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Advanced materials: Overview of the field and screening criteria for relevance assessment



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# Advanced materials: Overview of the field and screening criteria for relevance assessment

by

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# Abstract: Advanced materials – Overview of the field and screening criteria for relevance assessment

The project activities described in this report comprise a literature review, expert interviews, an online survey, desk research on relevance criteria and the organisation of the first of three thematic conferences that will take place in the context of this project. Based on the gathered information and experiences, advanced materials were clustered into different groups. Each group was characterised in form of factsheets. At the first conference, clustering approaches were discussed as well as the need to "define" advanced materials and aspects of including safety considerations into material design.

A number of advanced material types were identified that could be of relevance with regard to chemical safety. This could, for example, be due to indications of hazards and risks that might require adequate risk management or due to insufficient regulatory coverage or missing risk assessment methods and tools.

This report summarises the results of the project's first work package. It is discussion input to two further thematic conferences of the project as well as to discussions on approaches to cluster, describe and prioritize advanced materials in other contexts.

# Kurzbeschreibung: Advanced materials – Überblick über das Feld und Kriterien für die Relevanzprüfung

Die in diesem Bericht beschriebenen Projekttätigkeiten umfassen eine Literaturrecherche, Experteninterviews, eine Online-Umfrage, die Entwicklung von Relevanzkriterien und die Organisation der ersten von drei thematischen Konferenzen im Rahmen des Projektes. Auf der Grundlage der gesammelten Informationen und Erfahrungen wurden Advanced Materials in verschiedene Klassen eingeteilt. Jede Klasse wurde in Form eines Factsheets charakterisiert. Auf der ersten Konferenz wurden Ansätze diskutiert Advanced Materials in solchen Klassen zusammenzufassen sowie die Notwendigkeit, Advanced Materials und Aspekte der Chemikaliensicherheit in das Materialdesign einzubeziehen.

Es wurden einige Typen von Advanced Materials identifiziert, die im Hinblick auf die Chemikaliensicherheit von Bedeutung sein könnten. Dies könnte z. B. auf Indizien zu Gefahren und Risiken, die möglicherweise ein angemessenes Risikomanagement erfordern, eine unzureichende regulatorische Erfassung oder fehlende Methoden und Instrumente zur Risikobewertung zurückzuführen sein.

Der Bericht fasst die Ergebnisse des ersten Arbeitspakets des Projekts zusammen. Er ist ein Diskussionsbeitrag zu den weiteren zwei thematischen Konferenzen des Projekts sowie zur weiteren Entwicklung von Ansätzen zur Einteilung von Advanced Materials in Gruppen und ihrer Beschreibung und Priorisierung in anderen Kontexten.

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### List of abbreviations

AdMa	Advanced material
BMU	Bundesministerium für Umwelt, Naturschutz und Nukleare Sicherheit = Federal Ministry of the Environment, Nature Protection and Nuclear Safety
DAMADEI	Design and Materials As a Driver of European Innovation
L&M	Lukassen and Meidell
MatSEEC	Materials Science and Engineering Expert Committee
NV	No values
R&D	Research and development
TIP	Technology Innovation Program
TSB	Technology Strategy Board
UBA	Umweltbundesamt = German Environment Agency
WoS	Web of Science
WP	Work package

### Summary

The field of materials sciences is broad and highly dynamic. New and improved materials have been developed to overcome limits with regard to static performance as well as functional tasks (active and passive). To avoid the high efforts of late risk management which is confronted with path dependencies and technological lock-ins, a prospective analysis of potential risks of new and emerging materials is necessary. In the realm of materials sciences "advanced materials" has become a frequently used term for new materials which seems to meanwhile cover also the field of nanomaterials. Due to their complex or innovative structure and composition, advanced materials are worth investigating to check whether the current framework for risk regulation still covers the new developments in the materials sciences.

The aim of the present report is to identify relevant advanced materials in regard to chemical safety. Since the term advanced materials is not clearly defined, a major focus of this investigation is to characterize the use of the term advanced materials to obtain a reasonable separation within the materials sector. A set of criteria that could be applied to assess the relevance of advanced materials regarding chemical safety was developed and is provided for further discussion and refinement. In addition, a first description of identified advanced material clusters was performed. The resulting factsheets provide a short overview of the characteristic properties of the identified advanced materials along with notes on the application range and potential risks and their regulatory status, as far as it can be anticipated.

The report is divided into three main areas of investigation:

- 1) Structuring the field of investigation by
  - o screening of definitions and classification of advanced materials
  - quantitative screening of scientific activities related to advanced materials to identify material types by keywords and relevant authors as well as their interaction
  - o qualitative identification of present clusters of advanced materials
- 2) Identification of relevance criteria to evaluate advanced materials regarding four different relevant dimensions: science, economy and technology, risk and regulation
- 3) brief characterization of the identified clusters of advanced materials in the format of factsheets

In the following, after a description of the methodological approach, the results of the three parts of analysis will be summarized.

#### Methodological approaches

Three methodological approaches were used to characterize and screen the field of advanced materials for relevant material types.

#### LITERATURE RESEARCH

The literature research is divided in a quantitative and a qualitative part: First a quantitative bibliometric analysis containing a scientometric research of the Web of Science Core Collection and a network analysis was conducted. Second, a qualitative analysis of identified publications, reviews and technical articles on advanced materials was performed.

Assuming that scientific activity is an indicator for the relevance of a material type in terms of research and development, an analysis of scientific papers was conducted by using keywords from five different categorizations of advanced materials, which were identified in studies on the

whole field of advanced materials. Using the identified keywords separately and combined, a scientometric analysis of publications in the Web of Science Core Collection between 2000 and 2018 was conducted. The increase in numbers of publications in Web of Science between 2000 and 2018 was investigated. Using the yearly increase in numbers of publications as the main indicator for research activity, the most emerging research areas with regard to advanced materials were identified.

For the research areas with the highest increase of publication numbers, a qualitative analysis was conducted to identify the involved types of materials, their chemical and physical qualities, potential applications and associated production processes.

To further characterize the field, a network analysis of the scientific literature on advanced materials complements the scientometric analysis to identify key actors and relationships between the most relevant keywords. The network analysis and the thereby identified related keywords serve as supplement and control for the terms used in the quantitative literature research.

#### EXPERT INTERVIEWS

Experts were interviewed to obtain opinions on the field of advanced materials and the relevance of different material types in the research field. The selection of experts was not systematic but considered the most relevant authors of scientific publications identified from the literature research as well as experts with an expected broad overview of the field. Academia, authorities and industry were covered with a focus on EU actors.

#### ONLINE SURVEY

An online survey was conducted to obtain expert feedback on the identified advanced material types. The usefulness and applicability of various criteria to identify the relevance of particular advanced materials were addressed. In addition, the survey should contribute to information collection on the specific advanced material classes. The results of the survey were used to further develop the factsheets and elaborate criteria for the relevance assessment.

#### Structuring the field of investigation

A definition of advanced materials, considered by the EU dates back to 2013:

"An advanced material is any material that, through the precise control of its composition and internal structure, features a series of exceptional properties (mechanical, electric, optic, magnetic, etc.) or functionalities (self-repairing, shape change, decontamination, transformation of energy, etc.) that differentiate it from the rest of the universe of materials; or one that, when transformed through advanced manufacturing techniques, features these properties or functionalities." (European Commission 2013, p.25)

This description shows how broad a definition of advanced materials can be. In this way it covers nearly all areas of material development. Besides it, there are related concepts for advanced materials in recent studies on the field. From five of these studies (European Commission 2013; Lukassen and Meidell 2007; National Institute of Standards and Technology 2010; Materials Science and Engineering Expert Committee 2013; Technology Strategy Board 2008) classifications of advanced materials were identified, which partially covered the same classes, but also differed a lot. Six classes of advanced materials shown in Table 1 are derived from the classifications. Substance independent keywords, related to either activity (functionality), structure or the manufacturing process as well as their synonyms were used for the first quantitative literature research (cursive in the table).

