover different dimensional range of the materials and microstructures (from atomistic to macroscopic scale) and connect each other through well-defined input-output model parameters.

(iii) Advanced High-Throughput Experimental Testing and Characterisations will permit to accelerate the obtention of reliable datasets to aid the construction of predictive models and implement feedings to AI-tools.

(iv) Advanced AI Toolkits and Integrated Design Support Platform shall be constructed to integrate the above model functions and apply AI tools in an effective manner.

(v) New HEA-based Damage Barrier SSbD Coatings and Products will be produced experimentally on selected use cases: (a) hot forging and (b) machining of difficult to cut metals, both in order to quantify the benefits of the developed coatings and the lowering of the materials/processing environmental and economic impacts. References

[1] M2DESCO contract nr 101138397. web-link at the Horizon Europe site.

Molecular Dynamics Investigation into the binding mechanisms of PET polymer - enzyme PETase Complex

Athina Karaoli,[1] Co-Authors: Dimitris G. Mintis,[1,2] Haralampos Tzoupis,[1] Iseult Lynch,[2,4] Georgia Melagraki,[5] Antreas Afantitis[1,2,3]

1. Introduction

Plastic pollution has reached a point where traditional waste management can no longer mitigate the plastic waste problem effectively. The UN estimates that the annual global plastic production exceeds 400 million tonnes and is expected to triple by 2060. A significant portion of plastics (~85 %) is being disposed of in unregulated landfills or left unmanaged, and only 9 % is currently recycled [1].

Enzyme-based methodologies have emerged as an alternative for addressing plastic waste [2]. Advances in enzyme-based approaches hold great promise, as their integration into plastic degradation processes offers a sustainable and energy-efficient alternative to traditional mechanical recycling [3].

A breakthrough achieved in 2016 [4], showed that polyethylene terephthalate (PET), can be hydrolysed. During this process, two enzymes PETase and MHETase catalyse the degradation of PET to mono(2- hydroxyethyl) terephthalate (MHET) and then into terephthalic acid (TPA) and ethylene glycol (EG) (Figure 1) [5]. Building on these findings, the PhD project presented here aims to investigate the chemical processes involved in the degradation of plastic polymers such as PET using molecular simulation techniques.

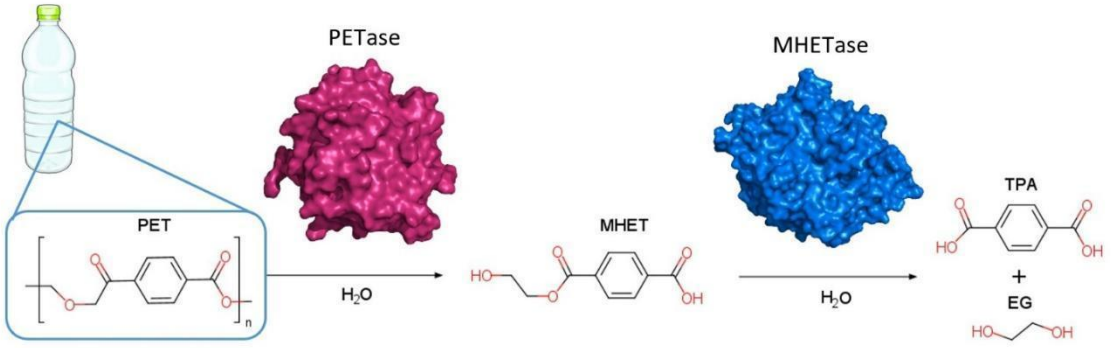

Figure 1. Representation of the degradation of PET into TPA and EG.

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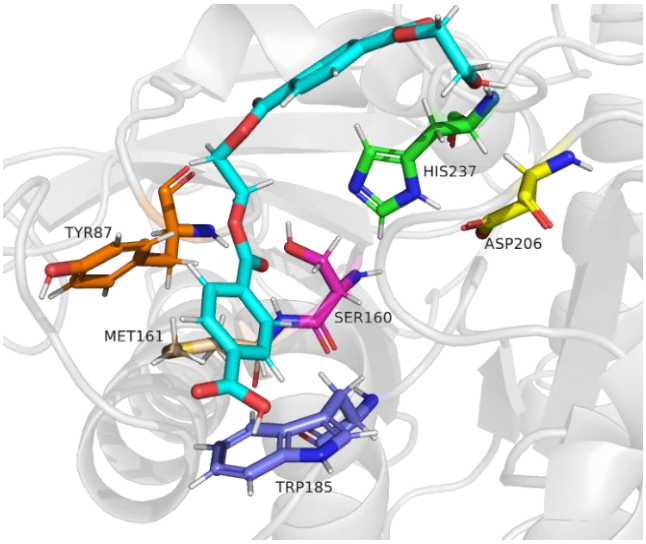
2. Methodology

Methodological Enhancement through Automation: The integration of Enalos Asclepios KNIME nodes (https://novamechanics.com/products/asclepios-knime-nodes/) with molecular dynamics (MD) studies represents a significant advance, offering a robust automation tool for complex computational chemistry tasks. The Asclepios KNIME nodes facilitate the streamlining and high-throughput processing of MD, which has been particularly instrumental in the field of small molecule drug design research.

A PET dimer was docked in PETase (PDB ID: 6EQE) using AutoDock Vina [6]. The Amber ff14sb and the GAFF2 force fields were employed to build the parameters for the protein and ligand, respectively, for the MD simulations. All MD simulations were performed using GROMACS [7]. Two production MD simulations were performed under constant temperature/pressure ensemble (T=300 K and P=1 atm) for: (i) the unrestrained complex and (ii) the complex with positional restraints on the ligand.

3. Results

The PET degradation process initiates through interactions between residues Ser160-His237-Asp206 [5, 8-10]. Table 1 shows a comparative analysis of the observed distances with those described in the literature. Figure 2 shows the conformation of PET with respect to the active site residues. Our results agree with those reported by Han et al (2017). PET forms hydrogen bonds with Tyr87 and Met161 residues that stabilise it in the active site.



Our MD simulations highlight the proximity between Ser160 and His237 that facilitates deprotonation of Ser160 by His237. Furthermore, our analysis showed the formation of an oxyanion hole involving the amine groups of Met161 and Tyr87 along with the O_3 of the PET in the restrained system, characterised by short H−O_3 contacts. Conversely, the unrestrained system displayed a disruption in this oxyanion hole.

Figure 2. Close-up view of the PETase active site with the PET substrate.

Table 1. Average Distances as calculated by molecular docking and MD simulations.

		Distances (Å)	SER160 HG - HIS237 NE2	HIS237 HD1 - ASP206 OD2	TYR87 NH - PET O3	MET161 NH - PET O3
Molecular docking		present study	3.70	1.70	2.30	3.00
		Han et al., (2017) [5]	3.70	1.70	1.90	2.30
		da Costa et al., (2021) [8]	2.64	1.79		
Molecular Dynamics	Unrestraint system	present study	2.24 ± 0.49	1.81 ± 0.10	11.53 ±0.66	10.92 ± 0.82
		da Costa et al., (2021) [8]	4.18 ± 0.78	7.97 ± 0.37		
	Restraint system	present study	3.56 ± 0.24	1.82 ± 0.10	3.40 ± 0.42	3.58 -± 0.26
		Jerves et al., (2021) [9]	1.76 ± 0.15	1.62 ± 0.15	2.68 ± 0.57	3.07 ± 0.44
		Garcia et al., (2023) [10]	1.92 ± 0.14	3.10 ± 0.30	1.94 ± 0.14	2.20 ± 0.20

4. Future work

The initial results highlight the importance of PETase in PET degradation and lead us to further analyse the system through Density Functional Theory (DFT) calculations. This approach allows us to model the reaction mechanisms, providing insights into the catalytic processes.

Future plans include investigating ThermoPETase [11] and FAST-PETase [12]. ThermoPETase has improved thermostability and longer activity at high temperatures, while FAST-PETase exhibits a more efficient degradation process at 40 °C. The limited data available regarding FAST-PETase and ThermoPETase highlight the importance of employing quantum mechanics/molecular mechanics (QM/MM) models to investigate the application of these enzymes for PET degradation in an industrial setting.

5. Conclusions

The findings show the presence of an oxyanion hole and the dynamic facilitation of proton transfer between the SER and HIS residues in the active site. The understanding of the principles in enzymatic degradation at the molecular level serves as a crucial step towards our aim, which entails the development of a structure-based machine learning algorithm for engineering resilient and highly efficient enzymes capable of rapidly decomposing environmentally persistent plastics.

The use of Enalos Asclepios KNIME nodes in this study underscores a commitment to enhancing computational efficiency and accuracy in MD investigations, especially in contexts requiring high-throughput data processing.

6. Acknowledgments

This work received funding from the European Union's Horizon Europe research and innovation program under the Marie Sklodowska-Curie Doctoral Network PLASTIC UNDERGROUND (Grant Agreement No. 101072777).

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Developing advanced biological models to anticipate possible side effects in next-generation antimicrobial coatings

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1. Introduction

The EU Nova Project is a consortium of highly motivated researchers to produce next-generation antimicrobial coatings to fight viral, bacterial, and fungal pandemics. In this context, we are anticipating the potential risk of these coatings causing unfavourable toxicological reactions for human health already during the material design stage. Currently, we are developing in vitro assays to assess the biocompatible and immunocompatible properties of coatings used in long-term implantable biomaterials like hernia meshes. This study aims to complement ISO standard 10993 and OECD guidelines by filling gaps through advanced methods. Our approach follows the 3R Principle and includes mimicking release situations from the coatings in physiologically relevant conditions using skin and immune models, and with advanced visualization technique FIB/SEM (Focused Ion Beam-Scanning Electron Microscopy). We aim to understand the biological response triggered by nanomaterials/coatings and their mode of action. We incorporate the expertise of research institutes specializing in nanomaterial biointerface interactions. The knowledge gained from previous projects in the field of nanosafety assessment is utilized to develop and expand nano-suitable assays within the NOVA project. The developed methods are highly recommended by authorities to reduce the need for animal assays. Suitable coatings identified in the NOVA project will be further investigated in animal experiments to validate our advanced models as standard procedures beyond the project.

2. Cell-based Assays conducted in NOVA

Our main objective is to evaluate the safety and efficacy of bioactive coating technologies developed in the NOVA project for medical applications. We conduct safety testing according to DIN EN ISO 10993-5, which covers a wide range of interactive surfaces. We also perform assays in NOVA using a human keratinocyte cell line (HaCaT) to simulate human exposure through skin contact (Empa). By applying artificial sweat and water as extraction solvents the coatings were treated in a worst-case sweat exposure scenario before cell culture evaluation (Figure 1).

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Skin irritation and sensitization will be assessed analogous to the respective OECD guideline ARE-Nrf2 Luciferse Method (KeratinoSense™) TG442D.

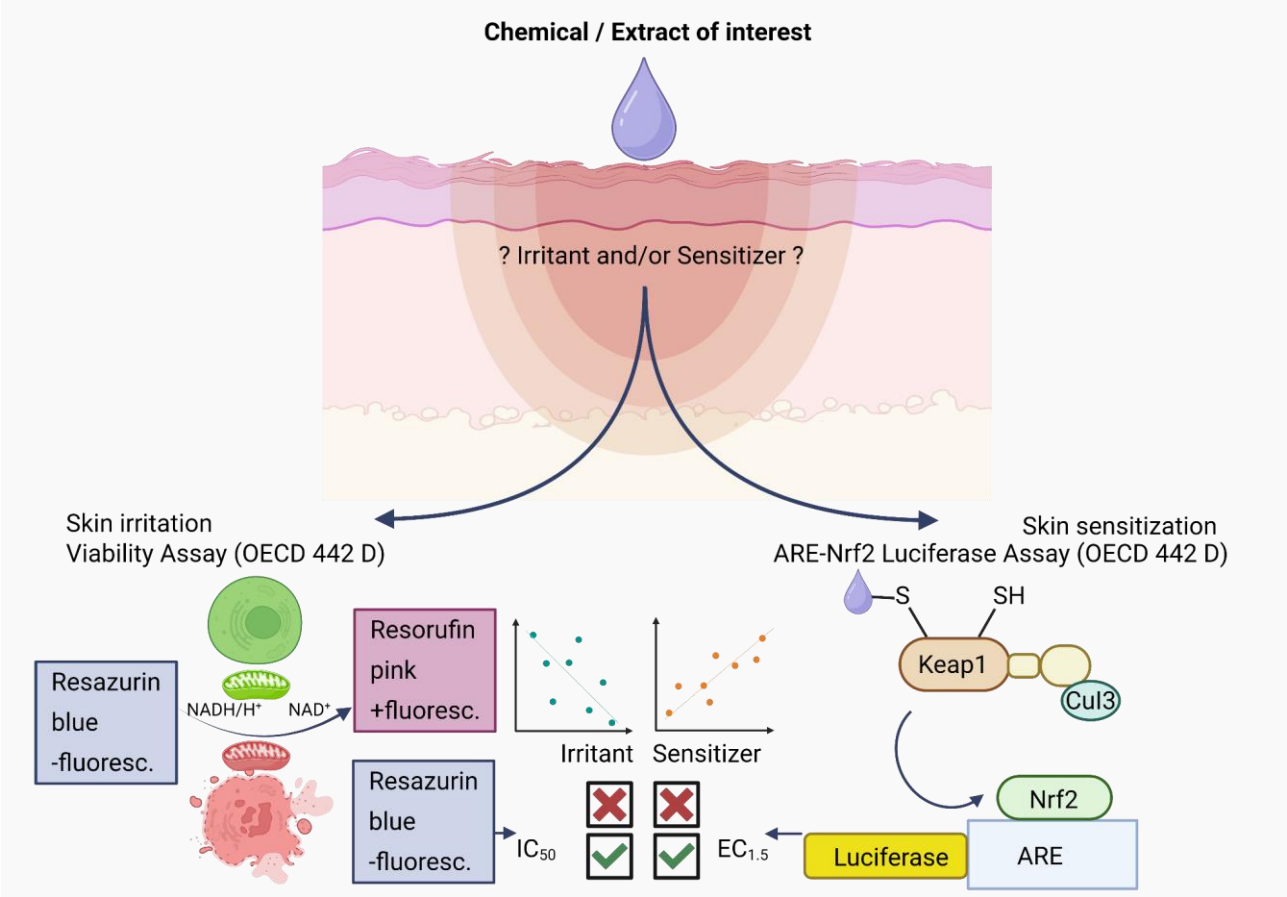

Figure 1: Basic mode of action of the applied KeratinoSense™ OECD guideline ARE-Nrf2 Luciferse Method.

Furthermore, if the KeratinoSense™ assay detects skin sensitization, additional assays such as the activation of dendritic cells (h-CLAT or IL-8 Luc) TG442E or OECD test guideline 439 using reconstituted human epidermis will be applied for confirmation.

For direct cell-material contact on solid surfaces, the Fraunhofer IKTS utilizes the patented in vitro test system "ClicKit-Well" and applies a quantitative viability and cell adhesion test procedure using the XTT assay at three different time points (Figure 2).

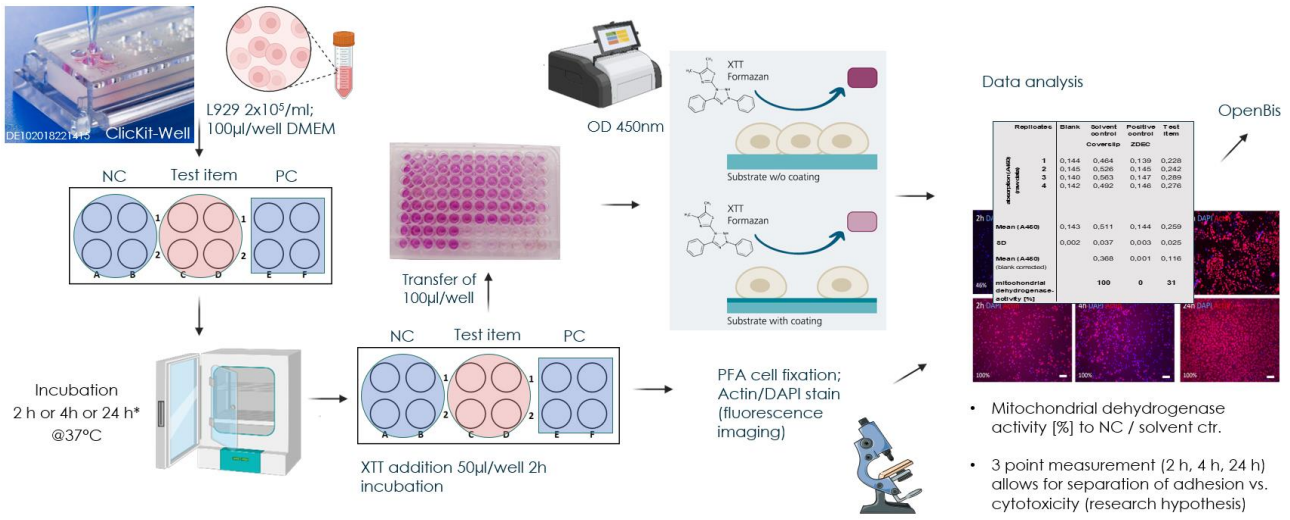

Figure 2: Scheme of quantitative cell adhesion/ direct cytotoxicity assay.

SEM is used for the evaluation of cell adhesion on the coated materials, cell orientation, migration, and cell morphology, which give an insight into cell behaviour on different surfaces (Figure 3). FIB milling and conventional SEM imaging of dried biological samples provides structural information and reveals morphological characteristics of the sample interior.

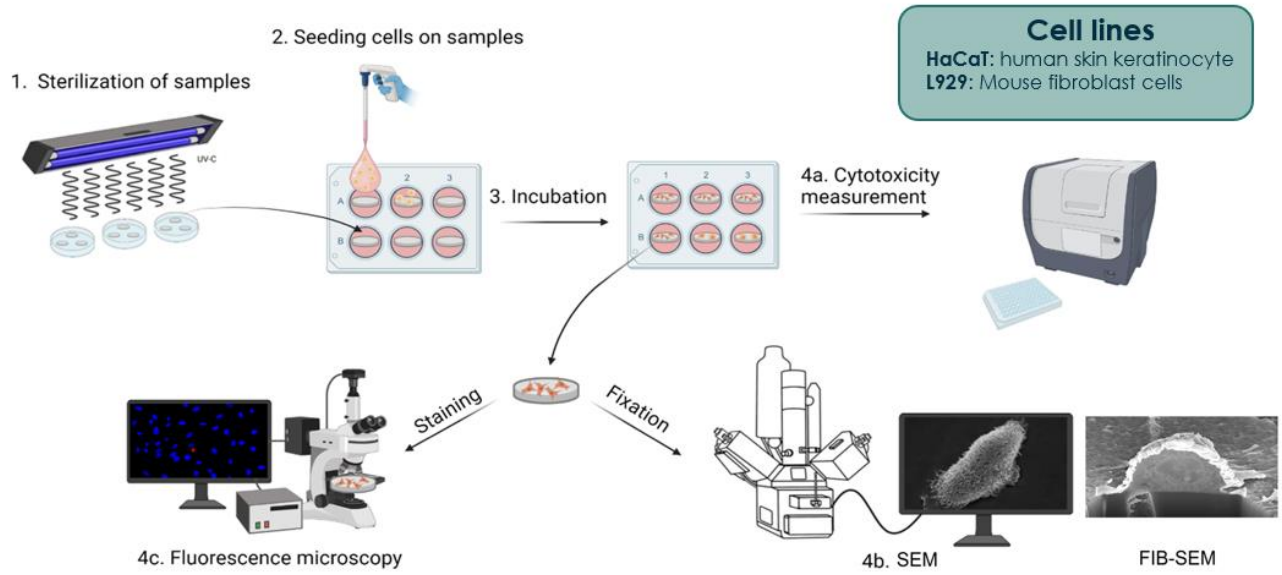

Figure 3: Scheme of FIB/SEM imaging experiments.

3. Conclusions

In conclusion, we have successfully developed and implemented a range of assays tailored to our specific objectives. These assays have allowed us to gain initial insights and generate data from the first samples tested. By using these assays, we can assist material and coating manufacturers in identifying specific candidates for further improvement and advancement toward becoming a viable product. Our assays enable

us to address specific scientific questions and reliably accompany the in vitro development of new coating ideas. This approach significantly reduces the number of promising candidates that would need to undergo animal testing in the next phase. Overall, our work contributes to the advancement of safe and effective coatings for medical applications, providing a valuable and ethical alternative in the product development process.

4. Acknowledgment

This research has received funding from the European Union's Horizon Europe Framework Programme under grant agreement No.101058554. This work was co-funded by the Swiss State Secretariat for Education, Research and Innovation (SERI) and the UK Research and Innovation (UKRI) under the UK government's Horizon Europe funding guarantee grant No. 10042534 & grant No. 10055606.

Application of Ionic Liquids (ILs) for the preparation of nanostructured carbons as oxygen reduction reaction catalysts

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1. Introduction

Porous carbons, especially nanoporous and nanostructured carbons, including Activated Carbons (AC), Carbon NanoTubes (CNTs), etc., have been standardized in many technological applications and become a hot scientific topic, due to their unique properties such as their high thermal and mechanical stability, electric conductivity, microwave absorption capacity, catalytic activity, tunable surface chemistry, enhanced and tailorable pore structure and wide availability[1].

On the other hand, Ionic Liquids (ILs) are lately considered amongst the most effective precursors for the preparation of nanostructured carbons, because they do not decompose completely into volatiles under pyrolysis but leave behind significant amounts of recalcitrant char. Moreover, there is a great variety of different IL structures that contain nitrile functional groups (−C≡N), either in the form of anion or cation, thus yielding highly nitrogen-rich carbon samples[2].

This work is primarily focused on the investigation of the catalytic performance of carbon materials developed through the template method. To this end, various types of enhanced pore size Vycor® (eps-Vycor®) have been employed as hard templates/molds in the nanocasting/pyrolytic treatment of [BMIM][TCM] as IL precursor. Upon dissolution of the hard template, the recovered N-doped porous carbons have extensively been characterized by bi-modal micro-mesoporosity[3]. Afterwards, C,N-networks prepared by this method have succesfully been studied as ORR electrocatalysts showing a prevalent $4e^-$ reduction process under operation.

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2. Materials and Methods

The IL used in this work was the 1-butyl-3-methylimidazolium tricyanomethanide ([BMIM][TCM]), which was provided by IoLiTech GmbH, with a purity over 98% and a moisture contamination of 150 ppm. Vycor® glass tube (Code 7913, Corning® USA), was selected as the hard template for the preparation of the nanostructured carbons.

Nanostructured carbon syntheses via templated precursor pathway include the casting of [BMIM][TCM] into raw and eps-Vycor® under vacuum, to facilitate the imbibition of the IL phase into the porous structure, followed by carbonization and template dissolution to recover the carbonaceous samples as Vycor® replica. The main target of etching process was to widen the pore necks and thicken carbon domains lying into Vycor®cavities.