Name	Synonyms	Description					
Active materials	smart, functional, multifunctional, adaptive	active materials are able to modify at least one of their properties in response to an environment variable					
Composites	advanced composites, composite materials	composites represent combinations of two or more materials					
Structural materials	structured materials, multi- structural, artificially structured	structural materials are structured in two or three dimensions					
Nanomaterials	nanotechnology	at least one of the dimensions nanomaterials is in the range of 1 to 100 nanometres					
Biobased materials	biomaterials	biobased materials either represent materials applied to a biological system or materials derived from a biological source					
Advanced manufacturing	advanced processing	advanced manufacturing relies on adding or removing material through virtual geometry, without the use of pre-shapes and without subtracting material					

# Table 1: Names of material classes derived from classifications of advanced materials.Cursive phrases were used as keywords in the scientometric analysis.

The overall results of the scientometric analysis indicate increasing research activity in the field of advanced materials. Besides the high diversity of material types that has already been reflected in the number of keywords from the studies on advanced materials, a close connection to the field of nanomaterials was identified. Most of the classes that seem to be relevant for the field of advanced materials belong to the composite-type of materials. The dimensions *structure, functionality* and *manufacturing* have been identified playing a significant role in defining materials as advanced.

With regard to a separation of advanced materials from other fields of materials most of the definitions presented so far remain time dependent with their focus on new or improved properties and the resulting (currently) outstanding performance (Kennedy et al. 2019). Here, an orientation at the design process represents a time independent approach for definition. As already suggested in an earlier study, advanced materials could be seen as being rationally designed as 'tailored materials' whose properties are aligned on a specific application (U.S. Congress 1988). Here *rational design* may consider two dimensions: a predetermined arrangement of new structures by a composition of either different materials or different structures.

For a further quantitative characterization of the field, the most cited keywords used to describe functionality, structure and manufacturing identified in the five studies mentioned above were connected with keywords for different material clusters. Table 2 shows what phrases have been used for the query. All keyword combinations, which showed to have less than ten publications every year between 2000 and 2018 were neglected (no values 'NV'). Blue fields indicate a large increase in publication numbers over the last 19 years. Especially nano-related keywords show a steep increase, but also biomaterials and soft materials. Overall, functionality related terms show a strong increase over the full period of analysis. Yellow indicates the steep increase over the last four years. For the keyword combination elastomer and functional materials the steepest increase from 2015 to 2018 was obtained.

# Table 2: Slopes (as percentage) of the number of publications in WoS for the combination of keywords for functionality, structure and manufacturing process (column) AND keywords for material types (row)

	"functional materials"19 yr	"functional materials"4 yr	"active materials" 19 yr	"active materials" 4 yr	"smart materials" 19 yr	"smart materials" 4 yr	"structural materials"19 yr	"structural materials"4 yr	"advanced manufacturing"19 yr	"advanced manufacturing"4 yr
"glass*"	4,8%	5,5%	4,1%	14,8%	5,2%	3,6%	2,9%	15,9%	NV	NV
"ceramic*"	3,9%	13,2%	3,3%	11,3%	2,1%	0,0%	2,5%	19,7%	NV	NV
"polymer*"	4,9%	13,6%	4,8%	10,3%	4,7%	11,3%	3,3%	15,9%	NV	NV
"metal*"	4,4%	16,6%	4,6%	13,0%	3,9%	12,7%	3,4%	7,5%	3,4%	20,4%
"elastomer*"	3,8%	27,0%	4,8%	12,7%	4,2%	24,4%	3,1%	-5,0%	NV	NV
"alloy*"	3,9%	16,8%	3,6%	-10,0%	4,2%	-0,6%	3,5%	10,2%	2,9%	10,6%
"coating*"	4,0%	18,3%	5,0%	12,2%	4,7%	5,9%	3,2%	23,4%	NV	NV
"electro active"	NV	NV	NV	NV	NV	NV	NV	NV	NV	NV
("electronic*" or "electric*")	4,4%	15,7%	4,9%	13,1%	4,1%	9,0%	3,0%	19,6%	2,2%	15,3%
"photo- active*"	4,5%	19,0%	NV	NV	NV	NV	NV	NV	NV	NV
"self-repairing"	NV	NV	NV	NV	NV	NV	NV	NV	NV	NV
"textile*"	4,6%	31,8%	3,4%	23,9%	NV	NV	NV	NV	NV	NV
"fibre*"	NV	NV	NV	NV	2,6%	-10,8%	NV	NV	NV	NV
"cellular*"	4,9%	-1,8%	NV	NV	NV	NV	2,2%	17,0%	NV	NV
"gels*"	4,7%	15,3%	NV	NV	4,8%	12,5%	NV	NV	NV	NV
"foam*"	4,2%	25,9%	4,8%	11,9%	4,2%	13,0%	3,7%	20,0%	NV	NV
"soft material*"	5,3%	1,7%	NV	NV	3,3%	23,0%	NV	NV	NV	NV
"nano*"	5,1%	13,3%	5,3%	10,0%	4,6%	12,1%	4,6%	15,0%	3,0%	10,0%
"nano- particle*"	5,6%	9,9%	5,2%	10,4%	4,9%	16,6%	5,7%	16,2%	NV	NV

	"functional materials" 19 yr	"functional materials"4 yr	"active materials" 19 yr	"active materials" 4 yr	"smart materials" 19 yr	"smart materials" 4 yr	"structural materials"19 yr	"structural materials"4 yr	"advanced manufacturing"19 yr	"advanced manufacturing"4 yr
"nano- material*"	4,2%	15,1%	4,8%	10,0%	3,4%	26,7%	NV	NV	NV	NV
"biobased*"	NV	NV	NV	NV	NV	NV	NV	NV	NV	NV
"organic*"	4,9%	13,5%	4,7%	13,5%	3,6%	14,3%	3,5%	15,0%	NV	NV
"bio- material*"	5,1%	11,6%	NV	NV	5,0%	22,7%	NV	NV	NV	NV

The blue shaded backgrounds represent the normalized slope within 19 years (2000 - 2018, darker shades for higher values), the yellow shaded backgrounds represent the normalized slope within 4 years (2015 - 2018, darker shades for higher values). NV= no values for neglected combinations; data from WoS Core Collection, July 2019

A qualitative analysis of 62 papers (mainly reviews) was based on the results of the quantitative analysis of research activity (Table 2). Only publications for keyword combinations with the highest increase in publication numbers were selected. The analysis showed that areas of application considering advanced materials are quite diverse. The main identified sectors are medical applications/pharmaceuticals, electronics (especially energy storage and sensors) as well as construction purposes. Polymers seem to play a major role in the field of advanced materials. With regard to their functionality in particular materials that tend to be small, adaptive (or even active) or flexible are frequently discussed. Nearly all materials mentioned in the analysed publications represent a combination of several different substances.

# Figure 1: Keywords of publications, which use "advanced materials" either in title, abstract or keywords



The size of words and dots represent the respective number of articles. Blue indicates a high number of citations for the retrieved articles, red a small number of citations. Keywords, which occurred less than three times are neglected. Data from Web of Science Core Collection, July 2019.

#### Source: Own presentation

Furthermore, a network analysis on the keyword "advanced materials" in Web of Science was conducted to examine related keywords and authors as well as their interactions. A total of 13,471 publications were identified. The network analysis showed a multi-centric author landscape with a main author group consisting of scientists from China and USA. There are also ongoing research activities in Europe, with a rather broad variety of authors, institutions and topics. Figure 1 shows the keywords used in the publications and their relatedness due to appearance in the same publications. The size of the dots indicates the publication number, while the size of the lines shows how often the keywords are used in combinations. Next to nano-related keywords, the term composite, self-assembly, microstructure, mechanical properties, biomaterial, polymer and graphene stand out. The map proves the findings from the scientometric analysis. Only the frequent appearance of the term self-assembly was unexpected, since it was not noticed by the quantitative literature research.

#### Relevance assessment

Relevance in this report is understood as either

- ▶ indication of potential risks,
- ▶ a lack of information on risks,
- a lack of legal coverage of the materials in their (intended) applications or the implementation and enforcement of the respective requirements,
- > a lack of applicability of risk assessment approaches and tools or
- challenges to circular economy, resource consumption or other environmental aspects.

As the above aspects only indicate potential challenges but not necessarily a "concern" with regard to chemical safety, the term "relevance" is used to show that reasons exist to prioritise an advanced material for further work.

The diversity and complexity of advanced materials and their applications require taking different perspectives and addressing various aspects to identify the "relevance" of an advanced material. Four dimensions of relevance are proposed:

- Scientific dimension: novelty of (the scale and/or combination of) properties
- *Economic and technical dimension:* potential of an advanced material to successfully reach the market and/or trigger innovations at process or product levels
- *Hazard and risk dimension*: indication of hazardous properties or critical exposure levels
- *Regulatory dimension*: lack of legal coverage and/or ability to conduct hazard or risk assessments.

**Fehler! Verweisquelle konnte nicht gefunden werden.**Figure 2 shows the four dimensions of the proposed relevance assessment approach and the core questions that can be addressed with information in this area.

#### Figure 2: Overview of the four dimensions of relevance assessment



#### Source: Own presentation

Apart from the four dimensions of relevance, additional criteria may be considered, which concern environmental and societal impacts of the use of advanced materials. These could relate, among others, to the recycling potential of advanced materials.

For each of the four dimensions, possible indicators of relevance have been identified. It is described what type of conclusions could be drawn from the indicator, whether or not the respective information is expected to be available and which practical challenges may have to be overcome in their use. Based on this evaluation, a set of criteria and related indicators have been proposed that could be used to identify the relevance of advanced materials for chemical safety and prioritise them for further work.

# Identification of critical areas of advanced materials and description of relevant materials in attached factsheets

Twenty-six classes of advanced materials, which are either frequently mentioned in the publications of the research field or regarded as an advanced material by experts were described and assessed in factsheets (cf. separate <u>Factsheets</u>). They represent a first approach to get an overview of the field, respective applications as well as first information on risk potential and regulatory gaps. The clustering of materials should support the analysis and assessment of common features of different material classes concerning the relevance criteria. The following (partly overlapping) clusters of advanced materials were described via factsheets in this project.

- 1. Biopolymers (Materials based on naturally occurring polymers, which are designed for a specific functionality)
  - a. DNA-based Biopolymers
  - b. RNA-based Biopolymers
  - c. Protein-based Biopolymers

- d. Sugar-based Biopolymers
- e. Lipid-based Biopolymers
- 2. Composites (combination of two or more materials)
  - a. Macroscopic Composites
  - b. Hybrid Materials (Materials that are a combination of organic and inorganic materials)
  - c. Fibre-reinforced Composites
  - d. Particle-reinforced Composites
- 3. Porous materials (Materials which show a porous structure, differentiated by pore size)
  - a. Microporous Materials
  - b. Mesoporous Materials
  - c. Macroporous Materials
- 4. Metamaterials (Materials with properties that go beyond the naturally occurring properties of their components)
  - a. Electromagnetic Metamaterials
  - b. Acoustic Metamaterials
- 5. Particle systems (properties of the materials are related to their particles' structure)
  - a. Quantum Dots
  - b. Supraparticle
  - c. Nanoflowers
  - d. Graphene
- 6. Advanced Fibres (fibres several  $\mu m$  or smaller in diameter with an intended functionality)
  - a. Organic Fibres
  - b. Carbon-based Fibres (incl. CNTs)
  - c. Inorganic Fibres (e.g. silica)
- 7. Advanced Polymers (Polymers with an intended functionality)
  - a. Electro-active Polymers
  - b. Magneto-active Polymers
  - c. Self-repairing Polymers
  - d. Co-polymers
- 8. Advanced Alloys (Alloys, which comprise more than two components; at least two components have a large share in the final material)
  - a. Advanced Alloys

To conclude, the main findings of the factsheets are: Many advanced materials contain (eco-)toxic substances that are combined with other substances. Based on the reviewed literature it is often unclear how stable the connections between the substances (building blocks) are. Therefore, it is unclear to which extent these (eco-)toxic substances could be released and create exposures that could cause risks to health or the environment. In addition to the (eco-)toxicity of the building blocks, further hazards can be related to the structure of the materials. Critical morphology (e.g. fibres), reactivity or particle size (e.g. nanocomposites) can lead to hazards and risks, even though the substances / building blocks are not hazard or risk relevant themselves.

Risk can further be enhanced by exposure, e.g. by persistence or ubiquitous use with releases into the environment and body uptake. For example, materials like DNA-based biopolymers show high uncertainties regarding their persistence in different ecosystems as well as the human body. This may induce risk relevance since the response of the immune system of the human body as well as other living organisms is unknown.

For some advanced materials it is not obvious which legal definition they fulfill (substance, mixture, article etc.). Therefore, the coverage by REACH and the related requirements to generate data for these materials is not fully clear. Other materials, such as advanced polymers which fall under the definition of polymers, may be exempt from registration under REACH. Here, apart from specific knowledge on the composition and molecular binding between the building blocks, a harmonized interpretation of the legal definitions is necessary to conclude on which of them applies.

A further reason for relevance of advanced materials is their potentially missing recyclability. Several classes of advanced materials consist of very different building blocks that are connected at molecular level and/or at nanoscale and can't be separated anymore. This may be the case especially for hybrids and nanocomposites as well as metamaterials. Thereby, recycling might become problematic.

Most of the identified advanced material types are still in a developmental stage. It is still uncertain in what products and in what amounts they will be used, which makes an estimation of potential exposures difficult. Nevertheless, some are already on the market even though risk related questions are unanswered (e.g. the application of microporous applications in health care products).

# Zusammenfassung

Das Feld der Werkstoffwissenschaften ist breit gefächert und ausgesprochen dynamisch. Neue und verbesserte Materialien werden entwickelt, um die Grenzen herkömmlicher Materialien hinsichtlich ihrer statischen Leistungsfähigkeit oder funktioneller Eigenschaften (aktiv und passiv) zu überwinden. Um den hohen Aufwand eines späten Risikomanagements zu vermeiden, welches mit Pfadabhängigkeiten (im Sinne einer technologischer Bindung – "Lock-in") konfrontiert ist, ist eine prospektive Analyse der potenziellen Risiken neuer und aufkommender Materialien notwendig. Im Bereich der Werkstoffwissenschaften ist "Advanced Materials" zu einem häufig verwendeten Begriff für neue Materialien geworden, der mittlerweile auch den Bereich der Nanomaterialien zu umfassen scheint. Aufgrund der komplexen oder innovativen Struktur und Zusammensetzung ist eine Untersuchung von Advanced Materials sinnvoll, um zu prüfen, ob der gegenwärtige regulative Rahmen für das Risikomanagement die neuen Entwicklungen in den Werkstoffwissenschaften noch ausreichend abdeckt.