Electrochemical measurements were carried out with a Rotating Ring Disk Electrode (RRDE working electrode, Pine Instrument Co) made of a disk of glassy carbon (GC, ∅ 5mm, A = 0.196 cm^2) and a platinum (Pt) ring with a surface of 0.11 cm^2. All carbonaceous samples produced were fabricated as RRDE electrodes and measurements were performed in a three-electrode cell operating in a 0.1M KOH solution, equipped with an [Ag][AgCl][KCl_{sat}] reference electrode and a Pt wire as counter electrode.

3. Results and Discussion

The porous structure of developed carbons was elaborated by interpreting the results of N_2 adsorption at 77 K. Adsorption isotherms were obtained on a Quantachrome porosimeter. BET (Brunauer-Emmett-Teller) method was applied to the calculation of the specific surface areas (SSA) of each sample while pore size distributions (PSDs) were obtained using the Quenched Solid Density Functional Theory (QSDFT) method. The PSDs were derived from both the adsorption and desorption (equilibrium) branches of the isotherm. QSDFT was selected as the most realistic theoretical analysis model for carbonaceous materials prepared via the templated precursor path and thus applied to samples featured by wrinkled and rough amorphous pore walls, the alternative NLDFT model being more appropriate in the case of porous carbons with flat and non-structured graphitic walls[4].

It can be argued that the carbons derived from the etched eps-Vycor® samples share common pore structural characteristics. However, there are distinct features related to the shape of the N_2 adsorption isotherms and the way the PSD curves decay at the region of large pore sizes (Figure 61a,b). The different shape of the N_2 adsorption isotherms and PSD curves is attributed to the different portion of the small and large fragments in the carbon samples.

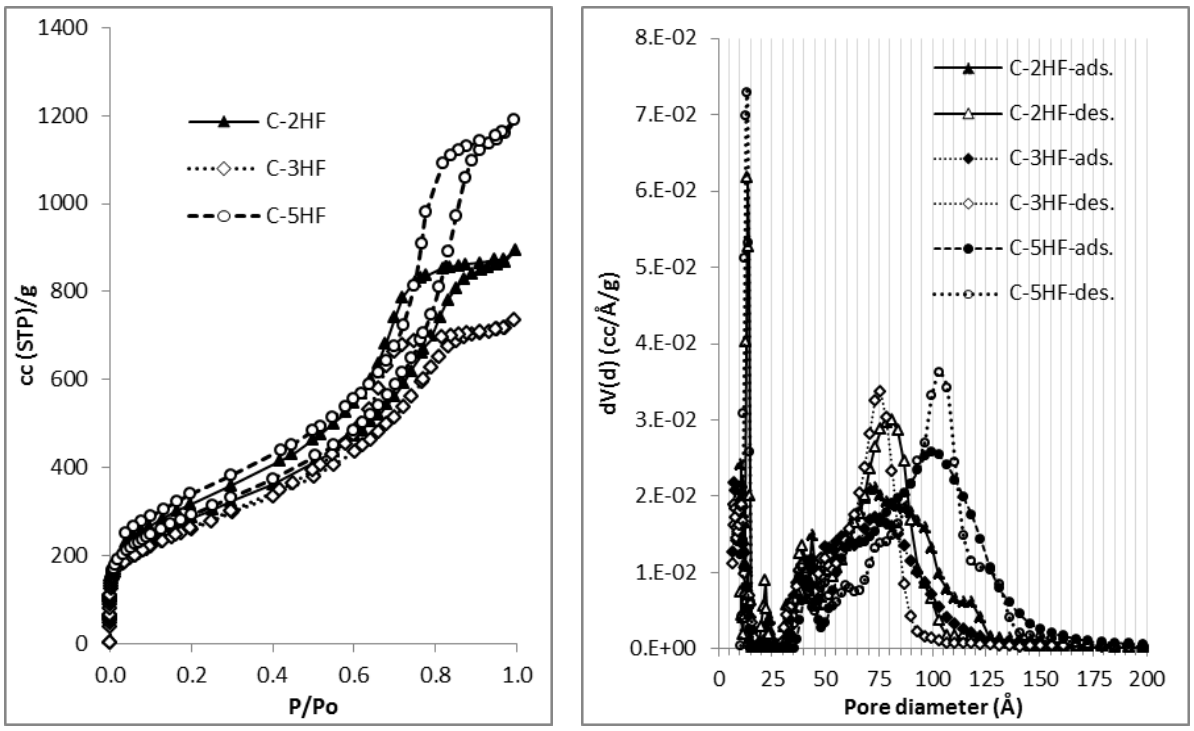

Figure 61: (a) N_2 adsorption isotherms at 77 K of the carbon samples derived from 2HF- Vycor®, 5HF- Vycor® and 7HF- Vycor®. (b) PSDs of the carbon samples derived from 2HF- Vycor®, 5HF- Vycor® and 7HF- Vycor®.

Table *1* summarizes the main properties of C-2HF, C-3HF and C-5HF samples related to their pore structural characteristics.

Table 1. Characteristics of the porous structure of C-4h and C-8h

Sample	S BET ($m^2\ g^{-1}$)	Total Pore Volume (TPV) ($cc\ g^{-1}$)	Mean pore diameter (d) (nm)
C-2HF	1012	1.38	1.4 and 7.5
C-3HF	930	1.14	1.3 and 7.5
C-5HF	1042	1.84	1.4 and 10

The prepared electrocatalysts were scrutinized with the Rotating Ring Disk Electrode (RRDE) and the corresponding voltametric curves are depicted in Figure 62. As it can be seen from the analysis of these electrochemical profiles, all electrocatalysts showed a well-defined ORR reduction peak with remarkable onset potential values (Eon).

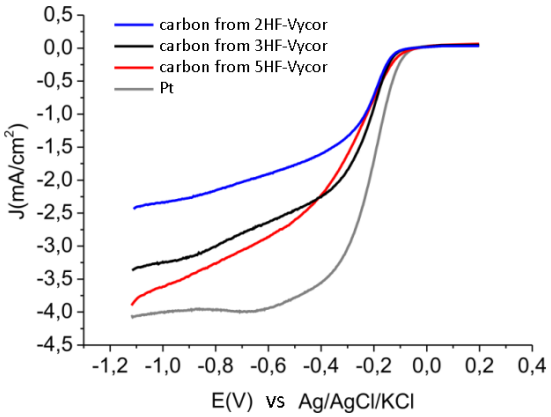

Figure 62: RRDE current-potential curves of carbon from 2, 3 and 5HF- Vycor® at 293 K in O_2 saturated 0.1 M KOH solution registered at GC disk (A = 0.196 cm²). All samples were measured at a working electrode spin rate of 800 rpm.

4. Conclusions

In this work we showed that templated IL pyrolysis and unconfined IL pyrolysis followed by activation with CO_2, brings to N-doped C-materials with different pore structural characteristics and pore surface properties. It has also been concluded that the pore size of the template, which in this work consisted of pore etched Vycor® with different degrees of pore etching, also affects the properties of the derived carbons.

The N-doped carbons produced with the templated IL pyrolysis method were tested as catalytic materials for the challenging electrochemical ORR. All materials exhibited remarkable efficiency in oxygen reduction with the sample produced from the template with the smaller pores being the most effective one.

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ZnO nanoparticles supported on mesoporous silica hosts as efficient antibacterial agents for nanocoating applications

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1. Introduction

Infectious diseases pose a significant threat to human health and the global economy, accounting for more than 20% of global mortality, while viruses are responsible for about one-third of these deaths.[1,2] To tackle with these threats, antimicrobial coatings are widely used, presenting however certain draw-backs related to: (i) the release of the active compounds that might slowly enter the ecosystem, (ii) the loss of their efficiency in short time, (iii) the resistance of the microbes to the commonly used agents and (iv) the high human toxicity of some antimicrobial agents (e.g., Ag). Addressing these challenges, the present study is focused on the developement of novel active nanomaterials (ANMs) based on ZnO nanoparticles (NPs) supported on mesoporous silica featuring different pore geometry. Specifically, mesoporous SBA-15 and KIT6 were used as non-toxic ZnO NPs hosts. Inclusion of ZnO NPs within the mesoporous networks provides various benefits related to higher NPs dispersion,[3] limitation of growth phenomena, as well as reduction of zinc amount and of the harmful release of zinc cations. To achieve a geometrically restricted deposition of ZnO NPs within mesoporous silica hosts special attention must be given to the employed metal loading method, since most of them usually lack control over particle size and distribution. Thereby, a novel dendritic polymer templating strategy called assisted impregnation (A.I.) was employed.[4] This technique relies on the use of hyperbranched polymers as metal entrapping and templating agents by taking advantage of their chemical and chelating properties. Particularly, in this study, the water soluble, low cost and commercially available hyperbranched polyethyleneimine (PEI) of 5,000 Da molecular weight was exploited. After the structural characterization of the synthesized nanomaterials, their antibacterial activity was investigated against Gram-positive Staphylococcus Aureus bacteria, while their biocompatibility was investigated through cytotoxicity on mammalian cell lines.

2. Experimental section

SBA-15 and KIT-6 mesoporous hosts were produced through the synthetic routes described Kosuge et al.[5] and Kleitz et al.[6] Inclusion of ZnO within mesoporous silicas was performed via assisted impregnation (A.I.) technique consisting of the following synthetic steps (Figure 1). The initial step involved the introduction of PEI within silicas'

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mesochannels through wet impregnation. Following PEI addition, a washing procedure was performed to remove the free polymer. Then metal sorption was carried out by adding the obtained organically modified mesoporous silicas into aqueous solution of $Zn(NO_3)_2{\cdot}6H_2O$ (with initial concentration 10,000ppm, pH ≈ 5) and left stirring for 24h. During this period, anchoring of Zn^{2+} ions in specific sites (tertiary and primary amino groups) supplied by the hyperbranched polymer took place. Finally, solids were obtained by filtration, dried and calcined at 550°C for 5h at a heating rate of $1^{o}Cmin^{-1}$ under air flow for the PEI decomposition and the acquisition of ZnO loaded silicas. The obtained nanomaterials were characterized by TGA, XRD, SEM, EDX and N_2porosimetry.

The antibacterial activity of ZnO NPs supported on mesoporous SBA-15 and KIT6 was investigated against Gram (+) Staphylococcus Aureus bacteria as model microorganism Their minimum inhibitory concentrations (MIC) and minimum bactericidal concentrations (MBC) of theses nanomaterials were determined by the broth dilution and colony counting methods according to M07-A9 and M26-A protocols issued by the Clinical Laboratory Standards Institute (CLSI), respectively.[7,8] On the other hand, their toxicity was evaluated on DU145 and PC3 human prostate adenocarcinoma cell lines, A549 human lung carcinoma cell line, and HEK293 normal human kidney cell line by MTT assays after 24h incubation time.

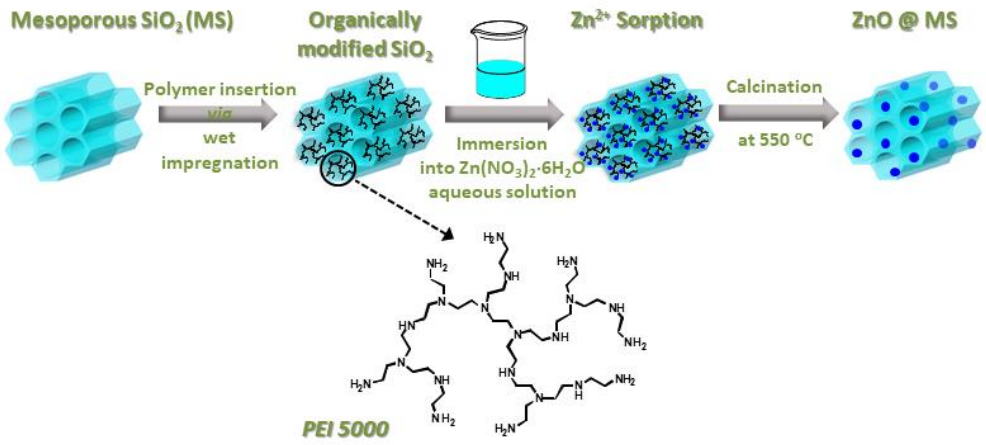

Figure 63: Schematic illustration of ZnO NPs supported on mesoporous SiO_2 through Assisted Impregnation

3. Results and Discussion

A hyperbranched polymer uptake of 17 and 27 wt.% in case of SBA-15 and KIT-6 respectively was determined by TGA technique, while polymer's presence was also verified by N_2 adsorption analysis. According to the values listed in Table 1, upon PEI addition a drastic drop in specific surface area and total pore volume was induced together with an increase in the average pore diameter, indicating the introduction of the polymer into the channels of the porous hosts. The same conclusion derives by comparing N_2 adsorption data of the parent and Zn loaded materials. SEM and EDS mapping analysis (Figure 2) reveals a very high uniformity and homogeneous spatial distribution of Zn species, without the detection of Zn rich domains or large ZnO aggregates. In addition, based on the values listed in Table 1, there is a good correlation between Zn and PEI loadings, with the highest Zn up-take, about 6 wt.%, attained for KIT-6. Finally, as demonstrated by low and wide angle XRD patterns, Zn addition did not

deteriorate the ordered mesostructure of the parent SBA-15 and KIT-6 materials, while the absence of peaks assigned to the ZnO crystal phase in the wide angle area evidences the high dispersion degree and the nanocrystalline nature of ZnO species.

Table 1: PEI content, Zn loading, pore and structural properties.

Samples	PEI content (wt.%)	Zn loading (wt.%)	SSA (m^2g^{-1})	TPV (ccg^{-1})	Average Pore Diameter (nm)
SBA-15	–	–	537	0.49	3.6
SBA-15_PEI	17	–	223	0.28	5
ZnO_SBA-15	–	2.6	511	0.56	4.4
KIT-6	–	–	876	1.16	5.3
KIT-6_PEI	27	–	297	0.57	7.7
ZnO_KIT-6	–	5.9	742	1.05	5.7

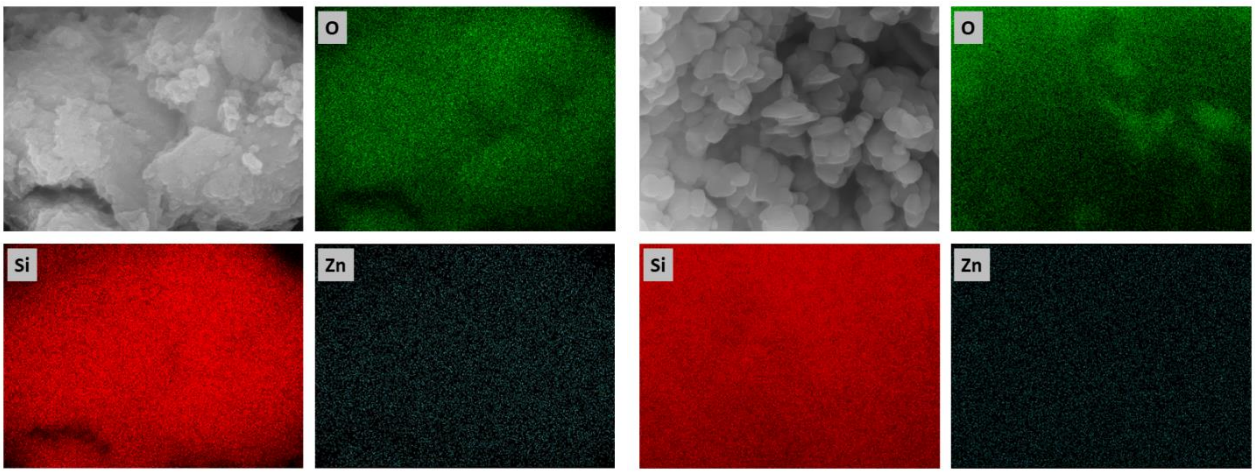

Figure 2: SEM micrograph and corresponding elemental maps of ZnO_KIT-6 (left) and ZnO_SBA-15 (right)

4. Conclusions

To conclude, a novel dendritic polymer templating strategy, called assisted impregnation, was employed for the development of highly dispersed ZnO species uniformly distributed within SBA-15 and KIT-6 mesoporous networks. As deduced, mesoporous host's pore structural characteristics affect polymer uptake and in turn the final Zn loading. Preliminary assessment revealed that the developed nanomaterials exhibited adequate antibacterial efficancy, at low concentrations (above 200 μg/ml), combined with low cytotocity.

5. Acknowledgements

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"Advances in combating antimicrobial resistance of materials via laser based techniques"

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1. Introduction

Antimicrobial surfaces are valuable in medical, and industrial applications, whereas contamination with pathogens and biofouling may cause a severe risk to human well-being. Conventional approaches used for bacteria treatment comprise coating the surface with antibiotics, and application of coating containing microbicidal polymers, or metal nanoparticles. Nevertheless, such coatings have a rather short lifetime and those raise concerns related to leaching and degradation percentage of the developed coating. Therefore, there is a considerable interest in designing persistent and non-leaching bacteria - free surfaces. To acquire an antimicrobial surface, we merge micro and nanoscale structuration of mirror polished stainless steel surfaces by ultra - short laser irradiation and subsequent deposition of magnetron sputtered layer of Ag and Cu. Laser surface patterning (LSP), represents an alternative approach to a variety of surface modification methods, and it has been successfully applied for antimicrobial applications to enhance the resistance of the materials surfaces against bacterial attachment.

The use of surface texturation and incorporation of additional antimicrobial agents of Ag and Cu demonstrated good results in view of most prominent bactericidal effect against *Staphylococcus aureus, Candida albicans, Pseudomonas Aeruginosa* and *Escherichia coli*. More expressive results were obtained for the Laser structured/Cu surfaces. The laser texturation and the deposition of magnetron sputtered layers of antimicrobial material are environmentally - safe processes that are applicable to a broad range of materials. This combined approach is appropriate for studies of bacteria-surface interactions, and could provide possibilities for future antimicrobial applications in everyday use.

2. Femtosecond laser patterning and magnetron post-modification of the stainless steel

Laser induced surface texturing was obtained by ablating the surface of mirror polished cold rolled stainless steel samples (2.5 x 2.5cm, 1mm-thickness). The radiation from a commercial Ti: Sapphire femtosecond laser source (Solstice ACE, Spectra-Physics) was focused to a spot of 25μm. The central laser wavelength is 800nnm laser, pulse duration of 70fs, and 1 kHz repetition rate. Maximum output power of 6W. Two types of textures were designed, one which contain only nanometric structures in the form of laser

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induced periodic surface structures (LIPSS), and one which possess micro and nanostructures (hierarchical).

The film deposition was performed by magnetron sputtering with pure Ag and pure Cu onto the surface of mirror polished and laser structured stainless steel. The working gas was argon at a pressure of p (Ar) ≈ 0.67 Pa in a constant flow mode (13-14 sccm) at room temperature. The final film thickness was established to the 500 nm.

3. Antimicrobial studies

To evaluate the antimicrobial properties of the laser modified surfaces, *S. aureus* ATCC 6538P at specified optical density was prepared from overnight grown LB agar plates and placed onto two types of laser patterned surfaces (LIPSS and hierarchical structures). 25 µl of bacterial suspension was pipetted onto 2.5 x 2.5 cm surfaces, covered with plastic 2 x 2 cm foil and incubated in a closed vessel for 4 and 6 h. After the incubation period, bacteria were washed off from surfaces by introducing the surface to 10 ml of SCDLP medium in 50 ml centrifuge tube and by vortexing the tube over 30 sec. the wash-off in SCDLP medium was seeded on LB agar medium and bacterial number was counted after 24 h of growth at 37ºC. Results showed that already after 4 h of exposure, more than 2 log less bacteria could be retrieved from the hierarchical surfaces than from control and after 6 h of exposure, no bacteria could be washed off from hierarchical surfaces.

A qualitative assessment of antimicrobial efficacy under semi-dry conditions was conducted, utilizing the following strains: *S. aureus* ATCC 6538P, *P. aeruginosa* ATCC 15442, *E. coli* ATCC 8739, and *C. albicans* DSM11225. Briefly, suspensions of each strain with defined optical density (OD) were prepared from overnight cultures, and subsequently plated on PC-agar plates to create microbial lawns. Following air-drying, laser patterned samples (LIPSS structures) were applied onto the bacterial lawns in triplicate and the plates were incubated at room temperature. After 2 hours, the samples were carefully removed, and the plates were further incubated overnight at 37°C to allow for the growth of viable cells. In the next day, pictures of each plate were taken to quantify colony-forming units (CFUs) for the areas in contact with the samples.

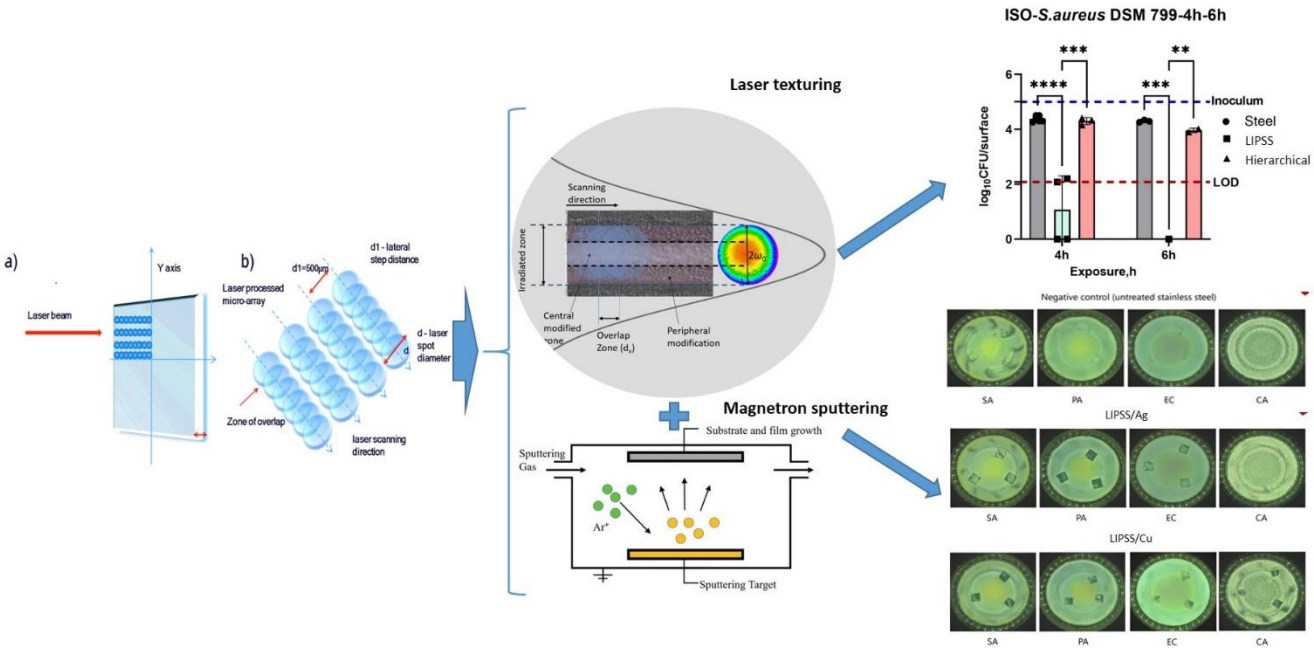

Figure 64: Effects of femtosecond laser texturing and and postmodification with magnetron sputtering and visualisation of bacterial assays and screening touch test performed on laser structured (in the form of LIPSS) magnetron sputtered samples with Ag and Cu. SA : S. aureus ATCC 6538P, PA: P. aeruginosa ATCC 15442, EC: E. coli, ATCC 8739, CA: C. albicans DSM11225

3. Discussion

Two approaches are known, that affect surface antimicrobial properties. One is the deposition of surface-repellent layers of chemical substances, and the other is to creation of an environment that acts as activating antimicrobial characteristics by creating contact between the surface and bacteria cells. The current study evaluated the combination of laser patterning with post-modification of the surface by magnetron sputtering. We first produced a set of diverse test textures (LIPSS and hierarchical structures) by femtosecond irradiation and the selected LIPSS and combined LIPSS/micro-column structures to analyse the effect of local stress imposed by the structures on the disruption of the bacterial cell membrane. After performing a bacterial viability test via a log10 CFU on laser patterned and mirror polished surface, we monitored a decrease of bacterial cell signal, with respect to control SS, and also concerning the surfaces that contain only nanometric (LIPSS) structures. The signal dropped drastically after 6h of exposition for the hierarchical structures. The performed screening test (Screen TT) only on laser-textured surfaces showed a limited effect. However, after exposition to laser structured in the form of LIPSS/magnetron sputtered samples, improved antimicrobial behaviour was clearly seen for Ag sputtered samples from the strains *S. aureus* ATCC 6538P, *P. aeruginosa* ATCC 15442, *E. coli* ATCC 8739. The LIPSS/magnetron sputtered Cu samples exhibit similar behaviour.

4. Conclusions

In summary, we have created a combined treatment approach by comprising femtosecond laser surface processing (using LIPSS and combined micro- and nano texturation) and magnetron deposition deposition to generate enhanced bactericidal surfaces. The results only from non-sputtered samples demonstrate good antimicrobial

effect. The interaction between the bacteria cells and the laser structured magnetron sputtered surfaces, have a synergistic effect simultaneously generating mechanical disruption due to the developed nanometric surface roughness, on the bacteria, and additionally adding the influence of known antimicrobial agents as Ag and Cu.

Acknowledgement: This work was funded by the European Union: Horizon Europe program under the Grant Agreement № 101057961, „Surface transfer of pathogens" (STOP), and EU H2020, Grant Agreement AIMed No. 861138.

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New Products from Waste PVC Flooring and Safe End-of-Life Treatment of Plasticizers

Tanja Bielmeier[1], Martin Schlummer[2], Marcus Süß[3]

1. Introduction

Our dependence on plastics, driven by affordability and convenience, has resulted in a global environmental issue. Every year, millions of tons end up in landfills, oceans, and ecosystems. The current "take-make-dispose" economic model is unsustainable for plastics. We need a circular economy. A circular economy for plastics prioritizes keeping materials in use for extended periods. This means recycling, reusing, and minimizing waste. This shift benefits the environment by reducing pollution, but also creates economic and social advantages such as job creation, resource efficiency, and lower greenhouse gas emissions.

The EU-funded project Circular Flooring aims to enable circular use of plasticized PVC (PVC-P) from waste flooring by developing recycling processes that eliminate plasticizers including hazardous phthalic acid esters (e.g. DEHP). End-of-life flexible PVC floor coverings potentially contain ‘legacy plasticizers’ which may no longer be used today for reasons of consumer protection and which in the meantime have been replaced in the EU by safer alternatives. State-of-the-art recycling of such flooring with recovery of PVC in virgin-like quality therefore requires a technically sophisticated separation of these ‘legacy plasticizers’. Circular Flooring meets this challenge with an innovative, dissolution based recycling process, which was developed by the Fraunhofer Institute for Process Engineering and Packaging IVV (Freising, Germany) and adapted to the special needs of plasticized PVC from old flooring.

2. Project Goals

Circular Flooring aims to enable a circular use of plasticized PVC from flooring waste by a recycling process (see Figure 1) that eliminates legacy phthalic acid esters that are not compliant with the EU REACH Directive. Additionally, a recycling process for recovering secondary legacy phthalate-free PVC from flooring waste will be developed, thus preventing usable resources from landfill or incineration. These are transformed into safe alternatives. Once recycled, a close cooperation with flooring manufacturers is planned to demonstrate that circular PVC and plasticizers are applicable in new flooring systems. Alongside the technical work, Live-Cycle-Assessments, health and safety assessments and economic feasibility studies accompany the work.

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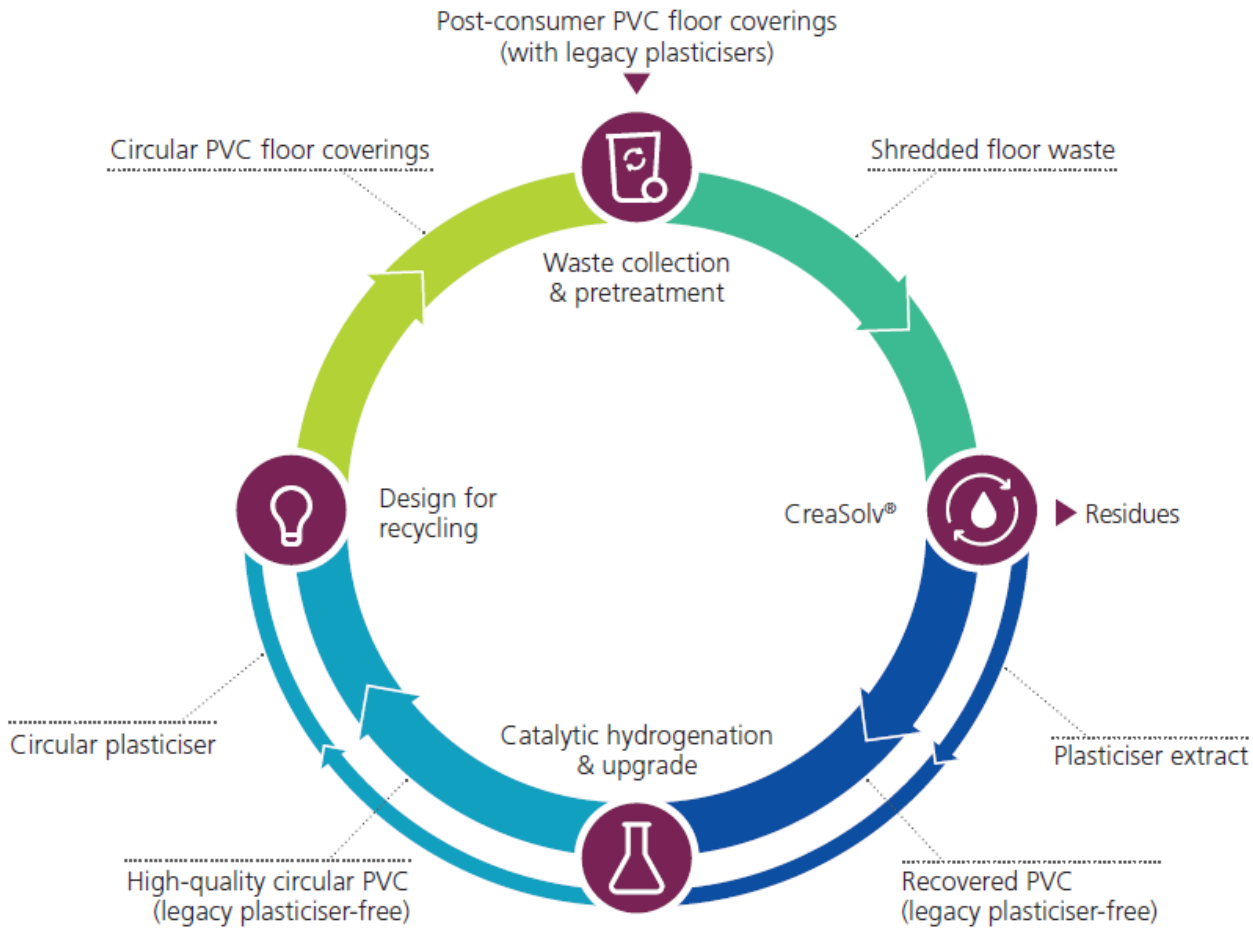

Figure 65: The recycling process

3. Impacts on European industry, society and the environment

In 2022, a total over 58.7 Mt of plastics were produced in Europe, whereas only estimated 13.1% of the production was gained from post-consumer material streams. The PVC share of the total European plastic produced is 9.1%, which corresponds to a total quantity of approximately 5.3 Mt[4]. Based on these figures, the impact of the project becomes clear as by implementing a dissolution based recycling process, the recycled share of the entire European plastic production would significantly be increased. Besides the raw materials consumption, current production of the vinyl chloride monomer entails a high energy demand and corresponding emissions, various by-products detrimental to the environment as well as an interrupted value chain in terms of resources recovery. PVC is often used for long-lasting products (> 25 years) and contributes already (because of its nature) to the environmental protection, in contrast to single-use or less durable plastics. Through a dissolution based recycling process, the PVC life cycle is considerably extended, and indispensable PVC usage would become more sustainable. The PVC industry, which employs > 500,000 people in Europe, will become stronger the future. In addition, the PVC recycling activities will create new jobs and by this strengthen the economy of European member countries.

[4] Plastics Europe - Enabling a sustainable future (The Fast Facts-2023)

4. Conclusion

The Circular Flooring project stands as a testament to the potential of innovative recycling technologies in creating a circular economy for plastics in Europe. By successfully developing a method to remove hazardous additives from waste PVC flooring and transform it into high-quality recycled material, the project offers a sustainable solution for a widely used material. The environmental benefits are clear: reduced reliance on virgin plastics, minimized waste generation, and lower greenhouse gas emissions. Additionally, the project offers economic advantages by strengthening the PVC industry and fostering job creation in the recycling sector.

However, achieving a truly circular plastics economy in the EU requires a multifaceted approach. While the Circular Flooring project demonstrates technological advancements, broader challenges remain. Continued efforts are needed to increase demand for recycled plastics, establish stable regulations for recycling technologies, and ensure robust safeguards against hazardous substances. This necessitates collaboration across all stakeholders – policymakers, industry leaders, and consumers – each playing their part in fostering sustainable practices. By combining innovative solutions like Circular Flooring with a comprehensive and collaborative approach, Europe can pave the way for a more responsible and environmentally friendly future for plastics.

Fraunhofer flagship project »ORCHESTER«: Digital ecosystem for a resilient and sustainable supply of functionally reliable materials

A. Kugele[1], M. Rabung[2], R. Tschuncky[2], C. Schweizer[1], D. Helm[1], P. Gumbsch[1]

1. Introduction

The interdisciplinary Fraunhofer flagship project »ORCHESTER«, scheduled to run for four years (2024-2027), addresses the challenges of the circular economy and security of supply, in particular with functionally reliable materials for the energy transition along the entire value chain.

2. Global challenges and regulatory requirements drive the need for sustainable and resilient materials

The European Critical Raw Material Act (CRMA) [1] is setting political framework conditions for a multitude of raw materials: by 2030, 10% are to be extracted in the EU, the further processing rate is to increase to 40% percent, the recycling rate to 15%, and a maximum of 65% of imports are to be sourced from just one country. Consequently, the objective is to move towards a circular economy, and to substitute critical elements [2].

Additionally, geopolitical and social crises lead to major uncertainties in industry and society due to disruptive material supply flows. Of particular importance is the implementation of the energy transition. The EU aims to achieve greenhouse gas neutrality by 2050 [3], which is dependent on a secure supply of raw materials and at the same time has a massive impact on material flows.

However, the reliable supply situation over the last decades has contributed to the value chains becoming increasingly optimized, specialized, and globalized. The result is an enormous variety of materials with closely defined process routes. As unexpected events such as the pandemic and the war in Ukraine have shown, the high degree of optimization and specialization makes value chains more susceptible to disruption. Even minor disruptions in the supply of materials lead to immense economic, ecological, and social consequences - in the event of bottlenecks, substitution solutions must be found quickly. However, the associated process routes currently come up against rigid and over-regulated standards and methods for the development and release of products and processes.

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3. Three demonstrators in the context of the energy transition

The challenges described are particularly significant for metal and magnetic materials with critical elements and widespread use. This applies to classic construction materials as well as light metal alloys and ultra-modern specialized functional materials, which are represented in this project by steel, aluminium and magnetic materials. We focus on material specification, recycling and criticality as well as a strong reference to the energy transition, thereby addressing the largest industrial sectors and future markets.

Figure 1: Three components in the context of energy transition used as demonstrators in this project.

4. Building a digital ecosystem to map the value chain

Recycled materials play a crucial role in material supply but can compromise the functional safety of components due to chemical contamination. Ensuring a sustainable and resilient supply of functionally reliable materials requires the entire value chain to be digitally and physically networked. Current market technologies do not yet support this level of integration.

Scientific and technological advancements indicate that a secure material supply for value chains can only be achieved through interdisciplinary concepts applied holistically. This involves raw material extraction and processing, metallurgy, process technology, materials science, mechanics, production technology, and recycling. It necessitates a comprehensive understanding of how chemical elements and compounds enter and interact within the cycle.

Thus, ensuring safe material supply demands rapid evaluation of process and functional safety, resilience, and sustainability within a digital ecosystem. To this end, we integrate experimental, simulation-based, process, sensor, and digital technologies into such an ecosystem. Additionally, tools such as high-throughput screening, sensor data, process simulations, and knowledge graphs for linking material and process data with models and expert knowledge will be utilized.

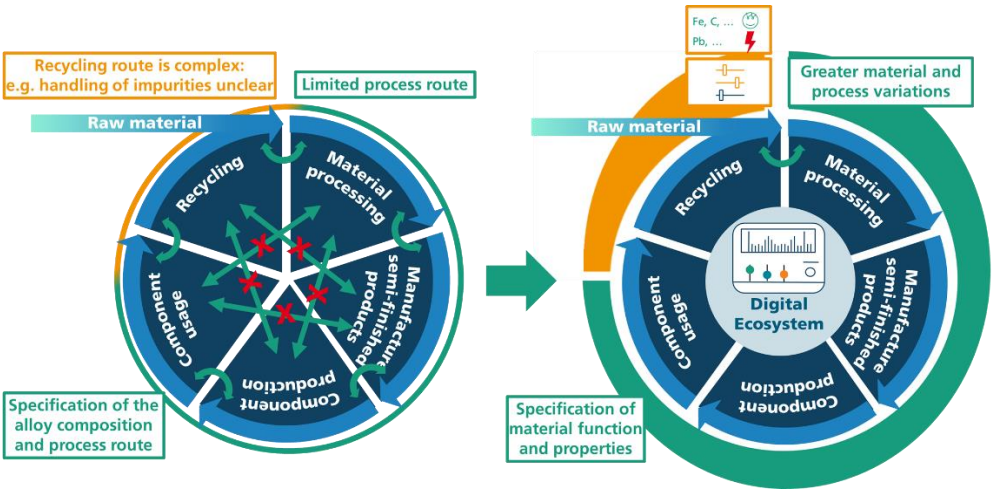

Figure 2: Representation of the value chain with the "state of the art" depicted on the left and vision of this project shown on the right.

5. Creating new opportunities with customized digital products

ORCHESTER will provide customers with a holistic offering to secure the supply of materials for resilient and sustainable value chains. The digital ecosystem to be created will provide integrated functional safety assessment solutions and recommendations for action based on a digital knowledge base. The solution approach is based on the digitalization and networking of information along the value chain. To this end, technical challenges in dealing with fluctuating material compositions in recycling routes, fast and efficient alloy variation, the integration of material flow models and computer-aided methods for predicting multifunctional material properties (e.g. mechanical, corrosive, producible and sustainable) must be solved.

6. Creating added value and measurable improvements

This project aims to show that a paradigm shift in material specification and the associated approval processes increases the selection of usable materials at least fivefold, increases the proportion of recycling in process routes by at least 50 % through methods for dealing with impurities in secondary metals. Moreover, the proportion of rare earths from primary production should be reduced by at least 25 %, and, in all demonstrators, the increase in resilience by more than 30 % is proven by a stress test.

Our targeted recommendations for action give the industry room for maneuver and evaluation options with regard to material supply and criticality as early as the development phase, proactively improving security of supply. In shortage and crisis situations, ORCHESTER will open up rapid response options for finding alternative materials and maintaining production via alternative routes or semi-finished products. This results in greater security of supply by reducing the proportion of critical alloying elements and by increasing the use of sustainable materials with a high proportion of secondary materials.

7. Conclusions

By driving technological advancements, the overarching goal of this project is to moderate the interplay between industry, associations, politics and research in the supply of functionally safe materials for the energy transition. In particular, we aspire a paradigm shift in material specification away from a definition based on material composition towards a function-based specification that enables faster substitution of critical materials and thus a more resilient material supply.

This work was funded as a Fraunhofer FLAGSHIP PROJECT.

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Session 9: Infrastructure & Methods Requirements for Materials Innovation

This Session is focussed on the requirements for novel and innovative infrastructures for characterisation- and measurement methods for organic and inorganic materials, hybrid, persistent, biodegradable and more materials to keep pace with the advancement in materials R&I. This includes, for example, clean room infrastructures, synchrotrons and other large-scale facilities, but also access to high end materials modelling infrastructures and testing. Innovative approaches for democratising access to expertise in experimental design and optimisation, as well as infrastructures for data management are also welcome.

The Session will include contributions on the implementation of the Safe & Sustainable-by-Design (SSbD) Framework or similar design-tools that aim at improving the safety, sustainability or circularity of a material, or material-including product or process.

Presentations (oral and poster) will also cover the following topics:

- Requirements for novel/innovative characterisation methods (incl. quantitative imaging, smart sensors),
- Automated, high throughput screening methods,
- Intra-scale characterisation methods,
- Digitalisation & data platforms along with FAIRness elements, and
- AI in experimental process/output (e.g. image/pattern recognition anomaly detection).

Detailed Programme

Start	End	Title	Presenter
14:30	14:45	Chemical Nanoscale Analysis of Mesoporous Mixed IrOx-TiOy Thin Films	Vasile-Dan Hodoroaba
14:45	15:00	Chemical Analysis of Functionalized Graphene along the Production Chain	Loay Akmal Madbouly
15:00	15:15	Correlation between size distribution, morphology and chemical analysis of Graphene Family materials	Kerstin Jurkschat
15:15	15:30	SUNSHINE Safe and Sustainable by Design (SSbD) approach and e-infrastructure	Lisa Pizzol
15:30	15:45	Score System for a Multi-criteria Decision Analysis based on the SSbD framework for MCNM/HARN Risk Management – The DIAGONAL Decision Support Tool Case	Blanca Pozuelo Rollón
15:45	16:00	Spectroscopic Approaches for Understanding Graphene Family Material interactions with Enzymes	Bashiru Ibrahim

16:00 16:20 24/7 Poster Presentations

Posters

S09_P02	Raman spectroscopy elucidates the transformation of single-walled carbon nanotubes following abrasive wear of epoxy coatings	Gunther Van Kerckhove
S09_P03	Morphological analysis and Sample preparation of Particulate Graphene oxide materials	Paul Mrkwitschka
S09_P04	NPCoronaPredict: Multiscale modelling of the nanoparticle biomolecular corona	Ian Rouse
S09_P05	Paper-based electrochemical sensor for the detection of essential oils and SARS-CoV-2 virus	Elisa Recchia
S09_P06	Beneficial effect of differently-coated Selenium Nanoparticles in 3D cell culture models mimicking the respiratory tract and intestinal epithelium	Pamina Weber
S09_P07	The “Navetta” in vitro aerosol exposure system for respiratory health monitoring as well as efficacy and safety testing of pulmonary delivered bio-based pharmaceutical formulations	Magdalena Weiss
S09_P08	Correlative chemical imaging to reveal the nature of different commercial graphene materials	Robert Schusterbauer
S09_P09	Holistic, reliable and practical Characterization Framework for Graphene-Family Materials, a correlated approach including Imaging-based techniques	Daniel Fernandez-Poulussen
S09_P10	Chemical Nanoscale Analysis of Mesoporous Mixed IrOx-TiOy Thin Films	Vasile-Dan Hodoroaba
S09_P11	Novel Two-Dimensional Magnets Synthesized in Graphene Oxide Under Ambient Conditions: Atomic Structure and Magnetic Properties	Viera Skakalova

Oral Presentations: Session 9

Role of Sample Preparation for Accurate and Automated Morphological Analysis of Nanoparticles proven in Interlaboratory Comparison Exercises

Vasile-Dan Hodoroaba[1], Christoph Salzmann[2], Francesco Pellegrino[3], Bénédicte Durand[4], Olivier Taché[5], Amaia Zurutuza[6]

1. Introduction

The accurate analysis of size and shape distribution of nanoparticles is a challenging task, which is strongly dependent on the complexity of the morphology of the particles and the type of material. Simple, model nanoparticles with spherical shape and narrow/monodisperse size distribution can be easily and accurately analysed basically by any sizing method (ensemble and counting). Nanoparticles which have a complex shape, are polydisperse in size, have a complex chemistry (including defined and unexpected outer shells/coatings), or provide a certain level of agglomeration and/or aggregation, are mostly prone to a faulty quantification regarding their particle size and shape distribution. Guidance for accurate measurement by electron microscopy techniques has been recently developed under ISO [1,2], however, the large variety of morphologies and chemistries of commercial nanoparticles cannot be covered with uniform guidance. Furthermore, one crucial point for an accurate determination of the size and shape nanoparticle distributions by imaging methods is the sample preparation, such that the individual particles are finally prepared as isolated particles on a suited substrate, not touching or overlapping each other.

In this contribution three examples of nanomaterials with different challenges for the morphological analysis will be highlighted: i) TiO_2 nano-bipyramides, ii) SiO_2 nanoparticles of spherical shape and a bimodal distribution with different relative concentrations, and iii) graphene oxide flakes.

2. Sample Preparation

The single-particle preparation of nanoparticles on a substrate for imaging guarantees not only an accurate dimensional measurement, but also enables the use of automated

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segmentation of the images. Hence, a more representative quantitative analysis of a statistically large number of nanoparticles by imaging methods becomes possible as a routine procedure.