Das Ziel des vorliegenden Berichts ist es, hinsichtlich der Chemikaliensicherheit relevante Advanced Materials zu identifizieren. Da der Begriff Advanced Material nicht klar definiert ist, liegt ein Schwerpunkt dieser Untersuchung auf der Charakterisierung der Verwendung des Begriffs Advanced Materials, um eine sinnvolle Trennung innerhalb des Werkstoffsektors zu erreichen. Es wurden zudem Kriterien entwickelt, die zur Beurteilung der Relevanz von Advanced Materials hinsichtlich der Chemikaliensicherheit angewandt werden können. Sie sollen in weiteren Diskussion geprüft, angepasst und ggf. präzisiert werden. Darüber hinaus wurden identifizierte Klassen von Advanced Materials strukturiert hinsichtlich ihrer Eigenschaften und Anwendungen beschrieben. Die so erstellten Factsheets geben einen kurzen Überblick über die charakteristischen Eigenschaften der identifizierten Advanced Materials, ihre Anwendungsbereiche und ihre potenziellen Risiken sowie zu ihrem regulatorischen Status, soweit dies möglich ist.

Der Bericht ist in drei Teile unterteilt:

- 1) Strukturierung des Feldes durch
  - o Überprüfung von Definitionen und Klassifizierungen von Advanced Materials
  - quantitative Überprüfung wissenschaftlicher Aktivität im Zusammenhang mit Advanced Materials, um Materialtypen nach Schlüsselwörtern und relevanten Autorinnen und Autoren sowie deren Verbindungen zueinander zu identifizieren
  - qualitative Identifizierung gegenwärtig genutzter Klassen von Advanced Materials
- 2) Identifizierung von Relevanzkriterien zur Bewertung von Advanced Materials in Bezug auf vier verschiedene Dimensionen: Wissenschaft, Wirtschaft und Technologie, Risiko und Regulierung
- 3) Charakterisierung der identifizierten Klassen von Advanced-Materials in Form von Factsheets

Im Folgenden werden nach einer Beschreibung des methodischen Ansatzes die Ergebnisse der drei Teile der Analyse zusammengefasst.

#### Methodisches Vorgehen

Drei methodische Ansätze wurden verwendet, um den Bereich der Advanced Materials nach relevanten Materialtypen zu charakterisieren und zu überprüfen.

#### LITERATURRECHERCHE

Die Literaturrecherche gliedert sich in einen quantitativen und einen qualitativen Teil: Zunächst wurde eine quantitative bibliometrische Analyse durchgeführt, bestehend aus einer szientometrischen Recherche der Web of Science Core Collection und einer Netzwerkanalyse. Danach wurde eine qualitative Analyse ausgewählter Publikationen, Rezensionen und technischen Artikel zu Advanced Materials durchgeführt.

Ausgehend von der Annahme, dass die wissenschaftliche Aktivität ein Indikator für die Relevanz eines Materialtyps im Hinblick auf Forschung und Entwicklung ist, wurde eine Analyse der wissenschaftlichen Arbeiten durchgeführt, indem Schlüsselwörter aus fünf verschiedenen Kategorisierungen von Advanced Materials verwendet wurden, die aus Studien zum gesamten Bereich der Advanced Materials ermittelt wurden. Unter Verwendung der ermittelten Schlüsselwörter, sowohl einzeln als auch kombiniert, wurde eine szientometrische Analyse der Publikationen in der Web of Science Core Collection im Zeitraum von 2000 bis 2018 durchgeführt. Die Zunahme der Publikationszahlen im Web of Science zwischen 2000 und 2018 wurde untersucht. Unter Verwendung des jährlichen Anstiegs der Publikationszahlen als Hauptindikator für die Forschungstätigkeit, wurden die am stärksten wachsenden Forschungsbereiche in Bezug auf Advanced Materials ermittelt.

Für die Forschungsbereiche mit dem höchsten Anstieg der Publikationszahlen wurde eine qualitative Analyse durchgeführt, um die entsprechenden Materialtypen, ihre chemischen und physikalischen Eigenschaften, die potenziellen Anwendungen und die damit verbundenen Produktionsprozesse zu bestimmen.

Zur weiteren Charakterisierung des Feldes ergänzt eine Netzwerkanalyse der wissenschaftlichen Literatur zu Advanced Materials die szientometrische Analyse, um Schlüsselakteure und Beziehungen zwischen den relevantesten Schlüsselwörtern zu identifizieren. Die Netzwerkanalyse und die dadurch bestimmten verwandten Schlüsselwörter dienen als Ergänzung und Kontrolle für die in der quantitativen Literaturrecherche verwendeten Begriffe.

#### EXPERTENINTERVIEWS

Um weitere Perspektiven zu Advanced Materials und zur Relevanz der verschiedenen Materialtypen im Forschungsbereich zu erhalten, wurden Expertinnen und Experten befragt. Die Auswahl der Expertinnen und Experten erfolgte nicht systematisch, sondern berücksichtigte die aus der Literaturrecherche ermittelten relevantesten Autorinnen und Autoren wissenschaftlicher Publikationen sowie Expertinnen und Experten mit einem erwarteten breiten Überblick über das Gebiet. Wissenschaft, Behörden und Industrie wurden abgedeckt, wobei der Schwerpunkt auf EU-Akteuren lag.

#### ONLINE-UMFRAGE

Mittels einer Online-Umfrage wurde Feedback von Expertinnen und Experten zu ausgewählten Advanced Materials erbeten. In der Umfrage wurde v.a. die Nützlichkeit und Anwendbarkeit verschiedener Kriterien zur Ermittlung der Relevanz bestimmter Advanced Materials in den Vordergrund gestellt. Darüber hinaus sollte die Umfrage zur Informationsgewinnung in Bezug auf die spezifischen Klassen der Advanced Materials beitragen. Die Ergebnisse der Umfrage wurden zur Weiterentwicklung der Factsheets und zur Ausarbeitung von Kriterien für die Relevanzbewertung verwendet.

#### Strukturierung des Untersuchungsbereichs

Eine auch in der EU diskutierte Definition von Advanced Materials stammt aus dem Jahr 2013:

"An advanced material is any material that, through the precise control of its composition and internal structure, features a series of exceptional properties (mechanical, electric, optic, magnetic, etc.) or functionalities (self-repairing, shape change, decontamination, transformation of energy, etc.) that differentiate it from the rest of the universe of materials; or one that, when transformed through advanced manufacturing techniques, features these properties or functionalities."<sup>1</sup> (Europäische Kommission 2013, S. 25)

Diese Beschreibung zeigt, wie umfassend die Definition von Advanced Materials sein kann. Hierdurch werden fast alle Bereiche der Werkstoffentwicklung abgedeckt. Daneben gibt es in neueren Studien auf diesem Gebiet auch verwandte Konzepte für Advanced Materials. Aus fünf dieser Studien (Europäische Kommission 2013; Lukassen und Meidell 2007; National Institute of Standards and Technology 2010; Materials Science and Engineering Expert Committee 2013; Technology Strategy Board 2008) wurden Klassifikationen von Advanced Materials identifiziert, die teilweise dieselben Klassen abdecken, sich aber auch stark unterscheiden. Sechs Klassen von Advanced Materials, die in Tabelle 1 dargestellt sind, sind von diesen Klassifikationen abgeleitet. Für die erste quantitative Literaturrecherche wurden stoffunabhängige Schlüsselwörter verwendet, die sich entweder auf die Aktivität (Funktionalität), die Struktur oder den Herstellungsprozess beziehen, sowie deren Synonyme (in der Tabelle kursiv dargestellt).

Bezeichnung	Synonyme	Beschreibung					
Aktive Materialien	Intelligent, funktional, multifunktional, anpassungsfähig	Aktive Materialien sind imstande mindestens eine ihrer Eigenschaften als Reaktion auf einen externen Parameter zu modifizieren					
Verbund- werkstoffe	Hochentwickelte Verbundwerkstoffe	Verbundwerkstoffe stellen Kombinationen von zwei ode mehr Materialien dar					
Strukturwerkstoffe	Strukturierte Materialien, multi- strukturell, künstlich strukturiert	Strukturmaterialien werden in zwei oder drei Dimensionen strukturiert					
Nanomaterialien	Nanotechnologie	Mindestens eine Dimension der Nanomaterialien liegt im Bereich von 1 bis 100 Nanometer					
Biobasierte Materialien	Biomaterials	Biobasierte Materialien werden entweder in einem biologischen System angewendet oder entstammen ein biologischen Quelle					
Fortgeschrittene Herstellung	Fortgeschrittene Verarbeitung	Fortgeschrittene Herstellung basiert auf dem Hinzufügen oder Entfernen von Material durch virtuelle Geometrie, ohne die Verwendung von Vorformen und ohne Materialabzug					

Fabelle 1: Bezeichnungen von Materialklassen, die aus den Klassifikationen der Advanced
Materials abgeleitet sind. Kursive Begriffe wurden in ihrer englischen Übersetzung
als Schlüsselwörter in der szientometrischen Analyse verwendet.