Another parameter of high relevance for nanoparticles is the number concentration. Here again, the more complex in morphology and chemistry the particles are, the more complex the accurate measurement of their number concentration is, regardless by the analysis method employed. Once suited sample preparation procedures resulting in single particles deposited on a substrate are available, the accurate counting by imaging methods becomes routine, too.

Various sample preparation procedures such as the substrate pre-treatment (with ozone, glow discharge or deposition of poly-L-lysine, etc), electrospray deposition, spin coating, etc., are available mostly depending on the type of nanoparticle material.

The alternative to the laborious, 'perfect' single-particles sample preparation for analysis would be the imaging of the nanoparticles as they are, directly deposited on a substrate, and application of machine learning approaches after appropriate manual training. First studies have showed success [3].

3. Measurements

Figure 1 illustrates the successful sample preparation as isolated particles for TiO_2 as a nanoparticulate material which usually tends to agglomerate and is difficult to completely deagglomerate [1,5].

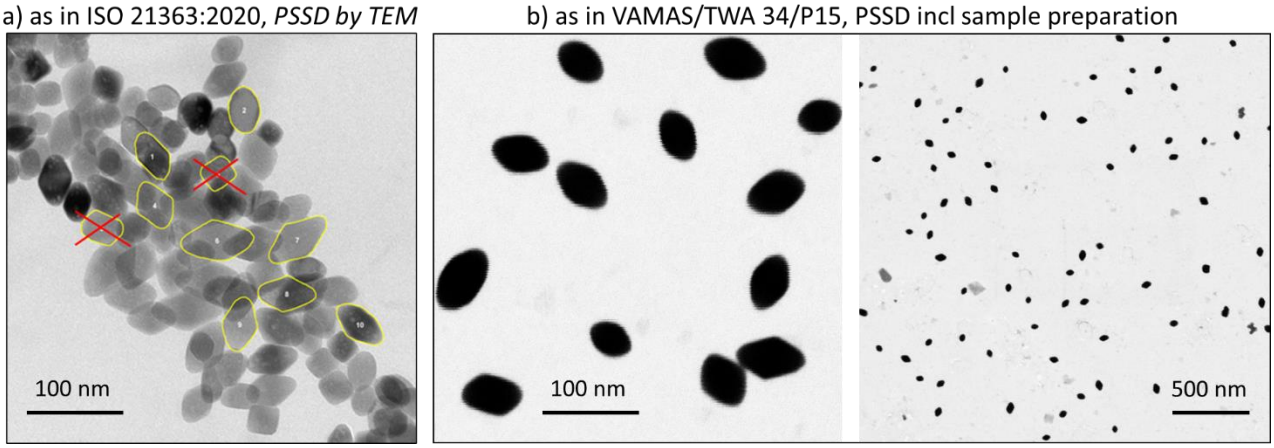

Figure 66: Result of the improved sample preparation of TiO_2 nanoparticles for more accurate imaging analysis, i.e. with almost only isolated nanoparticles, homogeneously deposited on the substrate

Whilst 2020 the sample preparation for standardized imaging analysis was not yet optimised (Fig. 1 left), [1] recently, progress in sample preparation of the same nanoparticles has been reached within the pre-standardisation platform of VAMAS [5]. Similar progress has been achieved in a parallel VAMAS interlaboratory comparison on SiO_2 bimodal nanoparticles [6], where the homogeneous and single-particle deposition on substrate has resulted in a significantly more accurate particle relative number concentration as measured by imaging methods (SEM, TEM, AFM).

A third case study, namely a graphene oxide 2D material in form of µm-large flakes of single monolayers, demonstrates the power of good sample preparation, see Figure 2

after optimisation of the sample preparation procedure. The study is conducted also as a (ongoing) VAMAS interlaboratory comparison, under TWA 41, project #13 [7].

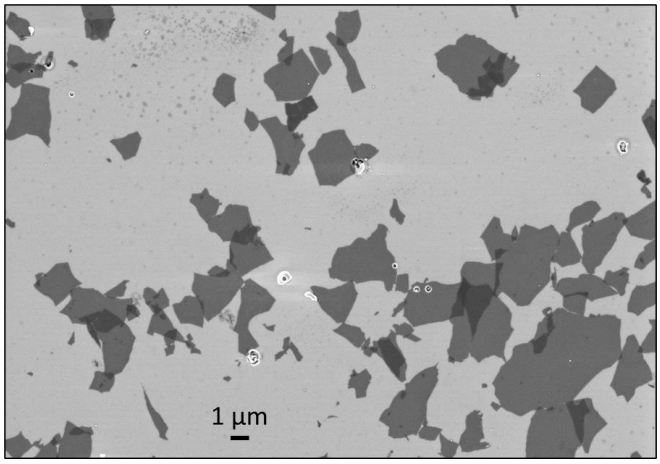

Figure 67: Result of improved sample preparation of graphene oxide monolayer flakes as measured with an SEM with an SE InLens-type detector

4. Results and Conclusions

After imaging of the particles deposited according to the optimised sample preparation protocols, the particle size and shape descriptors (minimum Feret, maximum Feret, ECD, aspects ratio) and the relative number concentration of the SiO_2 bimodal nanoparticles in the three interlaboratory comparisons described above have been measured. The image analysis approaches used and the final data will be presented, with a comparative discussion of the results obtained by individual laboratories and methods, and of the sources of measurement uncertainties observed. Relative deviations between laboratory mean values for the size and shape descriptors of max 10% could be reported particularly due to the improved sample preparation protocols. Significantly larger deviations have been reported for the (relative) particle number concentration by imaging and ensemble methods, the latter ones measuring the nanoparticles in suspension. The reasons for these deviations have been identified and will be also discussed.

5. Acknowledgements

The projects 17NRM04 nPSize and 19NRM04 ISO-G-SCoPe have received funding from the EMPIR programme co-financed by the Participating States and from the European Union's Horizon 2020 research and innovation programme. The contributions of all participants in the VAMAS interlaboratory comparisons are gratefully acknowledged.

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Chemical Analysis of Functionalized Graphene along the Production Chain

Loay Akmal Madbouly[1], Paul Mrkwitschka[1], Robert Schusterbauer[2], Elliot Jones[3], Vasile-Dan Hodoroaba[1], Jörg Radnik[1]

1. Introduction

In 2004 Geim and Novoselov successfully isolated and characterized graphene, which was proven to be groundbreaking discovery [1]. Graphene is a two-dimensional (2D) material consisting of a single layer of carbon (C) atoms arranged in a hexagonal lattice structure. It has attracted significant attention in the scientific and industrial communities due to its exceptional mechanical, thermal, electrical, and optical properties. Hence, graphene applications are immense, including electronics, energy storage, composites, and sensors. Its extraordinary electrical conductivity and high carrier mobility make it a prime candidate for next-generation electronic and optoelectronic devices, potentially overcoming limitations of traditional silicon-based technologies [2]. The material's strength, coupled with its lightweight nature, opens up new possibilities in the development of advanced composite materials for automotive, aerospace, and structural applications, where enhanced performance with reduced weight is constantly sought. Graphene shows significant promise, yet there is still much to uncover about its properties and industrial applications through ongoing research.

In this study, we characterize graphene materials with different types of functionalzation, in form of powder, suspension, and inks, using various characterization techniques such as X-ray photoelectron spectroscopy (XPS), scanning electron microscopy (SEM), energy-dispersive X-ray spectroscopy (EDX), time-of-flight secondary ion mass spectrometry (ToF-SIMS), and Auger electron spectroscopy (AES).

2. Experimental

In this study, we first analyze the chemical composition of starting material for commercial functionalized graphene (FG) that is in powder form. We then analyze the powders after functionalization (at Haydale) in various versions; dispersed in water forming suspensions. Finally, we investigate the behavior of this functionalised powders when inks are formed. The FG samples under investigation are functionalized using four different functionalization groups: fluorine (F), oxygen (O), ammonia (NH3), and carboxylic acid (COOH). Pure graphene (G) was also investigated as the reference sample.

XPS is a cornerstone technique in chemical surface analysis. Through the interaction of X-rays with material surfaces and emission of photoelectrons, it accurately identifies

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elemental composition, chemical states, and electronic structures. EDX excels in rapidly analyzing elemental analysis and mapping of materials. It also gives a valuable insight about the materials bulk (in the range of 1 micron). This is enabled by detecting characteristic X-rays emitted from the sample upon interaction with high-energy electrons of a SEM (or TEM). It is worth mentioned that EDX was carried out at 5 keV and 15 keV which gives a balanced insight about the near-surface as well as the bulk regions of the samples. SEM is a powerful analytical tool that has the capability to show the intricate details of surface morphology and structure with high resolution and clarity. The images created by SEM enables visualization of surface features down to nanoscale dimensions, such as the topographical characteristics, particle size distributions, and surface roughness or porosity. Finally, ToF-SIMS offers an unparalleled sensitivity for detecting trace amounts of surface composition (including contamination).

For the XPS analysis the powders were deposited onto a Tesa tape that is stuck on an aluminum substrate before entering the ultra-high vacuum chamber The same samples were later investigated by SEM, EDX, and ToF-SIMS in that order. The suspensions, which are graphene powders dissolved in water with approximately 50 mg/mL concentration, were let to sediment then using a micropipette, 6 µL from the sediment (i.e., bottom) suspension were deposited onto polished silicon wafers. The drop-casted samples were put into vacuum desiccator to dry overnight, then the samples were used for investigation in the same order as the powders. The inks were “spread” over silicon wafers and left to dry in vacuum overnight before analysis.

3. Results and Discussions

XPS analysis for the graphene powders showed presence of fluorine in the F-functionalized sample (F-FG) as well a high oxygen-to-carbon concentration ratio in the COOH and O functionalized samples. EDX analysis results – as bulk analysis - are in agreement with the surface-sensitive XPS results. The XPS analysis of the graphene suspensions also showed existence of F in the F-functionalized sample. The oxygen-to-carbon concentration ratio for the COOH- and O-functionalized samples were high as well. When compared to the powders, the oxygen -to-carbon ratio for all suspensions are higher than the ratios of the powder samples. For the inks, the EDX and ToF-SIMS showed the presence of F in the F-functionalized sample in certain areas of the sample. However, detection of the oxygen-to-carbon ratios proved to be very challenging. This is because the abundance of C in the resin and carbon black that are mixed with the graphene powders. Figure 1 shows a representative SEM micrograph and the corresponding EDX mapping of F result for the F-functionalized ink.

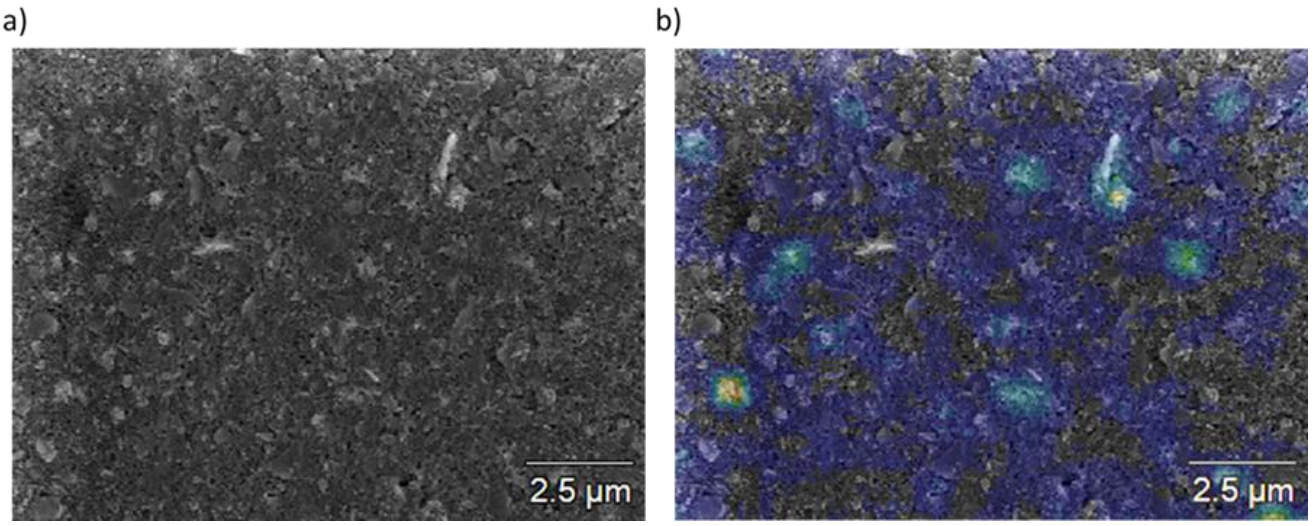

Figure 68: SEM image (a) and corresponding 5 kV EDX elemental map (b) of fluorine for an ink containing fluorine-functionalized - graphene within ink, after deposition of ink on silicon wafer, overlayed on (a)

4. Conclusions

Our results suggest a significant effect of water and commercial resins on the presence of graphene and associated functionalized group. For example, XPS analysis shows some significant differences between the chemical compositions of the solutions and the starting materials (powders). These changes can be explained by the location of the functionalization at the outermost surface as indicated by Chemello et al [3].

5. Acknowledgement

This project receives funding from the European Union's Horizon Europe Research & Innovation Programme under grant agreement no. 101092796 (ACCORDs - Green deal inspired correlative imaging-based characterization for safety profiling of 2D materials).

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Correlation between size distribution, morphology and chemical analysis of Graphene Family materials

Kerstin Jurkschat[1], Colin Johnston[2], Francesco Pellegrino[3], Elliott Jones[4]

1. Introduction

Two groups of GFM (graphene family) materials provided by University of Turin (UT) and Haydale Ltd. (HD) were analysed within the ACCORDs project (funded through Horizon Europe) for size distribution with different light scattering methods and morphology/crystallinity/ chemistry of individual flakes/ particles via transmission electron microscopy (TEM) in bright field and diffraction mode.

Comparison of results between imaging techniques and ensemble methods in liquid provides valuable insight into potential mechanisms of biological or environmental toxicity related to different size fractions and individual particle morphologies as well as surface modifications.

2. Materials and Methods

PSD

The Particle Size Distribution (PSD) was measured using a Malvern Panalytical Mastersizer 2000 laser diffraction instrument. The samples were measured in DI water, with a set of five measurements without sonication to assess the pristine PSD followed by 10 measurements with 30 sec US treatment between measurements. Samples were taken as received without any prior treatment. Additional measurements were carried out using Dynamic Light Scattering (DLS) on a Malvern Zetasizer NS instrument and Nano Tracking Analysis on a Malvern Nanosight instrument.

(S)TEM/EDX

TEM samples were prepared by drop casting 10µl of the dispersion (as received) onto 400mesh holey carbon coated copper grids (AgarScientific) and left to dry for at least 1 hour at RT prior to TEM examination. Images and diffraction patterns were obtained on a 200kV analytical JEOL 2100 instrument equipped with an OI EDS detector. Chemical composition was assessed with electron dispersive X-ray spectroscopy (EDX) in STEM mode.

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3. Results

Particle Size Distribution in liquid

The UT samples show mainly one very broad peak in the range between 1 and 100µm with some additional small peaks in the several hundred um range. Sonication can change the mean peak value to either higher or lower values. HD samples as received with no sonication show mainly two peaks: the larger size is in the range of 10-200µm and a smaller peak between approximately 1 and 10µm. After sonication an additional peak between approximately 100 and 500nm can be observed. Additional DLA and NTA measurements showed mainly peaks in the 100 to 1000 nm range, larger particles/agglomerates cannot be measured by either of these techniques.

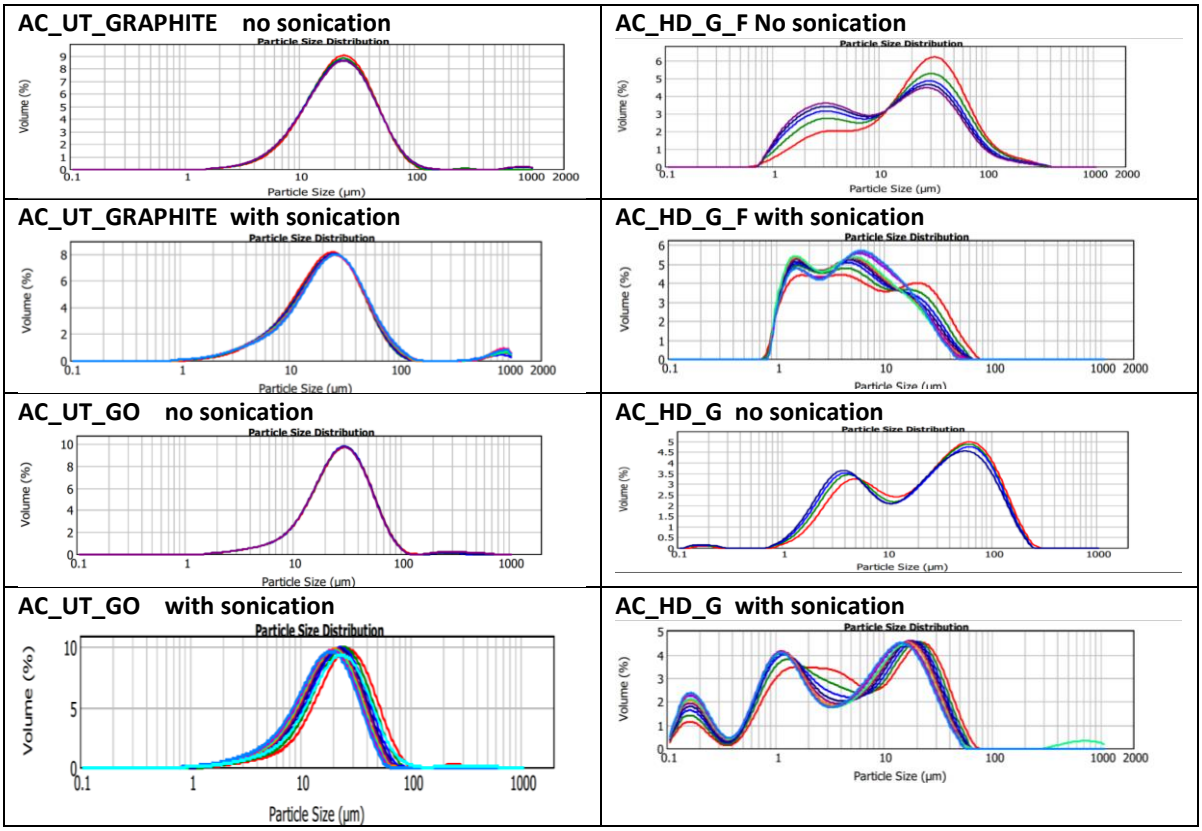

Figure 69: Examples of Particle (Agglomerate/Aggregate) Size distribution of two types of GFM samples with and without sonication

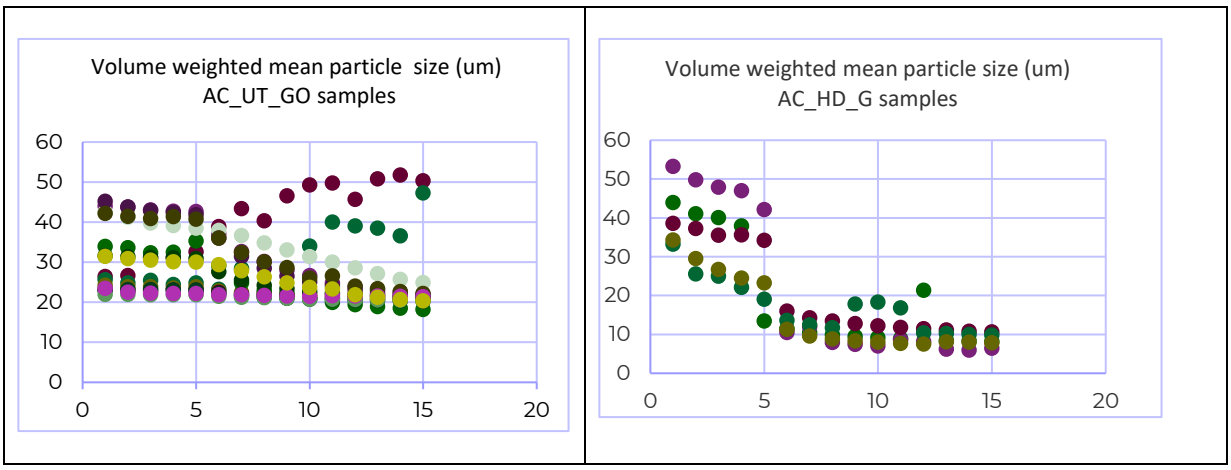

Figure 2: Volume weighted mean particle size change with stirring /pumping (measurement 1-5) and sonication (measurement 6-15)

4. Comparison of PSD in liquid versus imaging methods

The upper limit for particle size measurement in TEM is limited by the size of the TEM grid square (approx. 30µm. Overlapping particles as well as the irregular shapes make particle size estimates from TEM images difficult. Drying platelets or sheet like samples onto TEM grids may result in additional changes in perceived shapes. While the UT samples show large individual GFM flakes in the 10-50µm range, this size range is mostly associated with agglomerates or aggregates in the HD samples. Both sample groups also show much smaller particles which are primary particles or small agglomerates of GFM materials.

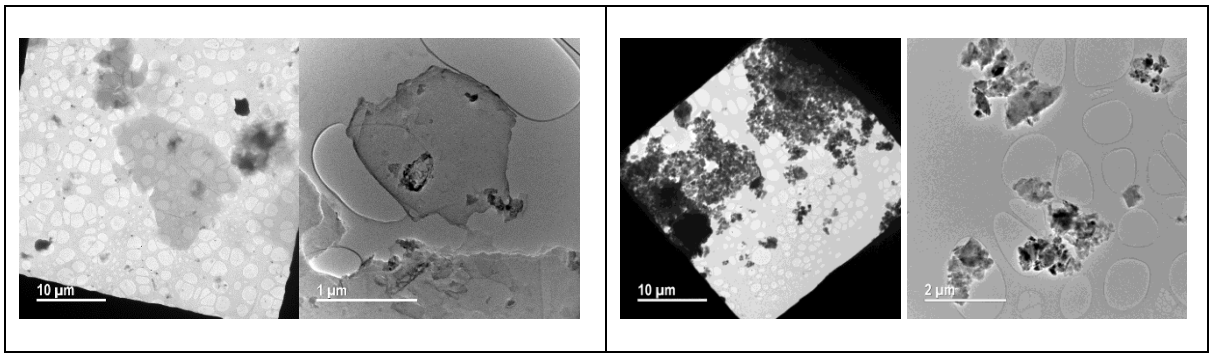

Figure 3: Low and medium magnification images of UT and HD samples

5. Comparison of chemical content (C/O ratio)

EDX maps were acquired from random areas and additional spectra were obtained from areas with no carbon support. Between 10 and 55 spectra were analysed for each sample and spectra where either oxygen or carbon had zero counts were excluded from the analysis. The amount of all additional elements detected was below 2at% in all areas.

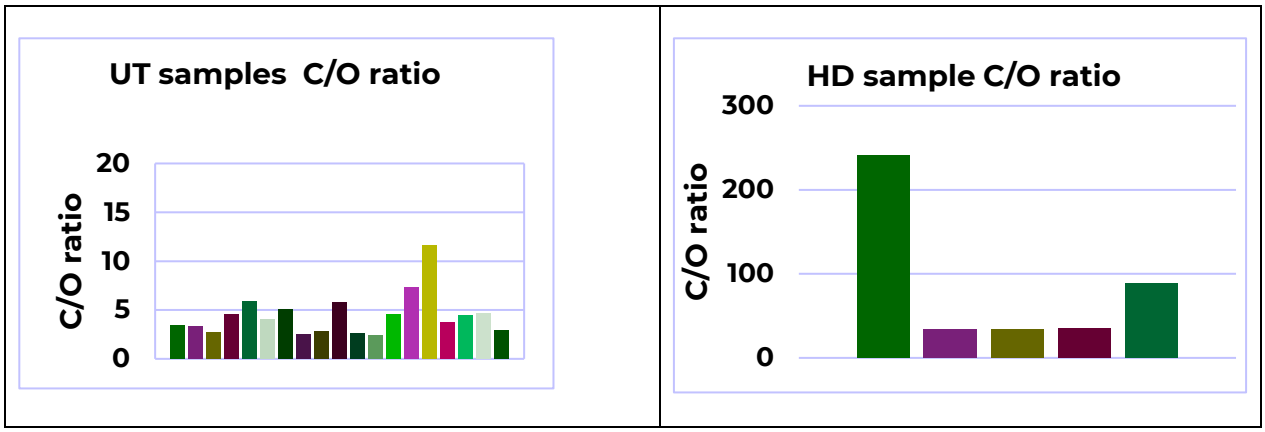

Figure 4: C/O ratios from EDX spectra in STEM mode

While the overall C/O ratio and the amount of impurities/ contamination was in good agreement with other techniques, the standard deviation error for all spectra from each individual sample was high. This indicates either a strong variation of the oxidation degree within each type of GFM material or a variation between different types of GFM

as present in each sample. Generally, the HD sample are more homogeneous in terms of morphology and chemical contents, whereas the UT samples show a stronger variation of C/O ratio overall and some correlation between the morphology and chemical contents.

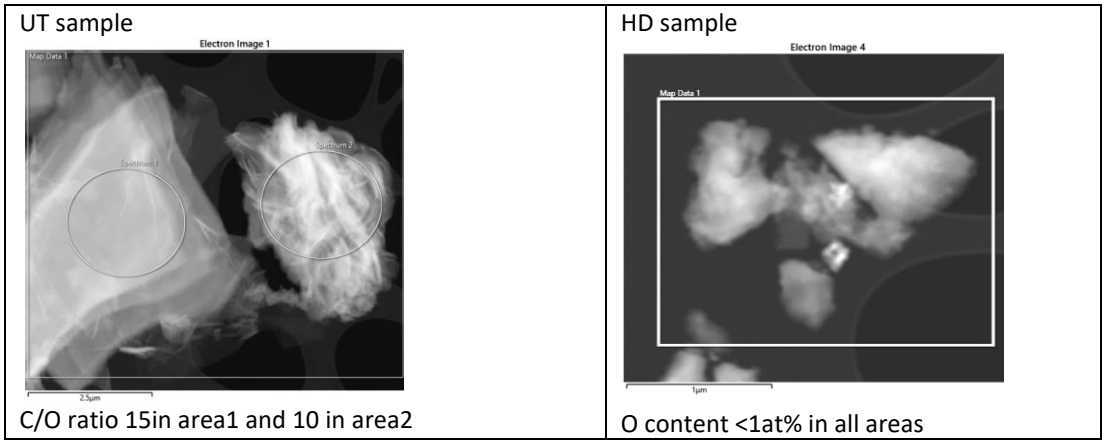

Figure 5: Morphology and C/O ratio variation within one sample of each group of GFM imaged with STEM

6. Conclusions

Particle sizes derived from methods in liquid (LD) appear to be significantly higher than from imaging and care needs to be applied to compare like with like, i.e. number based distributions and volume derived distributions for primary particles as well as agglomerates and aggregates. Energy transfer to the liquid sample during sonication can change the size distribution and this apparent PSD change is correlated not only to the shape of individual particles but also to their surface properties.

Different size fractions can be correlated with the help of imaging and spectroscopy techniques either to individual particles or agglomerates and aggregates. For the calculation of overall C/O ratios the morphology of individual particles as well as the amount and nature of impurities and or contamination needs to be considered.

7. Acknowledgment

This project receives funding from the European Union's Horizon Europe Research & Innovation Programme under grant agreement no. 101092796 (ACCORDs - Green deal inspired correlative imaging-based characterization for safety profiling of 2D materials).

SUNSHINE Safe and Sustainable by Design (SSbD) approach and e-infrastructure

Lisa Pizzol[1], Alex Zabeo[1], Arianna Livieri [1,2] , Matteo Carisi[1], Fabio Rosada[1], Danail Hristozov[3]

1. Introduction

The European Chemicals Strategy for Sustainability and the Zero Pollution Action Plan have called for a transition towards Safe and Sustainable by Design (SSbD) approach for chemicals and materials (EC 2019) (EC 2020). To support this policy ambition, the European Commission (EC) has recommended the establishment of a SSbD framework based on a holistic approach developed by the Joint Research Centre (JRC) (EC, 2022; C. Caldeira et al., 2022). Due to their inherently complex nature and interactions the advanced materials (AdMa) pose safety and sustainability concerns. Therefore, it is important to equip the European industries with the knowledge and tools needed implement the JRC SSbD framework for these materials. The EU H2020 SUNSHINE project has addressed this challenge by delivering a digital e-infrastructure designed operationalise the RC SSbD framework for AdMa.

2. Methods

The SUNSHINE digital e-infrastrucure has been aligned to all 5 steps of the JRC SSbD framework (Caldeira et al. 2022), enabling tiered assessment at each step of the innovation process represented by the *Agile Stage-Gate* model (Cooper, 2014; Cooper and Sommer, 2018; Hristozov et al., 2022). It has been designed as a digital platform to foster dialogue, collaboration and information exchange between industry actors along entire supply chains. It is also a place where innovators can communicate with regulators in a trusted environment already in the early stages of innovation. The e-infrastrucure is *Inclusive* as it has been developed by engaging key stakeholders (e.g. SMEs, large industry, academia, regulators) to ensure that it addresses their needs and requirements. It is *State-of-the-art* as it has been based on the latest knowledge and data and includes (1) guidance for cost-effective generation of new data; (2) approaches for grouping to enable read-across of existing information for SSbD purposes; and (3) a tiered approach for assessing the safety-sustainability-functionality balance of the materials/products at each stage of the innovation process to inform 'Go to development' and 'Go to market' business decisions.

The SSbD approach underpinning the e-infrastrucure has been developed to help industries to modify and assess advanced materials/products to increase their safety and sustainability, while keeping their intended functionality in commercially viable ranges. This approach is composed of two Tiers. Tier 1 uses a scoring system to calculate indices for health, environmental, social and economic impacts and plot those on a chart that clearly visualizes safety and sustainability-related 'hotspots of concern' along the

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lifecycles of the materials/products. These hotspots can be further assessed in Tier 2 which involves quantitative LCA (Life Cycle Assessment), LCC (Life Cycle Costing), and S-LCA (Social Life Cycle Assessment) (Pizzol et al., 2023). The SSbD approach is comparative, so innovative materials can be compared to a benchmark. Such a benchmark could be an alternative design option or a conventional material/product that has the same or a similar function.

The e-infrastrucure is *Open & FAIR* as it is connected to the SUNSHINE Open & FAIR database, which enables access to high-quality safety and sustainability data. The system is also *Secure* as it ensures controlled exchange of information between supply chain actors by means of a highly innovative blockchain technology. The e-infrastructure will be able to generate a SSbD digital pass for each product assessed by it.

3. Conclusion

The SUNSHINE e-infrastructure operationalises the EC SSbD framework, enabling the assessment of safety and sustainability impacts at different stages of the innovation process and from a lifecycle perspective. This user-friendly digital system has been designed to be relatively simple for industries to implement, acknowledging their limited time and resources for safety and sustainability assessment. Its two tiers (qualitative and quantitative) cater to different analysis needs and generate comparison matrices for informed SSbD decision making for products enabled by AdMa.

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Score System for a Multi-criteria Decision Analysis based on the SSbD framework for MCNM/HARN Risk Management – The DIAGONAL Decision Support Tool Case

Alberto Larraz Tejero[1], Blanca María Pozuelo Rollon[1], Arantxa Ballesteros Riaza[1]

1. Introduction

Within the European Green Deal[i], the Chemicals Strategy for Sustainability (CSS)[ii], which aims to reduce the harmful effects of chemicals on human health and the environment, introduces the Safe and Sustainable by Design (SSbD) framework[iii]. The European Union has proposed a framework that aims to go beyond legal requirements by providing standards for the sustainability and safety of materials and chemicals. The SSbD framework integrates dimensions, aspects, methodologies, and indicators to support research and innovation activities that evaluate and create environmentally friendly solutions, therefore advancing the goals of the Green Deal, from early stages. With its comprehensions into the framework's dimensions and techniques, this paper acts as a fundamental resource that will help shape future EU policies and activities.

Specifically, regarding DIAGONAL[iv] project, its main goal is bringing SbD knowledge and tools to a development stage which can be implemented in the MCNMs and HARNs related industries, relying on experimental (*in-vitro*) and modelling (*in-silico*) research, to study specific hazard and exposure properties that MCNMs & HARNs exhibit along their life cycle, with emphasis in the interactions between NM constituents, with other particles and the environment, as well as their release rate and fate. Within this project, the developing and integration of an interactive Decision Support Tool is contemplated with the aim of supporting regulators, industries and other stakeholders on the selection of the best available approaches to reduce risk at source and control the exposure at all stages of the life cycle; and to assess the benefit/risk balance of specific MCNMs and HARNs, and to propose suitable SbD alternatives and/or RMM dynamic charts and textual reports for decision making.

Consequently, the implementation of a comprehensive score-system based on a multi-criteria decision analysis for those steps addressed by the current SSbD framework seems to be the best solution for supporting the decision-making process of the final user.

The integration of every step of the SSbD framework in a user-friendly score-system is a challenging task which involves the development of experimental, modelling and literature research, to bring the cutting-edge knowledge of the MCNM/HARN in a same tool.

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2. Adapting the framework to the project

DIAGONAL (**D**evelopment and scaled **I**mplementation of s**A**fe by design tools and **G**uidelines for multic**O**mponent a**N**d h**A**rn nanomateria**L**s) start in May 2021, more than one year before the publication of the JRC Technical Report with the current Safe and Sustainable by Design chemicals and materials framework. Therefore, SSbD framework had to be adapted since the initial Grant Agreement was not align with the framework and criteria definition. Thus, the five-step approach was chosen for SSbD assessment of the MCNM/HARN and evaluating the suitability of the subsequent strategies.

In the same way, criteria and evaluation definition for MCNM/HARN was previously defined, so the expected experimental and modelling research had to be adapted and included in the new framework, including specificities for this kind for advance materials.

As a result, a new workflow was described to establish the connections between the experimental and modelling SSbD assessment with the SSbD Framework.

3. Score System

The 5-steps stepwise approach proposed in the SSbD Framework was included in the DIAGONAL score system, evaluating individually each step considering the work developed under the project:

- For Step 1 (*Hazard assessment of the chemical/material*), current criteria definition has been considered for grouping the MCNM/HARN under criterion H1-H2-H3, but only for those experiments which have been performed in DIAGONAL. The score will cover Human health, Environmental and Physical hazards.
- For Step 2 (*Human health and safety aspects in the chemical/material production and processing phase*) a control banding strategy is applied for obtaining a score value considering the nanoscale nature of the materials and the processing specifications.
- For Step 3 (*Human health and environmental aspects in the final application phase*) information derived from a specific MCNM/HARN environmental fate model is combined with information from step 1 to get a score value.
- For Step 4 (Environmental sustainability assessment) results from the LCA are used to express a score value based on the 16 impact categories.

However, within Step 5, some recommendations will be proposed but no score value will be given, unable to perform a general socio-economic evaluation in the DIAGONAL platform.

4. Integration of Decision Support Tool workflow

A good integration of experimental and modelling work performed as databases or models for a comprehensive evaluation of MCNM/HARN are directly related to the good performance of the score system. In Figure 1, we can observe the workflow of the Decision Support Tool involved in the score-system which supports decision making between a batch of SSbD strategies in comparison to the original material as a baseline.

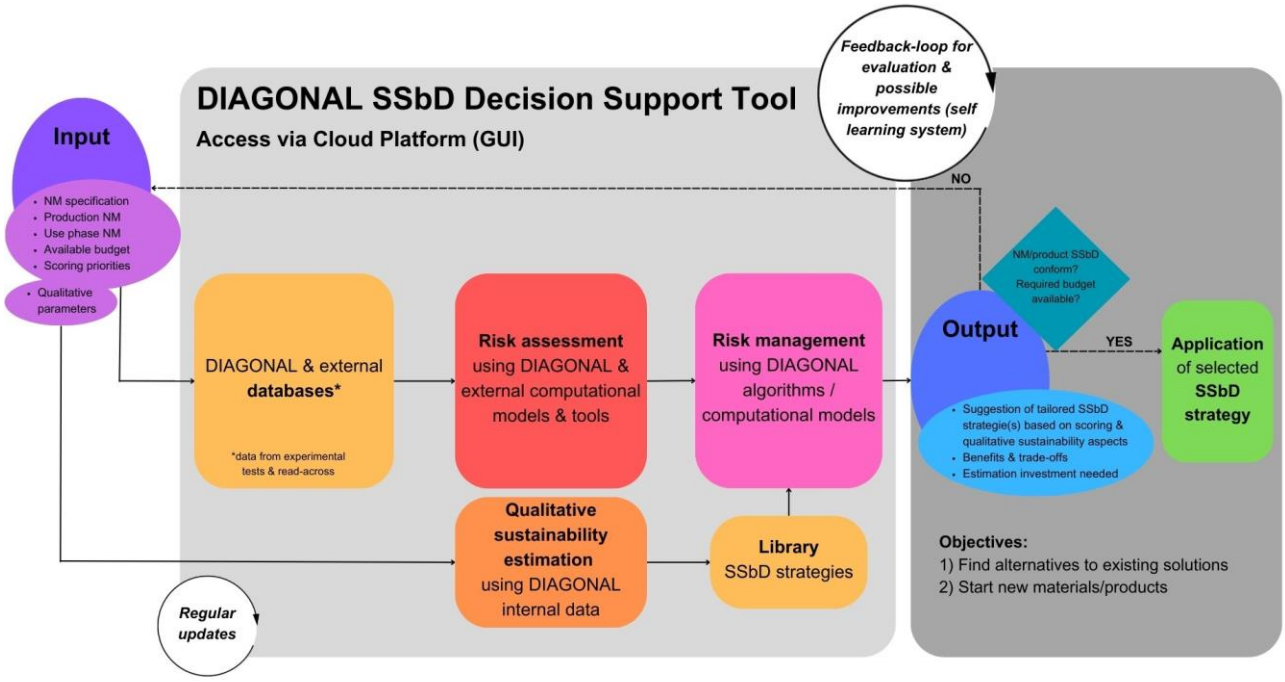

Figure 70: Decision Support Tool workflow

5. Conclusions

A multi-criteria optimization process based on proposed framework for SSbD has been implemented through a score system. The goal is to support decision making regarding SSbD strategies for MCNM/HARN using a software environment. This Decision Support Tool will evaluate the safety and sustainability of MCNM/HARN and classify different SSbD strategies according to their benefits.

For that, the proposed SSbD framework by EC has been adapted to DIAGONAL idiosyncrasy, using the proposed experiments and models to predict hazard and exposure related with safety and sustainability.

Finally, the score system will be presented in a user-friendly interface for an easy understanding of the SSbD framework and the criteria definition.

6. References

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[iv] Development and scaled Implementation of sAfe by design tools and Guidelines for multicOmponent aNd hArn nanomateriaLs (DIAGONAL) Grant agreement ID: 953152 doi:10.3030/953152

Spectroscopic Approaches for Understanding Graphene Family Material interactions with Enzymes

Bashiru Ibrahim[1], Divya Singh[1], Swaroop Chakraborty[1], Andrea Rossi[2], Francesco Pellegrino[2], Damjana Drobne[3], Eugenia Valsami-Jones[1]

1. Introduction

Graphene family materials (GFMs) are structural or chemical variants of graphene, a two-dimensional allotrope of carbon, that has attracted significant attention in recent years due to its remarkable properties and applications in various fields including biomedicine. Such applications include cellular imaging, drug delivery, biosensing and tissue engineering [1]. Despite the potential of graphene and GFMs in biomedicine, knowledge of their interaction with enzymes remains poorly understood. This interaction can occur through a range of mechanisms such as physical absorption, hydrogen bonding and π-π stacking interactions [2]. Such interactions can change the structural conformation of enzymes, impacting their stability, activity, specificity, and overall biological function [3]. Therefore, it is essential to investigate the interaction of GFMs with enzymes [4]. In the current study, circular dichroism (CD) spectroscopy was used to study effects of GFMs interactions with cholinergic enzyme-acetylcholinesterase (AChE). The technique provides an insight into the conformational structure of the enzyme and can elucidate the structural alterations induced by GFMs. The enzyme is a serine hydrolase that plays a critical role in degrading acetylcholine (ACh) and terminating neurotransmission. It is involved in cellular growth, apoptosis, drug resistance, response to signals and inflammation [5]. Understanding how GFMs change the structural composition and function of AChE can offer valuable insights into potential applications of GFMs in the treatment of neurological disorders.

2. Methodology

The studied GFMs were provided by the University of Torino, where they were synthesised using the Hummers modified method, which involves stirring high quality graphite in a mixture of concentrated sulphuric acid and phosphoric acid together with a strong oxidizing agent (potassium permanganate). The materials were characterised by dynamic light scattering (DLS), Fourier-transform infrared spectroscopy (FTIR) and UV-visible spectroscopy. The interaction of GFMs with AChE was studied by circular dichroism (CD). The CD spectra were recorded in a 1 mm path length quartz cell for the far UV (190 - 300 nm). The measurements were performed with step size of 1.0 nm, a spot

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[3] Biotechnical Faculty, University of Ljubljana, Večna pot 111, 1000 Ljubljana, Slovenia

width of 1.5 nm and an average time of 2s. The CD spectra of GFMs in 100 mM phosphate buffer (pH 8.0) were recorded and subtracted from the enzyme spectra. The enzyme was dispersed with GFMs (0 – 200 µg/ml) directly into the cuvette, and the spectra were corrected for dilution. The mean ellipticity was calculated using Dicroweb software [6].

3. Results and Discussion

The results revealed that the materials have hydrodynamic diameters ranging from 430-4,370 nm when dispersed in ultrapure water. Zeta potential measurements of the synthesised materials indicated negatively charged surfaces (-21-38 mV), suggesting good stability and dispersion. The absorption spectra (260-270 nm) confirmed the formation of GFMs using UV-vis. FTIR showed the formation of the following broad bands: 3212 cm^{-1} matching the O-H stretching vibrations that are typical of hydroxyl and carboxyl functional groups; 1719 cm^{-1} corresponding to C=O stretching vibrations implying the presence of carbonyl and carboxyl groups; 1622 cm^{-1} showing the contribution of cyclic aromatic groups; 1050 cm^{-1} matching the C-O stretching vibrations, which are the typical absorption bands of ethers.

Our results further revealed a distinct increase in the absorption spectra of AChE enzyme upon interaction with GFMs, suggesting the formation of enzyme-GFMs complexes. Interestingly, the concentration of GFMs (ranging from 0 to 200 µg/ml) did not significantly change the conformational structure of the enzyme (Figure 1). However, analysis using Dicroweb software revealed slight changes in the α-helix content of the enzyme, and β-sheet indicating subtle alterations in their secondary structure elements. Furthermore, the addition of GFMs led to significant peaks shift in the original spectra of AChE, which could be related to changes in the conformational structure of the enzyme.

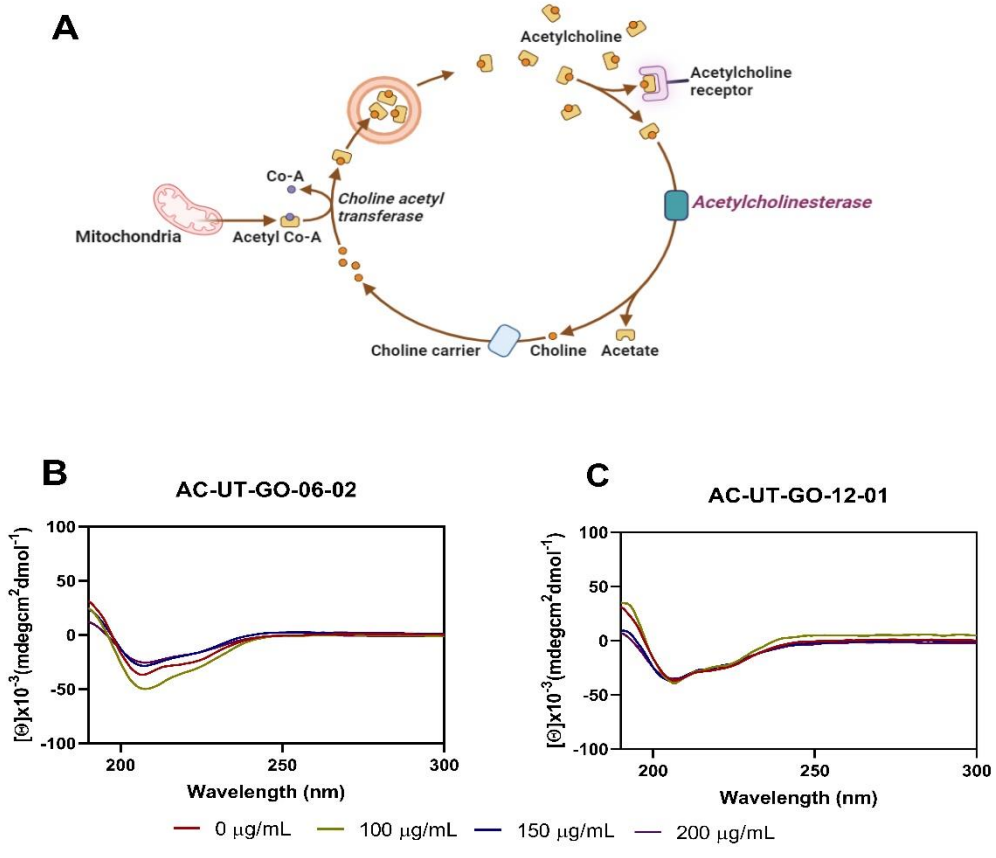

Figure 71: GFMs-AChE interaction (A) Schematic figure showing intermediates related to the biosynthesis of Acetylcholine and (B-E) mean residue ellipticity of AChE (0.5 mg/ml) titrated with increasing concentrations of GFMs (0-200 µg/ml) at room temperature.