<sup>&</sup>lt;sup>1</sup> "Advanced Materials sind alle Materialien, die durch die genaue Kontrolle ihrer Zusammensetzung und inneren Struktur eine Reihe außergewöhnlicher Eigenschaften (mechanische, elektrische, optische, magnetische usw.) oder Funktionalitäten (Selbstreparatur, Formänderung, Dekontaminierung, Energieumwandlung usw.) aufweisen, durch die sie sich vom Rest des Werkstoffuniversums unterscheiden, oder die, wenn sie durch fortgeschrittene Herstellungsverfahren umgewandelt werden, diese Eigenschaften oder Funktionalitäten aufweisen." (eigene Übersetzung)

Die Gesamtergebnisse der szientometrischen Analyse weisen auf eine zunehmende Forschungsaktivität im Bereich der Advanced Materials hin. Neben der hohen Vielfalt an Materialtypen, die sich bereits in der Anzahl der Schlüsselwörter aus den Studien zu Advanced Materials widerspiegelte, wurde eine enge Verbindung zum Bereich der Nanomaterialien festgestellt. Die meisten für den Bereich der Advanced Materials relevant erscheinenden Klassen, gehören zum Typ Verbundwerkstoff. Es wurde festgestellt, dass die Dimensionen *Struktur, Funktionalität* und *Herstellung* eine bedeutende Rolle bei der Definition von Werkstoffen als Advanced Materials spielen.

Im Hinblick auf eine Trennung von Advanced Materials von anderen Materialbereichen bleiben die meisten der bisher vorgestellten Definitionen zeitabhängig mit dem Fokus auf neue oder verbesserte Eigenschaften und der daraus resultierenden (derzeit) herausragenden Leistungsfähigkeit (Kennedy et al. 2019). Eine Orientierung am Designprozess stellt hier einen zeitunabhängigen Ansatz für die Definition dar. Wie bereits durch eine frühere Studie angedeutet, könnten Advanced Materials als rational konzipierte "maßgeschneiderte Materialien" angesehen werden, deren Eigenschaften auf eine bestimmte Anwendung ausgerichtet sind (U.S. Congress 1988). Dabei kann das *rationale Design* zwei Dimensionen berücksichtigen: eine vorgegebene Anordnung neuer Strukturen durch eine Zusammensetzung aus entweder unterschiedlichen Materialien oder unterschiedlichen Strukturen.

Für eine weitere quantitative Charakterisierung des Bereichs wurden die meistzitierten Schlüsselwörter zur Beschreibung von Funktionalität, Struktur und Herstellung, die in den fünf oben erwähnten Studien ermittelt wurden, mit Schlüsselwörtern für verschiedene Materialklassen verknüpft. Tabelle 2 zeigt, welche Phrasen für die Abfrage verwendet wurden. Vernachlässigt wurden alle Schlüsselwortkombinationen, die in jedem Jahr zwischen 2000 und 2018 weniger als zehn Publikationen aufwiesen (ohne Wert "NV"). Blaue Felder verweisen auf eine starke Zunahme der Publikationszahlen in diesen 19 Jahren. Vor allem nanorelevante Schlüsselworte, aber auch Biomaterialien und weiche Materialien zeigen eine steile Zunahme. Insgesamt zeigen die funktionalitätsbezogenen Begriffe über den gesamten Analysezeitraum eine deutliche Zunahme. Gelb zeigt eine starke Zunahme in den letzten vier Jahren an. Für die Schlüsselwortkombination Elastomer und Funktionswerkstoffe wurde die stärkste Zunahme von 2015 bis 2018 ermittelt.

#### Tabelle 2: Anstieg (in Prozent) der Anzahl von Publikationen in WoS für die Kombination von Schlüsselwörtern für Funktionalität, Struktur und Herstellungsprozess (Spalte) UND Schlüsselwörter für Materialtypen (Zeile)

	"Funktionswerk stoffe"19 J	"Funktionswerk stoffe"4 J	"Aktive Materialien"19 J	"Aktive Materialien"4 J	"Intelligente Materialie" 19 J	"Intelligente Materialie " 4 J	"Strukturwerkstoffe " 19 J	"Strukturwerkstoffe " 4 J	"Fortgeschrittene Herstellung"19 J	"Fortgeschrittene Herstellung" 4 J
"Glas*"	4,8%	5,5%	4,1%	14,8%	5,2%	3,6%	2,9%	15,9%	NV	NV
"Keramik*"	3,9%	13,2%	3,3%	11,3%	2,1%	0,0%	2,5%	19,7%	NV	NV
"Polymer*"	4,9%	13,6%	4,8%	10,3%	4,7%	11,3%	3,3%	15,9%	NV	NV
"Metall*"	4,4%	16,6%	4,6%	13,0%	3,9%	12,7%	3,4%	7,5%	3,4%	20,4%
"Elastomer*"	3,8%	27,0%	4,8%	12,7%	4,2%	24,4%	3,1%	-5,0%	NV	NV
"Legierung*"	3,9%	16,8%	3,6%	-10,0%	4,2%	-0,6%	3,5%	10,2%	2,9%	10,6%
"Beschichtung*"	4,0%	18,3%	5,0%	12,2%	4,7%	5,9%	3,2%	23,4%	NV	NV
"elektroaktiv"	NV	NV	NV	NV	NV	NV	NV	NV	NV	NV
("elektronisch*" or "elektrisch*")	4,4%	15,7%	4,9%	13,1%	4,1%	9,0%	3,0%	19,6%	2,2%	15,3%
"fotoaktiv*"	4,5%	19,0%	NV	NV	NV	NV	NV	NV	NV	NV
"selbstreparierend"	NV	NV	NV	NV	NV	NV	NV	NV	NV	NV
"Textil*"	4,6%	31,8%	3,4%	23,9%	NV	NV	NV	NV	NV	NV
"Faser*"	NV	NV	NV	NV	2,6%	-10,8%	NV	NV	NV	NV
"zellulär*"	4,9%	-1,8%	NV	NV	NV	NV	2,2%	17,0%	NV	NV
"Gele*"	4,7%	15,3%	NV	NV	4,8%	12,5%	NV	NV	NV	NV
"Schaumstoff*"	4,2%	25,9%	4,8%	11,9%	4,2%	13,0%	3,7%	20,0%	NV	NV
"weiches Material*"	5,3%	1,7%	NV	NV	3,3%	23,0%	NV	NV	NV	NV
"Nano*"	5,1%	13,3%	5,3%	10,0%	4,6%	12,1%	4,6%	15,0%	3,0%	10,0%
"Nano-Partikel*"	5,6%	9,9%	5,2%	10,4%	4,9%	16,6%	5,7%	16,2%	NV	NV
"Nano-Material*"	4,2%	15,1%	4,8%	10,0%	3,4%	26,7%	NV	NV	NV	NV
"biobasiert*"	NV	NV	NV	NV	NV	NV	NV	NV	NV	NV

	"Funktionswerk stoffe"19 J	"Funktionswerk stoffe"4 J	"Aktive Materialien"19 J	"Aktive Materialien"4 J	"Intelligente Materialie" 19 J	"Intelligente Materialie " 4 J	"Strukturwerkstoffe "19 J	"Strukturwerkstoffe " 4 J	"Fortgeschrittene Herstellung"19 J	"Fortgeschrittene Herstellung" 4 J
"organisch*"	4,9%	13,5%	4,7%	13,5%	3,6%	14,3%	3,5%	15,0%	NV	NV
"Bio-Material*"	5,1%	11,6%	NV	NV	5,0%	22,7%	NV	NV	NV	NV

Die Begriffe und Begriffskombinationen wurden in ihrer englischen Übersetzung für die Literaturanalyse verwendet. Die blau schattierten Felder zeigen die normierte Zunahme innerhalb der 19 Jahre (2000 - 2018, dunklere Schattierungen für höhere Werte), die gelb schattierten Felder zeigen die normierte Zunahme innerhalb von 4 Jahren (2015 - 2018, dunklere Schattierungen für höhere Werte). NV= ohne Wert für vernachlässigbare Kombinationen; Daten aus WoS Core Collection, Juli 2019.