4. Conclusions

In conclusion, our study highlights the ability of GFMs to interact with AChE and induce subtle structural changes. Through spectroscopic analysis, we elucidated the dynamics of enzyme-GFMs interactions and their effects on AChE structure. Further investigation into the underlying mechanisms of these interactions could pave the way for the development of novel biomedical applications harnessing the unique properties of GFMs.

5. Acknowledgment

This project receives funding from the European Union's Horizon Europe Research & Innovation Programme under grant agreement no. 101092796 (ACCORDs - Green deal inspired correlative imaging-based characterization for safety profiling of 2D materials).

Associated Partners (i.e. (a) Swiss Partners and (b) UK Partners) have received national funding from (a) the Swiss State Secretariat for Education, Research, and Innovation (SERI), and (b) Innovate UK.

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Poster Presentations: Session 9

Advancements in Surface Mapping Techniques for Characterizing Novel Materials in Battery Applications

Lukasz Nowicki[1], Malgorzata Celuch[1], Marzena Olszewska–Placha[1], Janusz Rudnicki[1]

1. Introduction

In recent years, there has been a noticeable interdisciplinary movement focused on improving the efficiency and sustainability of communication systems and new energy sources. This trend is exemplified by advancements in creating laminar substrates for 5G systems [1] and developing materials for energy storage, such as organic semiconductors [2] for photovoltaic cells and polymer-based conductive composites [3-4] for battery anodes. In addition to the progress in material innovation and fabrication, precise characterization methods, particularly concerning dielectric and electric properties, have attracted considerable attention [4-7] due to their direct impact on energy storage efficiencies. While traditional materials like laminar dielectrics, known for their bulk nature and uniform surface properties owing to established manufacturing processes, can often be adequately assessed through point-wise measurements [6-7], a diverse array of materials, including thin layers produced via various deposition may exhibit significant surface variability. Thin composite layers, for instance, demonstrate a notable sensitivity of electrical parameters to factors like thickness non-uniformities or dispersion homogeneity of conductive inclusions, necessitating the monitoring of parameter variations across the material surface. This need becomes particularly critical in applications like battery anodes, where electrical parameters directly impact battery cell efficiency. The utilization of 2D surface mapping techniques for assessing electrical parameters of battery anodes not only ensures quality testing during pre-manufacturing stages but also facilitates intermediate life-cycle testing. This enables the correlation of anode parameters with battery state of health (SOH) and the examination of the influence of the solid electrolyte interphase (SEI) layer on overall anode quality during battery operation, as well as the evaluation of anode aging post-usage. While standard dielectric resonator devices mainly allow point-wise measurements suitable for samples assumed to be homogeneous across their surfaces, ongoing advancements in novel materials and manufacturing techniques, such as printing techniques for carbon-based polymer composites [4-5] in battery cells or organic semiconductors [6] for photovoltaic cells, necessitate surface mapping to detect material parameter inhomogeneities.

2. Qualitative and quantitative imaging of electric properties

Dielectric resonator techniques have demonstrated high accuracy in non-destructive material measurements at microwave frequencies. Methods such as split-post dielectric resonator (SPDR) [6] and single-post dielectric resonator (SiPDR) [7] cover a wide spectrum of materials characterization. SPDR is recognized as a standard for

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characterizing low-loss laminar dielectrics and high resistivity semiconductors [8], while SiPDR configuration is tailored for surface impedance measurements of resistive films and contactless measurements of low-resistivity semiconductor wafers. These techniques involve extracting material parameters from measured resonant frequencies and Q-factors, both with and without the material sample inserted into the device.

A new measurement setup has been established as a part of action in I4Bags project [9]. It's featuring a Vector Network Analyzer (VNA), SPDR or inverted SiPDR (iSiPDR), and a laptop equipped with dedicated software. The VNA measures complex scattering parameters to interface with the SPDR or iSiPDR, employing the Keysight P5008 Streamline VNA with a broad frequency range. To ensure precise measurements, it is imperative that the samples under test are flat and uniform. Any deviations from flatness may introduce errors in the extraction of electrical parameters. An example of a measuring station is shown in Figure 1.

The scanner comprises an XY-motorized table and a 10 GHz SPDR or iSiPDR. These motors enable precise movement in both the X and Y directions, with the option to achieve high spatial resolution. Dedicated software aids in accurately positioning the SPDR or iSiPDR over the sample grid, enabling microwave measurements. The measurement procedure involves several steps: automatic frequency tracking to detect resonance, adjustment of the frequency range for precise parameter extraction, and performing a linear frequency sweep around the resonance frequency. Novel materials often exhibit variations in their electromagnetic properties across their surface due to production process variations, thickness nonuniformities, or inhomogeneously dispersed inclusions. To accurately characterize such materials, spatially resolved measurements are essential.

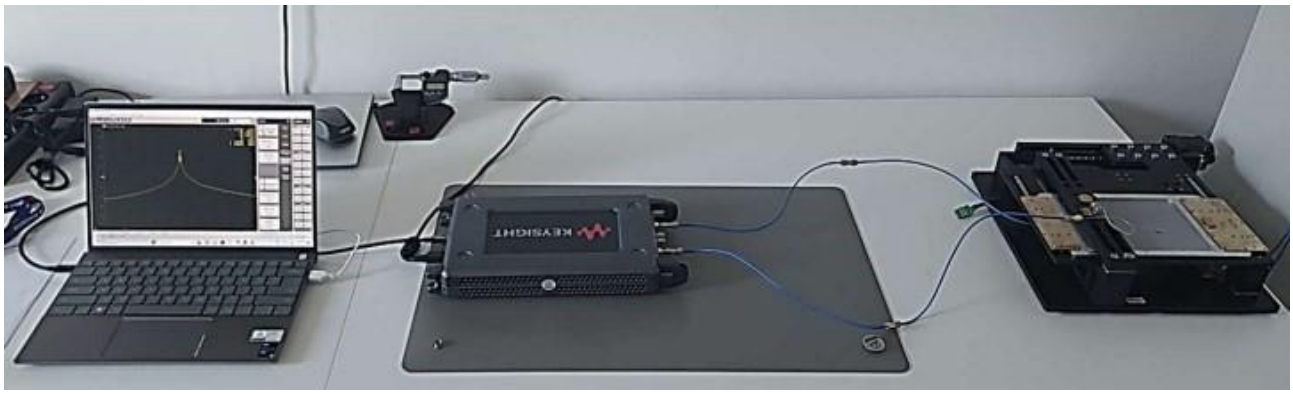

Figure 1: Measurement setup for imaging the electrical parameters of the tested material using a 10GHz iSiPDR scanner

3. Conclusions

The introduction of the 10 GHz iSiPDR and SPDR techniques, along with a new measurement configuration automated with dedicated software, represents a significant advance in materials testing capabilities. This configuration enables the extraction of two-dimensional maps of electrical properties, offering a comprehensive picture of the materials under test. The versatility of the measurement configuration using both techniques provides a wide range of material testing capabilities. This versatility ensures that different types of materials can be effectively analyzed, opening up possibilities for a variety of applications in different industries. Ongoing work involving the measurement of samples subjected to low-energy ion implantation as part

of the I4Bags project demonstrates the practical application of these measurement techniques.

At upcoming conference, the presentation of extracted 2D maps of electrical permeability, tangential loss using SPDR measurements, and surface resistance extracted using iSiPDR at 10 GHz will provide valuable insights into the electrical properties of the materials under study.

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Raman spectroscopy elucidates the transformation of single-walled carbon nanotubes following abrasive wear of epoxy coatings

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1. Introduction

Nanomaterials are integrated into consumer products to enhance specific properties [1]. However, concerns arise regarding their eventual release throughout the product lifecycle, particularly due to mechanical strains that can result in the generation of fragmented materials of **particulate matter (especially PM2.5)** or even nanomaterials. In this study, we investigated the potential release of single-walled carbon nanotubes (SWCNTs - brand TUBALL™) from epoxy composite materials. We utilized a pin-on-disk type tribometer to simulate accelerated mechanical aging of the nanocomposites (figure 1).

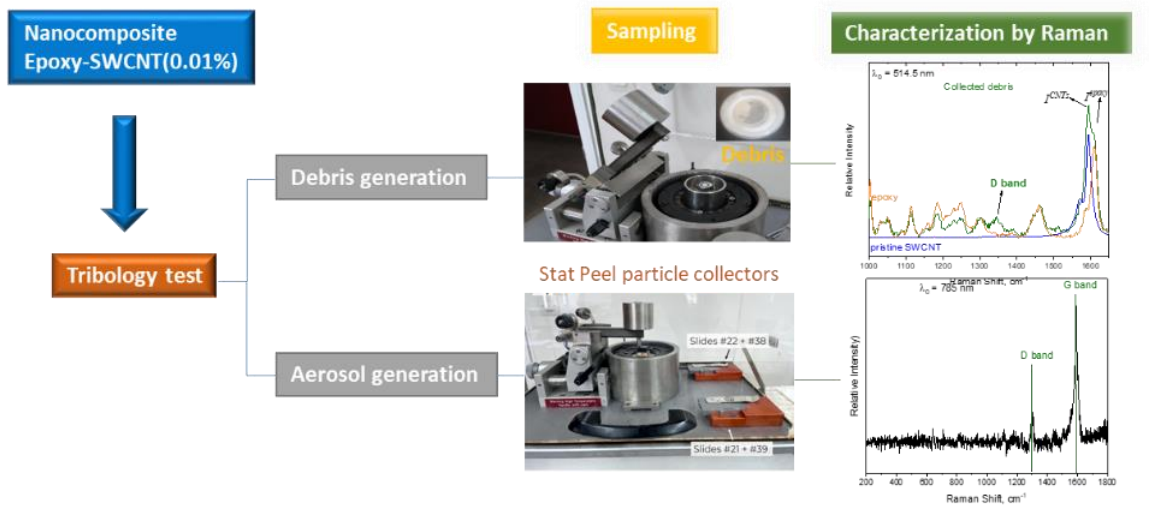

Figure 72: Schematic representation of experimental setup used.

2. Results

Raman spectroscopy was used to characterize pristine nanocomposite material, abraded material, and debris obtained from the tribometer, while airborne particles

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generated during the abrasion test were collected using the Stat Peel's Identifier C2 system (figure 2).

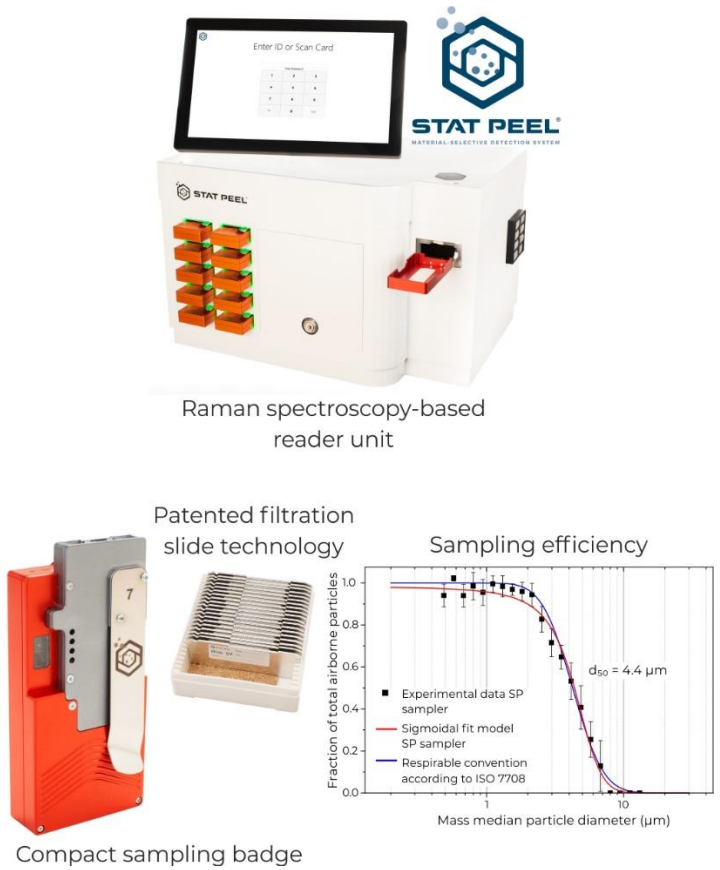

Figure 2: STAT PEEL Identifier system.

3. Conclusions

Raman spectra conducted on the Stat Peel filters revealed the presence of free SWCNTs released from the epoxy matrix, albeit in notably low quantities. All the SWCNT quantified masses are close to the LoQ of the system and the calculated exposures are three orders of magnitude lower than the NIOSH recommended exposure limit (REL) of 1 µg/m^3. Evidence of structural changes and degradation in SWCNTs within samples subjected to accelerated wear during abrasive tests was readily discernible in the Raman spectra proved by the intensity of the characteristic band associated with defects, D-band, in the nanotubes [2].

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Morphological analysis and Sample preparation of Particulate Graphene oxide materials

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1. Introduction

Graphene oxide shows immense potential due to its physico-chemical properties that can be further tailored to specific applications through functionalization[1]. The well-known Hummer method is a synthesis method that can be easily scaled up[2]. Applications such as catalysis, biomedicine, electronic devices, and water filtration enable GO as a promising material for the future[3]. The present study focuses on the morphological characterization of graphene oxide flakes. The complexity of these materials varies substantially. Within the European project ACCORDs a framework for the physico-chemical characterization of complex graphene-family materials (GFM) is developed, with the focus on methods capable of imaging and with final correlation to the biological behaviour of the analysed materials.

2. Materials

The materials investigated in this study are three types of GO flakes with different origins. The “ideal” case of GO flakes from Graphenea represents flakes which are well dispersed, non-overlapping when prepared on a substrate, and can, therefore, serve as a reference regarding size and shape analysis. More complex but well documented regarding synthesis conditions are samples that were synthesised by University of Turin (“UniTo”) within the ACCORDS project. These exhibit nanoscale characteristics such as porosity, edge roughness combined with significant degree of agglomeration/aggregation and the lateral size spans several orders of magnitude. The commercial samples from Haydale are provided as powders, dispersed in water, as inks as a mixture of resin and GO, with different functionalization and tend to agglomerate heavily.

3. Sample Preparation

Sample preparation must be tailored to the specific measurement employed and each material requires unique solutions regarding substrate, dilution, dispersion media and deposition technique to obtain separated flakes with minimal overlap.

i) Graphenea samples were prepared as dispersion in Millipore water isopropanol mix on both holey carbon TEM grids and silicon wafer.

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[4] Graphenea Semiconductor SLU, San Sebastián, Spain

ii) UniTo samples were prepared in Millipore water similar to i).
iii) Raw powder samples from Haydale were deposited as is on self-adhesive carbon. The same powders were further embedded in polyacryl resin and then ground and polished to investigate the cross-sectional area. The powders were dispersed in water and drop-casted on silicon wafer. They were also provided as inks which were brushed on top of silicon wafer.

4. Characterization method

A SEM of type Supra40 (Zeiss) equipped with a secondary electrons (SE) InLens detector was utilized for this study. For samples deposited on TEM grid a dedicated sample holder for the scanning transmission electron microscopy in SEM (STEM-in-SEM) mode was used. With the InLens, the SEs emitted within a very narrow solid angle (SE1) are detected with the option to correlatively analyse the transmitted electrons, which are detected by the conventional SE Everhart-Thornley detector.

5. Image analysis

To accurately measure the lateral particle size, the electron microscopy (EM) data was processed using the software package ImageJ[4]. For the Graphenea material semi-automatic evaluation with a pre-processing median filtering, ISOData thresholding followed by a manual correction of faulty segmentation were performed. The images of the dispersed Haydale samples were automatically processed with the StarDist algorithm[5] to obtain the regions of interest of the flakes/particles, accounting for limited amount of overlap with only minimal manual post processing. Embedded powder samples were analysed semi-automatically. For the UniTo materials we developed a particle classification scheme. Further, the pore amount within the GO particles was evaluated through semi-automatic analysis by measuring the ratio of flake area to defect areas within the flake visible in the EM images.

6. Results

For the Graphenea material (shown in Fig. 1) the area equivalent circle diameter (ECD), the minimum Feret and the (maximum) Feret were extracted. The ECD amounts to 1.34 µm, the minimum Feret to 0.91 µm and Feret to 1.47 µm.

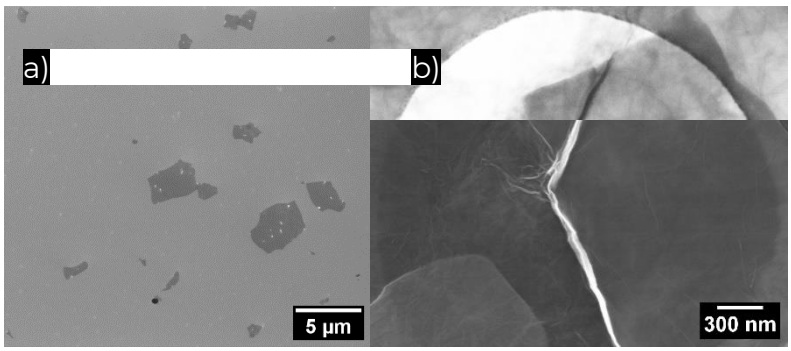

Figure 73: Graphenea sample as a) flakes on silicon wafer and as b) flake on holey carbon support (top: STEM in SEM; bottom InLens)

For the UniTo sample following dimensional properties have been determined: mean ECD ~1 µm, MinFeret ~0.47 µm, MaxFeret ~0.82 µm, with a pore area ratio of ~5% was obtained (with insufficient statistics as a proof-of-principle).

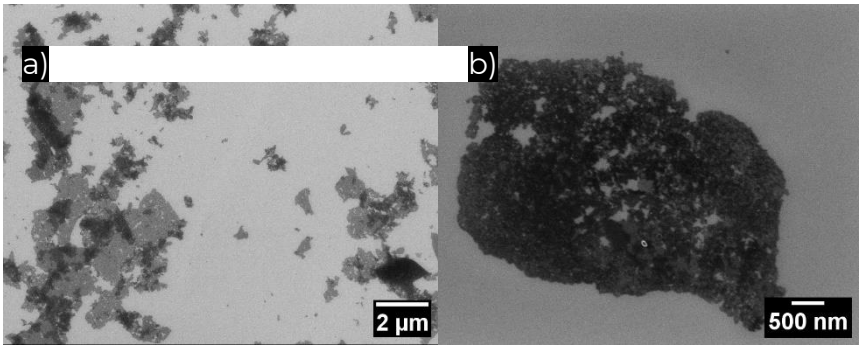

Figure 2: UniTo sample showing a) overlapping GO flakes and b) single flake with porous structure.

For the Haydale samples (Fig. 3) a distinction for the dispersed sample was made: the constituent particles were assessed separately from the agglomerated ones.

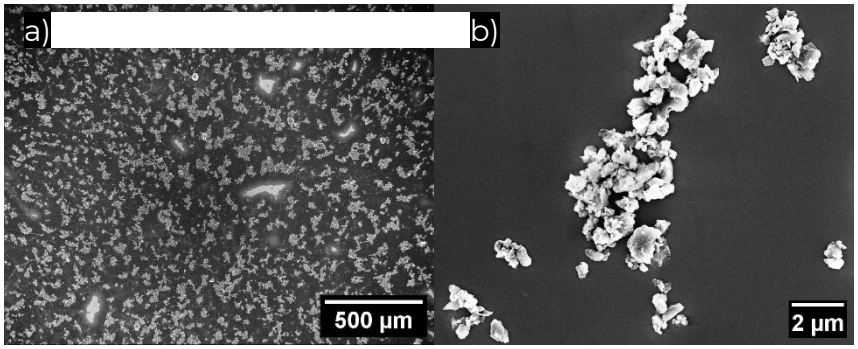

Figure 3: SEM of the Haydale sample powder dispersed in water a) at low magnifications showing agglomerations and b) at higher magnification showing constituent particles within an agglomerate.

Figure 4 shows the GO flakes embedded in resin (4 a) as part of the sample preparation process and within the inks as a mixture of resin and GO flakes.

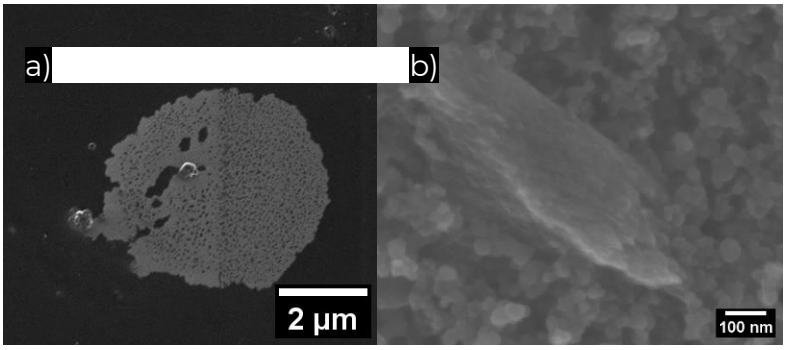

Figure 4: Haydale sample a) powder embedded in polyacryl resin b) GO flake as part of an ink.

7. Discussion

For each individual material each preparation method offers advantages and disadvantages or is not applicable. Drop casting works well for the Graphenea material allowing to accurately quantify the lateral particle size of the well-defined flakes. For the UniTo GO materials it is challenging to separate flakes from agglomerates and, therefore, only a qualitative assessment of the particle size distribution is currently possible. An additional feature, i.e., the pore amount/ area ratio, can be specified quantitatively within a certain error. For the Haydale samples agglomeration/aggregation of particles of the dispersed powders required to distinguish between the size of constituent particles and the size of agglomeration, leading to two different characteristic values per investigated sample.

The embedding preparation technique only works for powder samples but allows for the investigation of the particles in a similar environment to that of the inks (as the final nancomposite product).

8. Conclusion

It is imperative to find the suitable preparation method to enable the accurate and automatic analysis of the lateral size of GO flakes. Representativity of the analysis of EM images can be severely limited by non-optimal preparation, but also due to agglomeration/aggregation. These require both low and high magnification to capture the whole morphology picture. Existing automatic analysis algorithms are often too time-consuming, inflexible, and specific to completely assess the requirements of the shown complexity of GO materials.