Im Weiteren wurden 62 Artikel (hauptsächlich Reviews) qualitativ analysiert, die anhand der Ergebnisse der quantitativen Analyse der Forschungstätigkeit (s. Tabelle 2) ausgewählt wurden. Es wurden nur Publikationen für die Schlüsselwortkombinationen mit dem höchsten Anstieg der Publikationszahlen ausgewählt. Die Analyse zeigte, dass die Anwendungsbereiche unter Berücksichtigung der Advanced Materials recht vielfältig sind. Die wichtigsten identifizierten Branchen sind medizinische Anwendungen/Pharmazeutika, Elektronik (insbesondere Energiespeicherung und Sensoren) sowie der Baubereich. Polymere scheinen auf dem Gebiet der Advanced Materials eine wichtige Rolle zu spielen. Im Hinblick auf ihre Funktionalität werden insbesondere Materialien, die eher klein, anpassungsfähig (oder sogar aktiv) oder flexibel sind, häufig diskutiert. Fast alle Materialien, die in den analysierten Publikationen erwähnt werden, stellen eine Kombination aus mehreren verschiedenen Stoffen dar. Abbildung 1: Schlüsselwörter von Publikationen, die "Advanced Materials" entweder im Titel, im Abstract oder in der Verschlagwortung verwenden



Die Größe der Wörter und Punkte steht für die jeweilige Anzahl der Artikel. Blau zeigt eine hohe Anzahl von Zitaten für die abgerufenen Artikel an, rot eine geringe Anzahl von Zitaten. Schlüsselwörter, die weniger als dreimal vorkamen, werden vernachlässigt. Daten aus der Web of Science Core Collection, Juli 2019. Quelle: eigene Darstellung

Des Weiteren wurde eine Netzwerkanalyse zum Schlüsselwort "Advanced Materials" im Web of Science durchgeführt, um verwandte Schlüsselwörter und Autorinnen und Autoren sowie deren Beziehungen zueinander zu untersuchen. Es wurden 13.471 Publikationen identifiziert. Die Netzwerkanalyse zeigte eine multizentrische Autorenlandschaft mit einer Hauptautorengruppe, die aus Wissenschaftlerinnen und Wissenschaftlern aus China und den USA besteht. Auch in Europa gibt es laufende Forschungsaktivitäten mit einer ziemlich breiten Vielfalt von Autorinnen und Autoren, Institutionen und Themen. Abbildung 1Fehler! Verweisquelle konnte nicht gefunden werden. zeigt die in den Publikationen verwendeten Schlüsselwörter und ihre Verbindung in Bezug auf ihr Auftreten in diesen Publikationen. Die Größe der Punkte zeigt die Publikationsanzahl an, während die Größe der Linien zeigt, wie oft die Schlüsselwörter in Kombinationen verwendet werden. Neben den Schlüsselwörtern, die sich auf Nanotechnologie beziehen, fallen die Begriffe Komposit, Selbstorganisation, Mikrostruktur, mechanische Eigenschaften, Biomaterial, Polymer und Graphen auf. Die Karte bestätigt die Erkenntnisse aus der szientometrischen Analyse. Unerwartet war lediglich das häufige Auftreten des Begriffs Selbstorganisation (self-assembly), da dieser bei der quantitativen Literaturrecherche unbeachtet blieb.

#### Relevanzbewertung

Relevanz wird in diesem Bericht verstanden als:

- Hinweis auf mögliche Risiken,
- Ein Mangel an Informationen zu Risiken,

- Eine fehlende regulatorische Abdeckung der Materialien in ihren (beabsichtigten) Anwendungen oder der Umsetzung und Durchsetzung der jeweiligen Anforderungen,
- Mangelnde Anwendbarkeit von Risikobewertungsansätzen und -instrumenten oder
- Umweltaspekte.

Da die oben genannten Aspekte nur auf potenzielle Herausforderungen, aber nicht notwendigerweise auf ein "Bedenken" in Bezug auf die Chemikaliensicherheit hinweisen, wird der Begriff "Relevanz" verwendet, um zu verdeutlichen, dass Gründe dafür vorliegen, Advanced Materials im weiteren Vorgehen zu priorisieren.

Die Vielfalt und Komplexität der Advanced Materials und ihrer Anwendungen erfordert es, verschiedene Perspektiven einzunehmen und verschiedene Aspekte zu behandeln, um die "Relevanz" der Advanced Materials zu ermitteln. Es werden vier Dimensionen der Relevanz vorgeschlagen:

- *Wissenschaftliche Dimension*: Neuartigkeit der Eigenschaften (quantitative Veränderungen und/oder neue Kombination von Eigenschaften),
- *Wirtschaftliche und technische Dimension:* Potenzial der Advanced Materials, um erfolgreich auf den Markt zu gelangen und/oder Innovationen auf Prozess- oder Produktebene auszulösen,
- *Gefahren- und Risikodimension*: Hinweise auf gefährliche Eigenschaften oder ein hohes Expositionspotenzial,
- *Regulatory dimension*: Mangel an gesetzlicher Abdeckung und/oder fehlende Möglicheiten mögliche Gefahren- oder Risiken zu bewerten.

Abbildung 2 zeigt die vier Dimensionen des vorgeschlagenen Ansatzes zur Relevanzbewertung und die Kernfragen, die mit den Informationen in diesem Bereich beantwortet werden können.

#### Abbildung 2: Überblick über die vier Dimensionen der Relevanzbewertung (eigene Darstellung)

Was sind die wirtschaftlichen und technischen Potenziale eines Advanced Materials? Welche Funktionen könnte es erfüllen, wie könnte es zur nachhaltigen Entwicklung beitragen? Wirtschaft, Technologie Welche gefährlichen Eigen-Funktionalität schaften treten auf? Anwendung In welchem Ausmaß sind Mensch und Umwelt exponiert?? Wissen-Neue Gefahren Risiko Eigenschaften Exposition schaft Auf welche AdMas konzentriert sich die Wissenschaft? Geltungsbereich Welche Eigenschaften und Instrumente "Effekte" sind für F&E wichtig? Regulation Werden Advanced Materials (ausreichend) durch die Definitionen/Anwendungsbereiche der Gesetzgebung abgedeckt? Sind die Instrumente und Methoden des Risikomanagements (ausreichend) anwendbar?



Neben diesen vier Dimensionen einer Relevanz können zusätzliche Kriterien in Betracht gezogen werden, die die ökologischen und gesellschaftlichen Auswirkungen der Verwendung von Advanced Materials betreffen. Diese könnten sich u.a. auf das Recyclingpotenzial der Advanced Materials beziehen.