9. Acknowledgement

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NPCoronaPredict: Multiscale modelling of the nanoparticle biomolecular corona

Ian Rouse[1], David Power[1], Julia Subbotina[1], Vladimir Lobaskin[1]

1. Introduction

The layers of proteins and other biomolecules surrounding a nanoparticle (NP) in a biological environment – the nanoparticle corona – plays a vital role in determining the effective biological identity of the NP, its potential for adverse outcomes, and its eventual fate in the body [1]. The corona is a dynamic, mesoscopic entity formed over the course of hours, yet is highly dependent on fast, atomic-scale interactions between the surface of the NP and potential ligands. Consequently, it is extremely challenging to model the corona using conventional molecular dynamics. To overcome this issue, we have developed the NPCoronaPredict software package, which enables prediction of the contents of the nanoparticle corona via a multiscale modelling approach, employing a systematic scaling up of the system from the atomistic level of small molecules to nanomaterial surfaces, to coarse-grained modelling of the adsorption of proteins and other biomolecules, and finally to the evolution of the corona of an NP immersed in a mixture of these adsorbates [2,3].

2. Biomolecular adsorption

Although atomistic modelling of the adsorption of a protein or other large biomolecule is feasible via molecular dynamics simulations, the required time and computational resources render this unfeasible to carry out for the wide range of potential adsorbates present in realistic models of biological media. Thus, coarse-grained approaches are necessary to ensure that adsorption energies can be computed within an acceptable amount of time. We have previously developed the UnitedAtom methodology for protein adsorption, which precomputes the interactions between amino acids and NP surfaces and uses these to predict the adsorption of an entire protein by summation over all AA beads, taking into account their location in the protein relative to the NP in different orientations [4]. Recently, we have adapted this methodology to allow for modelling of the adsorption of essentially arbitrary biomolecules comprised of smaller organic molecular fragments to multi-component NPs consisting of well-defined single NPs, greatly expanding the range of systems which can be explored. The required input is a set of potentials representing the interaction between an organic fragment and a given nanomaterial, with over one hundred fragments parameterised to over fifty chemically distinct nanomaterials with multiple variants of these.

3. Corona formation

The initial corona, primarily small biomolecules with a high concentration in the medium, forms within milliseconds, while the final corona evolves over the course of several hours. To capture these dynamic processes over this extended time period we

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employ a kinetic Monte Carlo method, which treats adsorbates as hard spheres and simulates their random sequential adsorption and desorption for a pre-defined length of time [5]. This methodology uses the adsorption energies output from UnitedAtom together with collision rates computed from kinetic theory to produce a set of adsorption and desorption rate constants for each possible orientation of each biomolecule relative to the surface of the NP, accounting for proteins with multiple binding sites or elongated structures. Using these rate constants, the steady-state corona is obtained, and quantities of each adsorbed biomolecule provided. These are of direct interest in terms of mass abundance, and we provide further post-processing tools to produce corona-averaged descriptors, e.g., the total charge of adsorbed molecules normalised by the surface area of the NP or the total number of residues of a certain type present in the corona. These descriptors provide further insight into the nature of the corona and the identity presented by the NP to its biological environment for use as input to QSAR and other machine-learning methods as they provide a convenient and biologically meaningful representation of the NP.

4. The NPCoronaPredict package

To streamline the use of our models, we have developed the NPCoronaPredict package which contains both UnitedAtom and CoronaKMC, while supplying a set of tools and interfaces to enable corona prediction with minimal user effort, and is freely available open-source [2,3]. This package contains a set of input potentials generated via metadynamics and augmented with additional potentials produced using machine-learning methods. A Python script, NPCoronaPredict.py, is supplied which automates running UnitedAtom for a selected NP and set of biomolecules, converts the output into rate constants, and runs the CoronaKMC script for final corona prediction. We also provide a simplified GUI to perform some of the most common tasks: downloading requested structures from either the Protein DataBank or AlphaFold DB as required, running UnitedAtom calculations for selected biomolecules and nanoparticles, and visualising the results as shown in Figure 1. To assist in designing complex multi-component nanoparticles we also provide the graphical tool NPDesigner for step-by-step construction of these composite NPs for use in UnitedAtom.

5. Conclusions

We have developed a multiscale methodology for predicting the contents of the biomolecular corona surrounding a nanoparticle, enabling rapid scanning of a wide range of NPs and biological media. This methodology is implemented in the open source NPCoronaPredict software package, which provides both a simplified graphical interface and a suite of command-line tools for the prediction of biomolecule adsorption affinities and the resulting corona. The output from this software package is immediately useful in characterising the nature of the nanoparticle corona and is of use in bioinformatics and predictive modelling of nanoparticle toxicology due to providing convenient numerical descriptors quantifying the biological identity of a given nanoparticle in a target organism.

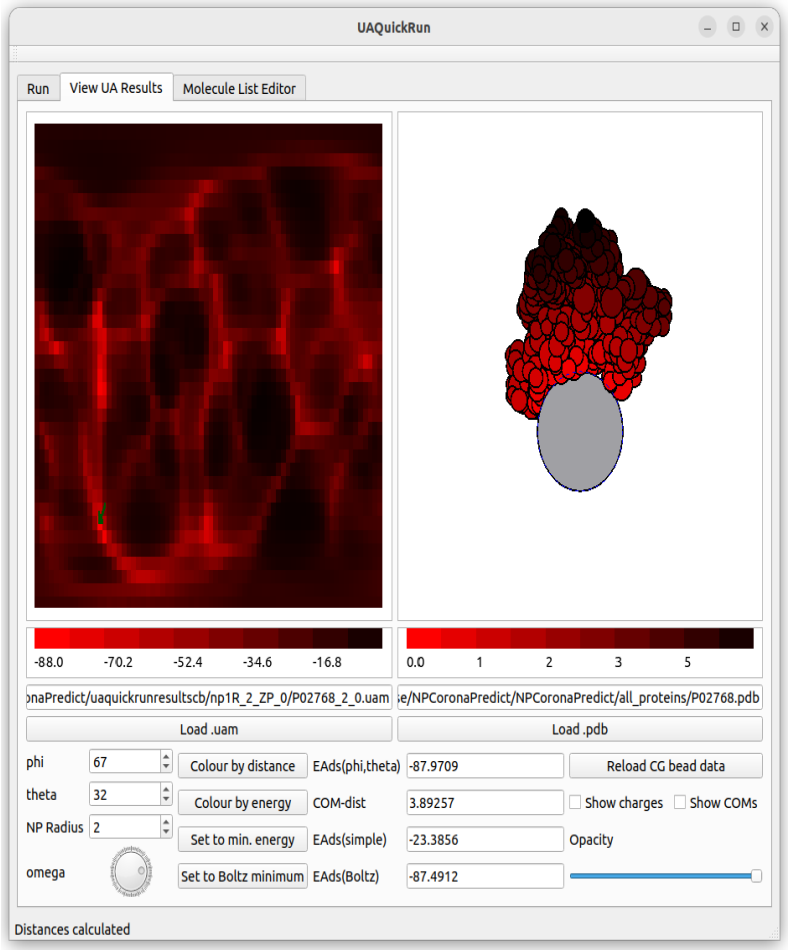

Figure 1: A snapshot of the graphical interface provided to compute biomolecule – nanoparticle adsorption energies, shown here for human serum albumin on a 2nm carbon black NP. The graphic on the left-hand side shows a computed adsorption heatmap, with red indicating strongly adsorbing orientations. The right-hand figure shows a schematic of the selected conformation of the protein, here chosen to be the most favourable binding conformation.

6. Acknowledgements

We acknowledge funding from EU Horizon2020 framework under grant agreements No. 686098 (SmartNanoTox project), No. 731032 (NanoCommons project), No. 814572 (NanoSolveIT project), and No. 101008099 (Marie Curie RISE CompSafeNano project), Horizon Europe (grant No. 101092741, nanoPASS project), and by Science Foundation Ireland (grant 16/IA/4506).

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Paper-based electrochemical sensor for the detection of essential oils and SARS-CoV-2 virus

Elisa Recchia[1], Laura Fabiani[2], Arianna Antinucci[2], Giorgia Leotta[2], Pierluca Galloni[2], Riccardo De Santis[1], Andrea Ciammaruconi[1], Giorgia Grilli[1], Florigio Lista[1], Fabiana Arduini[2]

1. Introduction

Paper-based sensors have emerged as promising platforms for the detection of various analytes due to their affordability, simplicity, and portability. Utilizing the inherent properties of paper, such as its porous structure and compatibility with functionalization processes, we developed in the last years several sensors and biosensors capable of selectively detecting target analytes in different fields including biomedical, environmental, agrifood, and defence [1].

It is worth noting that these sensors have demonstrated effectiveness in detecting both chemical and biological compounds, thus expanding their potential application field. The ability to detect analytes of different natures, such as organic molecules or biomolecules, makes these sensors extremely versatile and useful in a variety of contexts, from medical to environmental, from food industry to food safety.

2. Results

Herein, we present the results obtained within European Project Horizon Europe Reliance for monitoring the efficiency of the environmentally friendly antimicrobial coating developing a paper-based sensor for the electrochemical detection of essential oils namely thymol, eugenol, and carvacrol and a sandwich-type immunosensor to reveal SARS-CoV-2 virus in a paper-based origami configuration.

For the electrochemical measurement of both analytes, we functionalized the working electrode by drop casting with carbon black, demonstrating improved sensitivity using this affordable nanomaterial, in agreement with our previous articles [2].

The essential oils are revealed in solution by adding a drop directly on the sensor, as well as by sampling the target analyte on the surface and in the aerosol phase. The detection limit was 0.4, 0.4, and 0.6 ppm, with RSD % equal to 2 %, 1 %, and 3 % for thymol, eugenol, and carvacrol respectively.

For SARS-CoV-2 detection, a paper-based origami immunosensor has been designed. This biosensor incorporates specific recognition elements namely magnetic beads coated with a capture antibody against spike protein and a recognizing antibody labelled with alkaline phosphatase enzyme. SARS-CoV-2 virus is revealed after the

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addition of the substrate on paper-based screen-printed sensor, enabling rapid and sensitive detection. It's important to note that all immunorecognition steps are merged in one single step conducted inside waxed paper wells permitting the origami configuration.

3. Conclusions

Our results demonstrate the successful fabrication and characterization of these paper-based (bio)sensors, showcasing their potential for diverse applications in healthcare, environmental monitoring, and beyond. This work highlights the versatility and effectiveness of paper-based sensors as robust tools for real-time analyte detection, paving the way for advancements in sensor technology.

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Beneficial effect of differently-coated Selenium Nanoparticles in 3D cell culture models mimicking the respiratory tract and intestinal epithelium

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1. Introduction

Selenium (Se) is an essential trace element that plays a crucial role in various physiological processes, including enhanced immunity[1] (Avery and Hoffmann, 2018) and antioxidant defense[2]. Ingested as well as inhaled Se nanoparticles (SeNP) can be absorbed by epithelial and resident immune cells and being incorporated into selenoproteins that scavenge reactive oxygen species (ROS) and protect against oxidative stress-induced damage. Moreover, Se has been shown to modulate the release of inflammatory cytokines, and Se deficiency has been associated with impaired intestinal barrier function and increased susceptibility to intestinal infections and inflammation. Therefore, Se serves as a valuable micronutrient in protecting against oxidative stress and inflammation. Understanding the mechanisms of Se metabolism and its effects on intestinal and lung physiology is crucial for developing therapeutic strategies to combat gastrointestinal and respiratory disorders. However, the direct administration of Se as an antioxidant is not advised due to its narrow therapeutic window[3].

2. Objective

The objective of this study was to evaluate the toxicity as well as the antioxidant and anti-inflammatory capacity of SeNPs in 3D cell culture models. The respiratory tract can be resembled by an alveolar *in vitro* test system called ALIsens®[4] built on a microporous membrane of hanging inserts by seeding human alveolar type II epithelial cells (A549) and endothelial cells (EA.hy926), as well as macrophage-like (Mφ-THP1) and dendritic-like cells (DC-THP1). The physiologically relevant architecture of the system favors the development of a tissue-like microenvironment and facilitates exposures at the air-liquid-interface (ALI). The *in vitro* intestinal epithelium is based on a tri-culture model consisting of human intestinal epithelial cells (Caco-2) and mucus-secreting HT29-MTX cells, as well as hematopoietic cells (Raji B) able to promote Caco-2 conversion in specialized microfold cells (M-cell)[5,6].

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3. Conclusions

The treatment shows that the SeNPs are well tolerated in both cell culture systems without inducing neither a strong basal cytokine release nor increasing oxidative stress measured by ROS formation.

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The "Navetta" in *vitro* aerosol exposure system for respiratory health monitoring as well as efficacy and safety testing of pulmonary delivered bio-based pharmaceutical formulations

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Exposure of lung epithelia to aerosols is omnipresent. The unintentional exposure to exhaled droplets expelled during speaking, sneezing, or coughing is part of our daily life. Such aerosols contribute to the airborne transmission of infectious diseases. Additionally, exposure to aerosols or airborne particulates can occur in workplaces or in environmental settings. Along this line the World Health Organization (WHO) claimed: *"In 2019, 99% of the world's population was living in places where the WHO air quality standards were not met."* (1). For instance, a significant portion for air pollution derives from car tire wear and tear with an estimated global average *per capita* emission of 0.81 kg/year accumulating to 3-7% of the particulate matter ($PM_{2.5}$) in air. In humans, the permanent exposure to polluted air leads to the development of various pulmonary diseases that become a growing problem. The top ten leading causes of deaths in 2019 included three lung diseases (chronic obstructive pulmonary disease (COPD), lower respiratory infections, lung cancer) (4). Focusing on prevention and treatment of lung diseases is a hot topic, and the development of pulmonary delivered pharmaceutics is of great interest. Budesonide, for example, is a commonly used glucocorticosteroide applied to treat asthma and COPD. The application with a dry powder (DPI) or metered dose inhaler (MDI) allows local application, downregulating inflammation in the affected lung tissue. Moreover, the thin epithelial barrier (0.1-0.2 µm) in the alveoli, the large surface area of the lung (70-100 m^2) and the good blood supply enable a swift transfer of drugs into the circulatory system, making the pulmonary administration an interesting application route, less invasive than intravenous administration and hence better-compliant. In the context of nanomedicine, carrier systems are investigated that increase therapeutic efficiency, reduce toxicity, and achieve targeting delivery. Following the 3 R principle to reduce, refine, and replace animal experiments, we developed an *in vitro* aerosol exposure system, called Navetta, to test the environmental impact of air pollution on human lung as well as efficacy and safety of therapeutic aerosols intentionally administered *via* the pulmonary route. The Navetta enables the exposure of air-liquid interface (ALI)-cultured human lung epithelial cells (here the A549 cell line was used) to a low, laminar, horizontal air flow simulating the situation in the alveoli as closely as possible. *Via* electrostatic deposition of beforehand charged aerosols this system allows a very efficient deposition. The efficacy of the electrostatic deposition was tested using aerosolization of a sodium fluorescein solution showing a reproducible deposition across the 4 positions inside the Navetta, as well as by FITC-labelled silica,

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ZnO, CeO_2, or Ag-containing nanomaterials. To generate the aerosols from an aqueous suspension a 4-jet low-flow Blaustein atomizer was used to ensure a particularly gentle aerosol generation suitable for therapeutics and biological materials. For pharmaceutic efficacy testing we established a therapeutic model simulating airway inflammation using ALI-cultured A549 cells pre-incubated with tumour necrosis factor (TNF)-α. As efficacy readout the inflammation suppression after the administration of budesonide aerosolized from dry powder was determined. For safety profiling, cell viability and immune responses after exposure were determined. Additionally, a scanning mobility particle sizer and an optical particle counter were used to determine the size distribution of the generated aerosols over a size range from 10 nm to 35 µm. The particulate number concentration mode was 50 nm, and the particulate mass concentration was below 2-5 µm resulting in a deposition in the alveolar area. This data further allowed to perform *in silico* prediction of pulmonary drug deposition (5). For optimizing the efficacy of therapeutic administration into deep lung budesonide packaging into next-generation carrier systems based on biomaterials are of interest. One type of biological material offering great drug-loading opportunities are extracellular vesicles (EVs), which are regarded as safe and effective (6). EVs are a heterogenous group of membrane vesicles secreted by eukaryotic and procaryotic cells and participate in communication and signalling. Their lipid bilayer enables the loading of EVs with therapeutics such as RNA, DNA, or small molecular weight drugs (7). Tissue targeted drug delivery can be reached due to specific surface modifications of the EVs. Here we studied bio-derived EVs, which indeed enabled efficient uptake of fluorescently double-labelled EVs into the cells, with several post-incubation times being tested for efficiency optimization. In summary, we herewith demonstrate the suitability of the Navetta *in vitro* aerosol exposure system for testing cyto- and immunotoxic pulmonary effects derived from environmental pollutants and for efficacy and safety testing of pharmaceutical applications.

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Correlative chemical imaging to reveal the nature of different commercial graphene materials

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1. Introduction

Since Novoselov and Geim's seminal report in 2004[1], Graphene has attracted immense attention owing to its extraordinary properties[2]. Over the last two decades, the synthesis and functionalization of graphene have significantly advanced[3]. Various synthesis methodologies have emerged, giving rise to the development of related materials such as graphene oxide (GO) or elemental-doped graphene[4]. Additionally, chemical functionalization of the material surface can augment or modify specific graphene properties. Accurate physico-chemical characterization using diverse analytical techniques is indispensable for elucidating the nature of these materials[5]. Particularly those analytical methods equipped with imaging capabilities can derive greater analytical insights from these specific 2D materials. Nevertheless, a dedicated sample preparation is the prerequisite for a meaningful outcome.

2. Well-defined monolayer Graphene Oxide in µm range

Single-layer GO flakes, generously provided by Graphenea (Spain), were meticulously prepared for systematic imaging analysis. These flakes were carefully arranged on an alignment-marked SiO_2 substrate and sequentially imaged using scanning electron microscopy (SEM), atomic force microscopy (AFM), time-of-flight secondary ion mass spectrometry (ToF-SIMS), Raman spectroscopy, and additionally analysed with X-ray photoelectron spectroscopy (XPS). The exceptional lateral resolution and surface sensitivity of these techniques was crucial for accurate imaging of single-layer GO flakes. The ToF-SIMS images exhibited strong correlation with the SEM and AFM images (Figure 1a, c and d), offering valuable insights into the chemical composition. Employing 2D Raman spectroscopy, the number of overlapping single-layer flakes could be distinguished. Such structures were further visualized by Raman microscopy in a 3D image (Figure 1b). These GO flakes are good candidates for reference materials not only for imaging graphene-like structures, but also for exploring other types of 2D materials.

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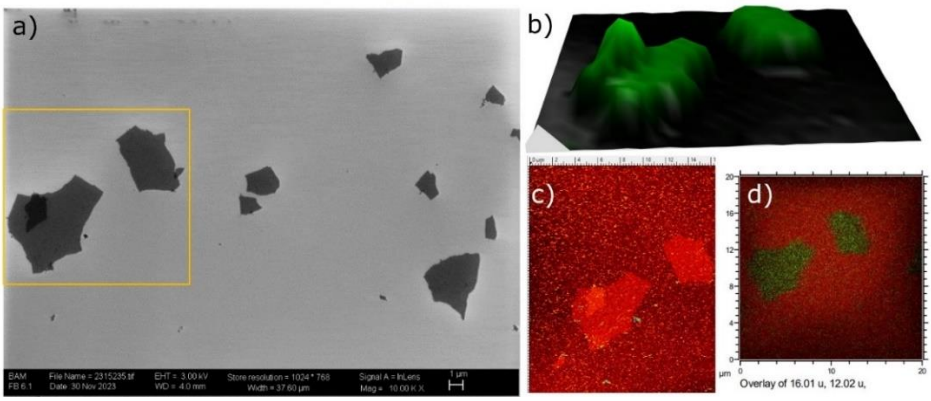

Figure 74: Correlative images of GO flakes a) SEM image, b) Raman intensity of G peak scanned over the area in (a) marked with yellow, c) AFM image and d) ToF-SIMS overlay image of C^- (green) and O^- (red) fragments.

3. Suspensions and Inks containing commercially fluorinated and nitrogenated GO Powder

In addition to the clearly defined monolayer graphene oxide (GO) flakes, we also examined commercial GO-containing suspensions and inks (from Haydale) with a more complex morphology, by using correlative imaging techniques. The basis of the inks and suspensions is GO powder which was functionalized e.g. with fluorine and nitrogen. To identify the source of various chemical fragments, ToF-SIMS and Auger electron spectroscopy (AES) were combined with SEM images of the same analysis area on the sample. Interestingly, not all GO flakes from the powder were homogeneously functionalized suggesting that the functionalization reaction takes place preferably on specific sites. It was also shown that the fluorine functionalization is a more effective process than the nitrogenation.

To obtain the inks, carbon black was mixed with functionalized GO powder and resin. SEM imaging showed that, based on morphological information, the GO sheets seem to be uniformly embedded into the resin/carbon black matrix (Figure 2a). The final confirmation proving a homogenous distribution of functionalized GO flakes was found by ToF-SIMS imaging and Energy-Dispersive X-ray Spectroscopy (EDX) elemental mapping. The results align closely with the nominal distribution of 10 % of specific functionalizations (marked by fluorine) solely associated to the graphene flakes, as indicated in the SEM images. While fluorine and oxygen signals are only visible on GO flakes, signals for carbon clusters (e.g. C_2^-) are noticeable on the whole surface as expected (see Figure 2). EDX mapping of Fluorine operated at low energy values could be correlated with these findings, albeit with lower resolution compared to ToF-SIMS, as EDX analysis probes deeper regions in the sample (roughly 1 µm) and ToF-SIMS only analyzes the outermost layer. Notably, AES on the same region could not identify the fluorine since the concentration is near the detection limit and the functionalized GO flakes “lie” mostly unparallel at the sample surface but rather being embedded deeper in the ink matrix. On one hand the GO powder is diluted by an order of magnitude with carbon black/resin and on the other hand the powder used for this specific ink was not as highly fluorinated as others according to XPS and EDX bulk analyses.

Besides the functionalization, traces of elements such as Na, K and Fe coming from the production process could be found and localized at the flakes sites when measuring ToF-

SIMS in positive mode. Intriguingly, as in the case of different functionalizations, the impurities were also detected on different areas/locations of graphene flakes.