Für jede der vier Dimensionen werden mögliche Relevanzindikatoren identifiziert und es wird diskutiert, welche Art von Schlussfolgerungen aus einem Indikator gezogen werden könnten, ob die entsprechenden Informationen voraussichtlich verfügbar sein werden und welche praktischen Herausforderungen bei ihrer Verwendung zu bewältigen sind. Auf der Grundlage dieser Bewertung werden einige dieser Kriterien und die sie konkretisierenden Indikatoren vorgeschlagen, die für eine erste Relevanzprüfung von Advanced Materials bezüglich der Chemikaliensicherheit verwendet werden könnten um die auf diesem Wege identifizierten Materialien für eine weitere Bearbeitung zu priorisieren.

#### Identifizierung kritischer Bereiche der Advanced Materials und Beschreibung relevanter Materialien in Factsheets

26 Klassen von Advanced Materials, die entweder in den Publikationen des Forschungsgebietes häufig Erwähnung finden oder von Expertinnen und Experten als Advanced Material angesehen werden, wurden in den Factsheets beschrieben und bewertet (vgl. separates <u>Dokument</u>). Sie sind ein erster Ansatz, um einen Überblick über den Bereich der Advanced Materials zu gewinnen und Informationen über ihre jeweiligen Anwendungen sowie mögliche Risikopotenziale und Regelungslücken zusammen zu stellen. Die Klassenbildung soll die Analyse und Bewertung von Gemeinsamkeiten verschiedener Materialklassen hinsichtlich der Relevanzkriterien unterstützen.

Die folgenden (sich teilweise überschneidenden) acht Klassen von Advanced Materials wurden in diesem Projekt mittels Factsheets beschrieben.

- 1. Biopolymere (Materialien auf der Basis natürlich vorkommender Polymere, die für eine bestimmte Funktionalität ausgelegt sind)
  - a. DNA-basierte Biopolymere
  - b. RNA-basierte Biopolymere
  - c. Protein-basierte Biopolymere
  - d. Biopolymere auf Zuckerbasis
  - e. Lipid-basierte Biopolymere
- 2. Verbundwerkstoffe (Kombination aus zwei oder mehr Materialien)
  - a. Makroskopische Verbundwerkstoffe
  - b. Hybridmaterialien (Materialien, die eine Kombination aus organischen und anorganischen Materialien sind)
  - c. Faserverstärkte Verbundwerkstoffe
  - d. Partikelverstärkte Verbundwerkstoffe
- 3. Poröse Materialien (Materialien, die eine poröse Struktur aufweisen, differenziert nach Porengröße)
  - a. Mikroporöse Materialien
  - b. Mesoporöse Materialien
  - c. Makroporöse Materialien
- 4. Metamaterialien (Materialien mit Eigenschaften, die über die natürlich vorkommenden Eigenschaften ihrer Bestandteile hinausgehen)
  - a. Elektromagnetische Metamaterialien
  - b. Akustische Metamaterialien
- 5. Partikelsysteme (Eigenschaften der Materialien hängen mit der Struktur ihrer Partikel zusammen)
  - a. Quantenpunkte
  - b. Suprapartikel
  - c. Nanoblumen
  - d. Graphen
- 6. Fortschrittliche Fasern (Fasern mit einem Durchmesser von mehreren μm oder kleiner mit gewünschter Funktionalität)
  - a. Organische Fasern
  - b. Fasern auf Kohlenstoffbasis (einschl. CNTs)
  - c. Anorganische Fasern (z.B. Kieselsäure)
- 7. Fortschrittliche Polymere (Polymere mit gezielt hergestellter Funktionalität)
  - a. Elektroaktive Polymere
  - b. Magnetoaktive Polymere
  - c. Selbstreparierende Polymere

- d. Co-Polymere
- 8. Fortschrittliche Legierungen (Legierungen, die aus mehr als zwei Komponenten bestehen; mindestens zwei Komponenten haben einen großen Anteil am Endmaterial)
  - a. Fortschrittliche Legierungen

Abschließend werden die wichtigsten Ergebnisse der Factsheets zusammengefasst: Viele Advanced Materials enthalten (öko-)toxische Stoffe, die mit anderen Stoffen kombiniert sind. In der analysierten Literatur ist oftmals unklar, wie stabil die Verbindungen zwischen diesen Stoffen (Bausteinen) sind. Es ist daher unklar, in welchem Umfang diese (öko-)toxischen Stoffe freigesetzt werden und zu Expositionen, die Gesundheits- oder Umweltrisiken verursachen, führen könnten. Neben der (Öko-)Toxizität der Bausteine können weitere Gefährdungen mit der Struktur der Materialien zusammenhängen. Kritische Morphologie (z. B. Fasern), Reaktivität oder Partikelgröße (z. B. Nanokomposite) können zu Gefahren und Risiken führen, auch wenn die Stoffe/Bausteine selbst nicht gefahr- oder risikorelevant sind.

Darüber hinaus kann das Risiko durch besondere Expositionsbedingungen weiter erhöht werden, z. B. durch Persistenz oder ubiquitäre Anwendung mit Freisetzungen in die Umwelt und Aufnahme in den Körper. Beispielsweise bestehen für Materialien wie DNA-basierte Biopolymere hohe Unsicherheiten hinsichtlich ihrer Persistenz in verschiedenen Ökosystemen sowie im menschlichen Körper. Dies kann eine Risikorelevanz induzieren, da die Reaktion des Immunsystems des menschlichen Körpers wie auch anderer lebender Organismen unbekannt ist.

Bei einigen Advanced Materials ist es nicht offensichtlich, welche rechtliche Definition sie erfüllen (Stoff, Gemisch, Erzeugnis usw.). Daher sind der Geltungsbereich von REACH und die damit verbundenen Anforderungen zur Generierung von Daten für diese Materialien nicht vollständig klar. Andere Materialien, wie z. B. diejenigen fortschrittlichen Polymere, welche auch die rechtliche Definition von Polymeren erfüllen, können von der Registrierung unter REACH ausgenommen werden. Hier ist neben spezifischem Wissen über die Zusammensetzung und die molekulare Bindung zwischen den Bausteinen eine gemeinsame und allgemein akzeptierte Interpretation der rechtlichen Definitionen notwendig, um zu einem Ergebnis zu kommen.

Ein weiterer Grund für die Relevanz von Advanced Materials ist ihre potenziell fehlende Recyclingfähigkeit. Mehrere Klassen von Advanced Materials bestehen aus sehr unterschiedlichen Bausteinen, die auf molekularer Ebene miteinander verbunden sind und nicht mehr getrennt werden können. Dies kann insbesondere bei Hybriden und Nanokompositen sowie Metamaterialien der Fall sein. Dadurch kann das Recycling problematisch werden.

Die meisten der identifizierten Advanced Material Typen befinden sich noch im Entwicklungsstadium. Es ist noch unklar, in welchen Produkten und in welchen Mengen sie verwendet werden, was eine Abschätzung der potenziellen Expositionen schwierig macht. Einige sind jedoch bereits auf dem Markt, auch wenn risikobezogene Fragen noch unbeantwortet sind (z. B. die Anwendung mikroporöser Materialien in Produkten des Gesundheitswesens).

# **1** Introduction and aim of the study

Innovations can be divided into several stages from a first relevant discovery in basic research to applied research, via the development of a prototype to the final product. With progressing stages path dependencies increase and options to correct e.g., in terms of risk prevention become more expensive and difficult to enforce.

If the regulatory framework is adapted, established applications and corresponding infrastructure may have to adapt to new rules that may limit the possibilities of implementing or continuing the use of an innovation. Moreover, with a view to potentially long lasting impacts of late action e.g., as visible for organic pollutants (Bettinetti 2016), it is an urgent necessity to accompany innovation processes already in the first stages by a prospective analysis of potential risk relevant aspects of a new technology.