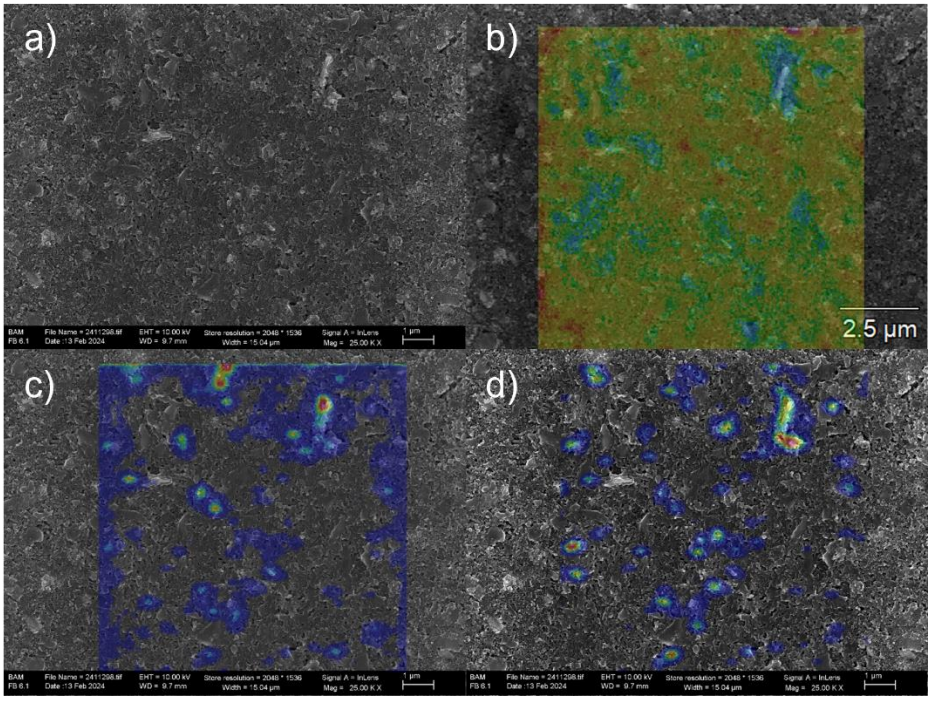

Figure 2: Correlative images of an ink containing fluorinated GO flakes: a) SEM micrograph, b) C_2^-, c) O^- and d) F^- SIMS maps overlayed on the SEM image in thermal colour representation (blue= low intensity, red=high intensity).

4. Conclusions

GO flakes and GO flakes containing commercial materials were chemically imaged at high resolution with different analysis techniques. In a first case study, single layer and overlapping sheets could be precisely visualized after dedicated preparation on a substrate. As these sheets have a highly defined structure, their potential exploitation as a reference material is considered.

Chemical imaging on functionalized GO flakes of commercial grade showed different fragments from surface functionalization, but also residual elements from the production process. The distribution of the functionalization over the flakes is rather inhomogeneous. Within the inks as the final product, the flakes were homogeneously distributed in accordance with the manufacturer specifications.

These findings demonstrate that ToF-SIMS is a powerful method in regard to surface sensitivity and detection sensitivity with excellent lateral resolution (well below 100 nm) making it an optimal method for imaging monolayer and few-layer graphene 2D materials.

5. Acknowledgements

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Holistic, reliable and practical Characterization Framework for Graphene-Family Materials, a correlated approach including Imaging-based techniques

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1. Introduction

ACCORDs is an Horizon Europe project working in the development of an imaging-based characterization framework (ACCORDs framework) for the holistic correlative assessment of Graphene Family Materials (GFMs) as a representative of 2D nanomaterials (NMs) to assess and predict 2D NMs health and environmental risks.

The ACCORDs framework will operationalise safe and sustainable by design (SSbD) strategies proposed in past or ongoing H2020 projects or within OECD by **correlating low-, medium-, and high-resolution physico-chemical-biological imaging-based methods with non-imaging methods in a tiered approach**. ACCORDs will deliver the ACCORDs framework and user guidance, new imaging-based characterisation methods, reference in vitro tests, new reference 2D NMs for different matrices, a new minimum information reporting guideline for FAIR data sharing and reuse of images as well as an atlas with reference images for diagnostics of compromised safety of GFMs / GFM products. The new guidelines and standard proposals will be submitted to standardisation bodies to allow creation of regulatory ready products. The novelty of ACCORDs is in **translating the principles of medical imaging-based diagnostics to 2D material hazard diagnostics**. ACCORDs will accelerate industrial sectors in the area of aviation, marine construction, drone production, flexible electronics, photovoltaics, photocatalytics and print inks-based sensors. The value ACCORDs proposes to the graphene industry are practical, easy, imaging-based tools for GFM quality monitoring next to the production line with a possibility to be correlated with advanced high-resolution imaging characterization methods in case hazard i.e. deviation from controls (benchmark values) are diagnosed. The ACCORDs framework and tools will contribute

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to the European Green Deal by addressing the topic: “Graphene: Europe in the lead” and to a new European strategy on standardization, released on 2nd February, 2022.

2. Objectives

- To develop purpose-oriented correlative approaches for the characterization and quantification of 2D nanomaterials as produced and in complex matrices and determination of their transformations in such environments.
- To increase the availability of validated protocols to advance both nanosafety studies and material characterisation and deliver improved data reporting guidelines.
- To ensure appropriate, realistic in vitro models to address current gaps in nanotoxicology.
- To deliver reliable data to support computational modelling and the development of grouping and read-across methods.
- Worldwide accepted risk assessment tools for establishing a robust supply chain for GFMs.

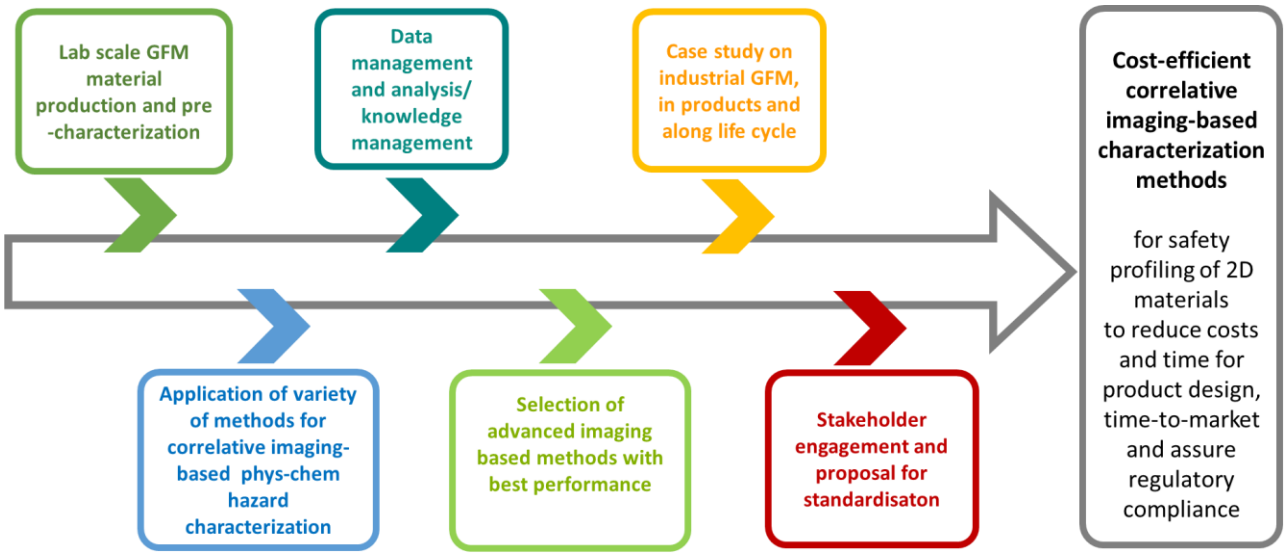

Figure 1 ACCORDS Workflow

3. Ongoing activities

- Graphene Oxide Materials produced, characterised and distributed to the consortium.
- Wide array of Physico-Chemical and Biological-Hazard characterisation techniques are being performed.
- Omero installed and discussions on image uploading.
- Engagement with International Standardisation Organisations & Identification of gaps in available literature.
- Design & Execution of a Dissemination Plan and identification of exploitable results.

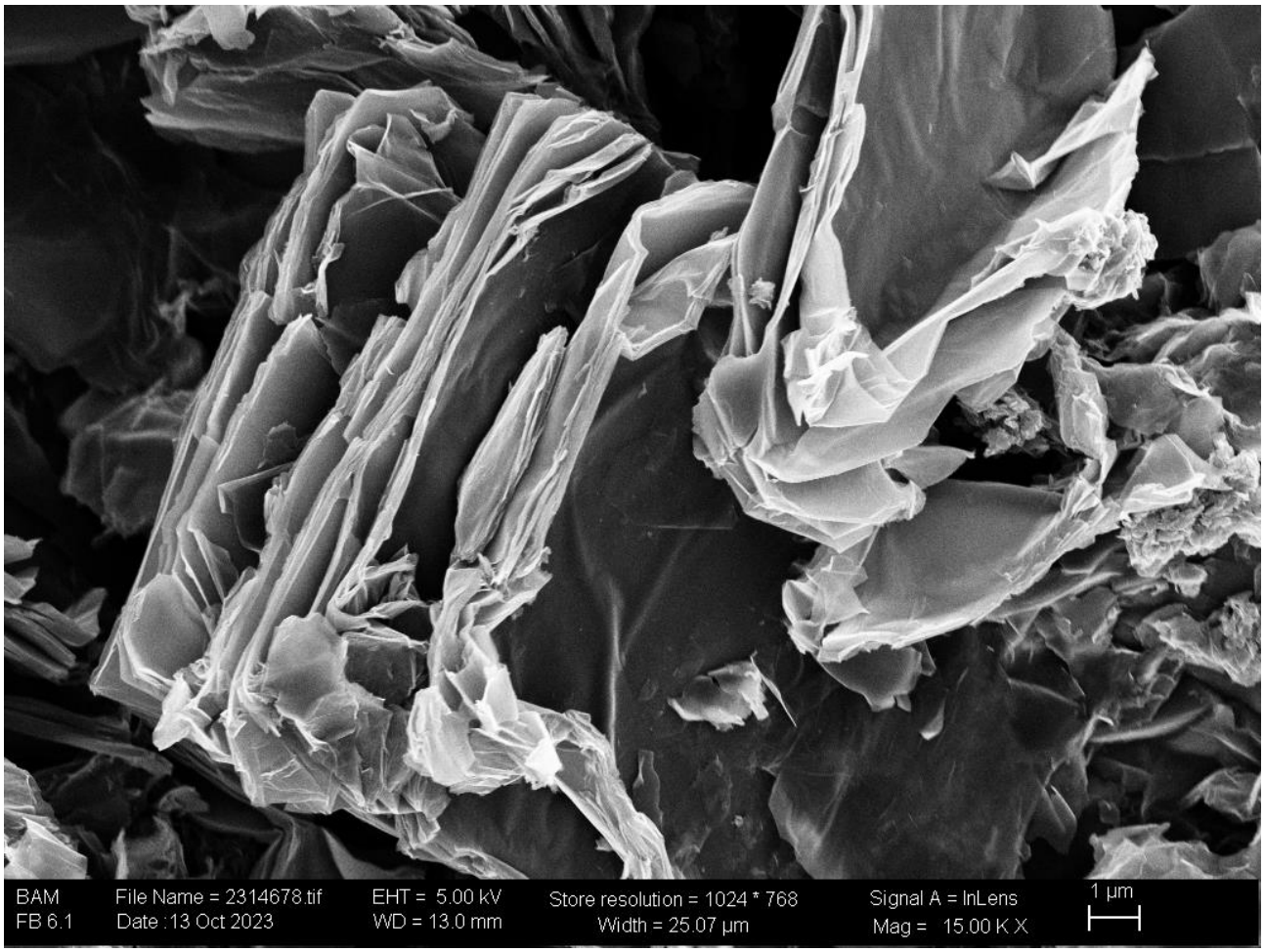

Figure 2: GFM Image from SEM technique at BAM

4. Expected Outcomes

- ACCORDs will deliver a new imaging-based correlative characterisation framework including **new regulatory compliant characterization methods** (5-10 **new** methods).
- Up to 10 **new** standard operating procedures (SOPs), new TMDFs along with TDRFs as a basis for data/images FAIRification, and decision-making workflows, computational modelling, and grouping and read-across.
- New imaging-based protocols (up to 5 **new** protocols are expected) will
- be integrated with already available ones to assure a correlative and tiered approach to advance nanosafety testing.
- Artificial Intelligence (AI) and machine learning-based analysis of material properties will provide new models supporting product design and decision-making.
- Up to 5 proposals for new technical documents for standards and guidelines to international standardisation bodies.
- A reliable and practical imaging-based characterization **framework** for the holistic imaging based correlative characterisation of 2D to allow creation of **regulatory ready products**.
- A user guide (for 2D nanomaterial producers, downstream users, and consultants).
- A catalogue (Atlas) of reference physico-chemical and biological /safety characteristics for 2D nanomaterial for practical **safety diagnostics to simplify**

monitoring of 2D nanomaterials along the value chain (quality and safety control) in analogy with medical imaging-based diagnostics.

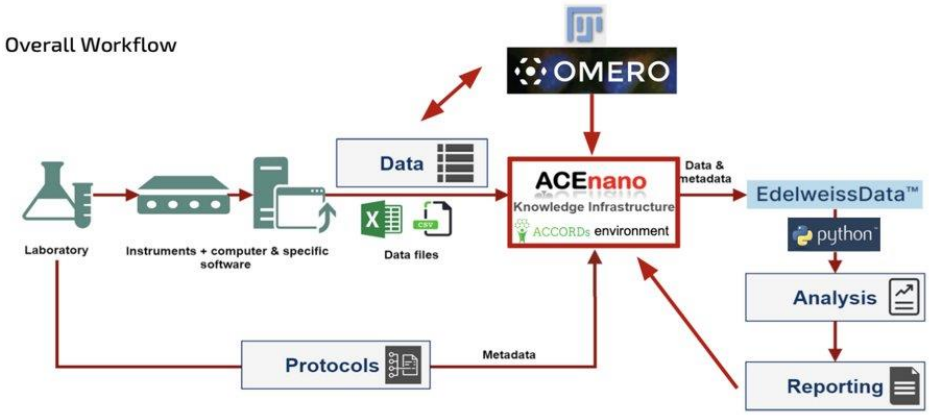

Figure 3: Digital workflow for the development of a knowledge infrastructure

5. Acknowledgements

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Chemical Nanoscale Analysis of Mesoporous Mixed IrOx-TiOy Thin Films

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1. Introduction

Porous films play an important role particularly in energy applications like photovoltaics, electrolysis, or batteries. Thin film properties such as thickness, chemical composition, crystallinity of the framework, and porosity define the activity of the porous films. The accurate morpho-chemical characterization of mesoporous thin films is a challenging analytical task which requires the consideration of new analytical approaches based on the combination of data of different methods able to address the structure and chemical composition at the nanoscale.

In this contribution we characterize thin mesoporous iridium-titanium mixed oxide film properties by EDS at an SEM applied in the dedicated “thin film analysis” approach [1]. Thus, the film mass deposition, film thickness and the film density can be determined [2]. Further, by dividing the measured film density to an assumed (theoretical) metal oxide framework (skeletal) density, the thin film porosity can be extracted, too [3,4].

2. SEM/EDS Analysis

To assess the lateral homogeneity of the morphology and chemistry of the mixed IrOx-TiOy thin films, first, high-resolution electron microscopy in conjunction with EDS elemental mapping have been applied on detached, free-standing films. Figure 1 shows an example of a mesoporous film with laterally inhomogeneous morphology, with islands-like structures of 150-200 nm size, of no templated mesoporosity, and which could be identified by EDS as IrOx-rich regions in the layer.

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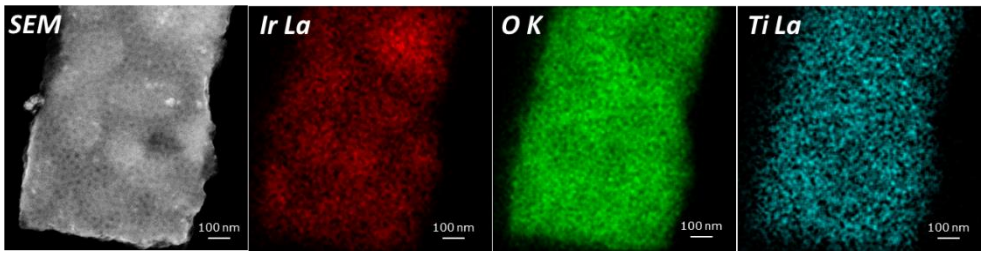

Figure 75: 5 kV SEM and EDS elemental maps of an IrOx-TiOx thin layer prepared as free-standing sample. Note the IrOx-rich domains within the mesoporous TiOx-rich matrix.

3. ToF-SIMS Analysis

A more surface and elemental sensitive analysis of the chemistry of a film like that presented in Figure 1, including a superior lateral resolution (of <100 nm) has been attained by mapping the sample surface with ToF-SIMS. Figure 2 displays the distribution of IrO+ and TiO+ ions at the surface of the film, demonstrating IrOx-rich islands observed with SEM and indicated by EDS in Figure 1. Further, the depth profiling mode of SIMS has been applied on homogeneous and inhomogeneous IrOx-TiOy films, revealing significant differences in the courses of Ir+, Ti+ and TiO+ ions along the film depth, with direct correlation to the synthesis conditions: the water content in the dip coating solution might lead to a separation of the IrOx and TiOy precursors, and provides a TiOy network with a templated mesoporosity and IrOx domains with a “native” porosity at the interfaces. In contrast, a dip coating solution without additional water results in an ordered pore network with a uniform distribution of IrOx and TiOy.

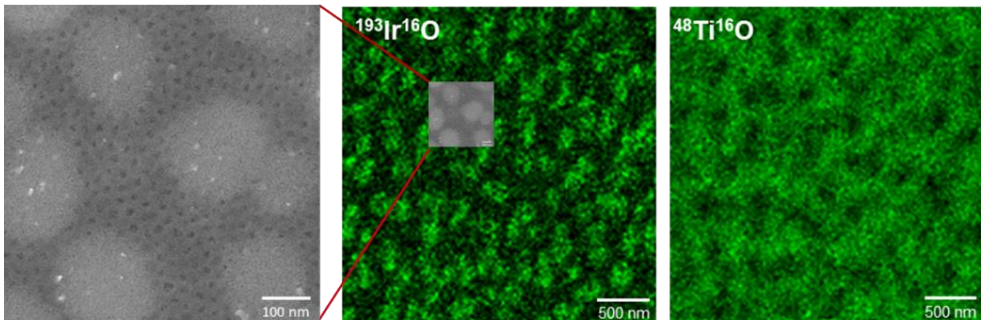

Figure 76: Chemical imaging of an IrOx-TiOx thin layer by ToF-SIMS. Note the IrOx-rich domains within the mesoporous TiOx-rich matrix at the surface.

4. Auger Electron Spectroscopy Analysis

Auger electron spectroscopy, with its excellent lateral resolution of <20 nm has been employed with the dedicated purpose of investigating the in-depth elemental distribution within the island-like structures in the inhomogeneous IrOx-TiOy films. The result of such an analysis is illustrated in Figure 3 and confirms basically the findings with ToF-SIMS. Slight enrichments of Ir are observed at the surface of the IrOx domains, but also at the interface thin film/ (Si) substrate in the IrOx-islands-free film matrix, the latter being accompanied by a decreased signal of oxygen.

Novel Two-Dimensional Magnets Synthesized in Graphene Oxide Under Ambient Conditions: Atomic Structure and Magnetic Properties

V. Skákalová[1,2,3], P. Kotrusz[1,2], K. Mustonen[3], T.A; Bui[3], M. Precner[1], P. Hutár[1], M. Hulman[1,2], M. Orendač[4] and M. Gmitra[4]

We have recently developed a simple chemical method SinGO (Synthesis in Graphene Oxide) that, under ambient conditions, can provide novel two-dimensional (2D) materials in a macroscopic scale [1]. The SinGO method opens an avenue to a new class of 2D magnetic and non-magnetic metal-iodides (2D-MI) encapsulated between graphene monolayers. Such vdW stacks would serve as a novel platform for nanotechnological devices in which 2D magnets hold spin whereas graphene as a conducting channel of Dirac electrons can guide the encoded relevant information. Noting that graphene spintronics has been aiming to exploit the extraordinary Dirac electronic properties but weak spin orbit-coupling limits its applicability for generating spin currents or spin torques. The proximity-induced spin-orbit coupling and exchange interactions in graphene-encapsulated 2D-MI magnets heterostructure might enable spin transport with unexplored yet physical mechanisms.

Here we will present the wide range characterization of 2D (magnetic and non-magnetic) metal-iodides encapsulated in graphene including their atomic structures (STEM), magnetization and electrical transport properties for possible applications.

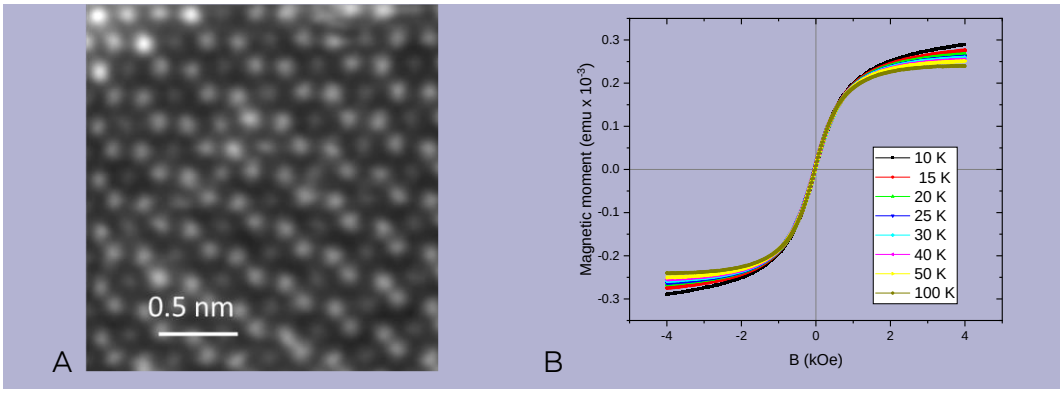

Figure 1: A. Scanning Transition Electron Micrograph of 2D FeI2 atomic structure embedded between graphene layers (carbon contrast is too low to be visible), B. Dependence of magnetization on magnetic field of 2D FeI2 - graphene heterostructure.

References

[1] K. Mustonen et al., Toward Exotic Layered Materials: 2D Cuprous Iodide, Advanced Materials 34, 2106922 (2022).

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Session 10: MaterialsWeek 2024 Closing- & Awards-Ceremony

This Session will provide a summary of the sessions, presentations, posters and discussions of the previous three days and close the conference with a festive act of Award Ceremonies:

- 2 oral and 2 poster presentations will be awarded a prize of EURO 250 each, kindly sponsored by CSBJ: Nanoscience and Advanced Materials Section, and
- 1 award for the winner of the 'Data Tool & FAIRness Competition Award', kindly sponsored by PARC.

Detailed Programme

Start	End	Title	Presenter
16:00	16:05	Conference Summary and Look into the Future	Steffi Friedrichs
16:05	16:15	Poster Presentation Award 1 & 2	Gupta Udatha
16:15	16:25	Oral Presentation Award 1 & 2	Gupta Udatha
16:25	16:30	FAIR Competition Award	Iseult Lynch
16:30	16:40	Closing Remarks	Steffi Friedrichs