However, prospective technology assessment is confronted with uncertainty about the nature of possible application contexts and thus also vague knowledge about critical stages during the phases of manufacturing, use and end-of-life. Prospective technology assessment therefore tends to gain orientation from the investigation of general qualities of the technology which most probably will determine the hazard or exposure potential in later applications. These qualities can be assessed by criteria for concern or relief. The early governance of nanotechnology is a prime example for an accompanying process where respective criteria have been derived from an investigation of the hazard and exposure-relevant qualities of the technology (Reihlen and Jepsen 2012).

Besides the benefits of the nanoscale with ongoing progress in materials science, new promising opportunities with regard to the design or the combination of condensed matter appeared in the horizon. Here at first glance, "advanced materials" seem to play a role as an umbrella term for the development of outstanding performance and new functions. Some of these new techniques, as e.g., supraparticles make use of nanomaterials as a basis for new combinations whose scale is above the nanoscale (cp. Wintzheimer et al. 2018). Others, e.g. metamaterials, can be totally independent of nanostructures (Kadic et al. 2019). The present study is dedicated to an analysis of these new developments in order to identify new materials that might have a significant impact on science, technology and economy on the one hand and bear a risk potential and/or are not yet covered by regulation on the European level.

This study aims at providing an overview of advanced materials and potential needs to act on chemical safety. The core addressees of the work are regulators and national authorities. However, also other stakeholders were involved in the project work and all stakeholders interested in advancing their knowledge of and involvement in discussions on advanced materials may use the information.

In order to ensure involvement of stakeholders, three thematic conferences were conducted during the project. The first conference took place in December 2019 in Dessau, Germany and was dedicated to discussing the need and options for defining advanced materials and differentiating them into distinct clusters as well as providing more in-depth information on distinct types of advanced materials, such as supraparticles or biopolymers. Information provided in presentations and obtained during the discussion is included into this report.

The current report is based on a literature search and analysis, expert interviews, an online survey and presentations and discussions at a national stakeholder workshop on advanced materials as well as an international conference conducted in the context of the study. Information from these activities is compiled in three different forms:

- a) a detailed description of the methodology and outcomes of the literature analysis (Section 2 and Section 3)
- b) an introduction to and discussion of potential criteria to assess the relevance of advanced materials (Section 4) and a proposal of criteria set for an initial priority setting regarding the relevance of advanced materials and
- c) an introduction to a possible clustering of advanced materials (Section 5) complemented by a number of factsheets exemplifying how the various advanced material types could be characterised (cf. separate background document)

# 2 Methodological approach

### 2.1 Literature research

It is assumed that a broad majority of scientists publish their results and thereby scientific literature represents scientific activity (Merton 1942). Therefore, a structured bibliometric analysis was conducted at the beginning of the project to identify and structure the field of investigation of "advanced materials". The bibliometric analysis contained a quantitative literature research and a network analysis. Additionally, in a qualitative analysis of identified publications, reviews and technical articles on advanced materials have been examined.

The identification of relevant keywords for search queries is the most important step in a bibliometric analysis. For that purpose, meta-studies comprising classifications of advanced materials were used to identify keywords related to the field of investigation. Five different classifications were examined. All terms for material classes of these five categorizations of advanced materials were used in the first query to keep the focus of the initial query as open as possible.

Using the identified keywords separately and combined, a scientometric analysis of publications in the WoS Core Collection between 2000 and 2018 was conducted. The WoS Core Collection contains over 21,100 peer-reviewed journals published worldwide (including Open Access journals) in over 250 disciplines (Web of Science Group 2019). For all queries the search field "topics" was used, which refers to all publications with the keyword in the title, abstract, the author keywords or the KeyWords Plus®<sup>2</sup>. In the query results no document types have been excluded. The results consist mainly of articles and reviews, but also meeting abstracts, proceeding papers and other types of documents. The increase in the number of publications in WoS within 2000 and 2018 as well as between 2015 and 2018 with regard to the dimensions 'structure', 'functionality' and 'manufacturing' as well as different material types were investigated. Using the number of publications per year and their positive slope over different time periods as the main indicators for progress, the most emerging research areas with regard to advanced materials were identified.

For the research areas with the highest increase of publication numbers, a qualitative research was conducted to identify the involved materials, their chemical and physical qualities, potential applications and associated production processes. Sixty-two recent articles were examined.

Further, a network analysis of the WoS results for the term "advanced materials" in the search field "topics" (see above) was conducted to identify key actors and their related keywords. The identified keywords of authors serve as complement and control for the terms used in the quantitative literature research. In contrast to the bibliometric analysis, no time period was enclosed, but all available publications were used. The network analysis is a visualization of two different indicators: Keywords or authors are shown as "Nodes" whose size indicates the number of their occurrence within the query results. "Edges", shown as lines of different width, indicate a connection between authors or resp. and keywords. A connection is assumed, if authors or keywords appear in the same publication.

## 2.2 Expert interviews

A number of experts were interviewed to obtain additional qualitative information on the initial findings of the literature analysis and the relevance of advanced materials in general. The

<sup>&</sup>lt;sup>2</sup> According to Web of Science KeyWords Plus® in addition to the author keywords contain relevant words and phrases from the titles of the cited articles. KeyWords Plus are selected by editors of Web of Science.

selection of contacted experts was not systematic but considered a) the most relevant authors of scientific publications identified from the literature research, b) experts with an expected broad overview of the field and which were (partly) already known to the consultants and where access was therefore easier, c) coverage of academia, authorities and industries as well as focus on EU actors. The selection of the interviewed experts finally depended on their interest in contributing to the present study.

A brief and rather open interview guideline was developed, but the actual content of the interviews very much depended on the background of the expert. The interviews contributed to structuring the field at a fundamental level, as well as to preparing the online survey and collecting ideas for the first conference.

# 2.3 Online survey

The aim of the online survey was to obtain expert feedback on the clustering approach developed by the project team and the usefulness and applicability of various criteria to identify the relevance of particular advanced materials. In addition, the survey should contribute to information collection on the specific advanced materials and hence feed into the respective fact sheets (cf. separate document).

The questions were structured into four sections (for the complete set of questions see Appendix A):

- 1. General information on the person/institution
- 2. Questions to assess the usefulness of various relevance criteria;
- 3. Questions on the project approach of clustering of advanced materials
- 4. Questions to collect information on specific types of materials

An invitation to participate in the survey was sent to all persons and institutions identified as relevant during the project, including participants to the first thematic conference. In addition, invitations were sent to the OECD WPMN as well as competent authorities at EU level.

The survey was launched February 12 and remained open for 3 weeks. Thirty-one persons answered the survey. The majority of answers was provided by public authorities (45 %) followed by industry and academia (both around 20 % of the answers). Answers were received from 6 EU Member States, the UK, the US and EU institutions. The responses to the specific types of advanced materials were used to further develop the factsheets. A brief summary of the responses to the general questions of the survey is provided in Appendix B.

## 2.4 Development of factsheets

A central aim of the project was to structure the field of advanced materials in order to enable authorities and other stakeholders to get a better overview and prioritise advanced materials that might cause a concern.

Based on the information collected from the above described activities, factsheets were developed to present that information in a standardised and structured form. Thereby it is available as a discussion input to the further thematic conferences. The factsheet development was an iterative process concerning both the clustering of advanced materials and the structure and information content to characterise them. While the clusters were partly discussed with an international audience at the first thematic conference, the structure of the factsheets was discussed only within the project team and UBA. A more detailed introduction to the factsheets is included in Section 5.
# 3 Structuring the field of investigation "advanced materials"

In recent years some approaches on defining and structuring advanced materials have already been published. In the European "Support for 3<sup>rd</sup> regulatory review on nanomaterials" a first effort on defining and systematically categorising advanced materials for EU regulation is presented. The review gives an overview on six definitions differing essentially by focussing either on the product ("value-added"), the properties of the material ("superior" or "exceptional") or their R&D stage and sales volume (Broomfield et al. 2016). Romanow and Gustafsson (2012) propose a further differentiation and define "value added materials"<sup>3</sup> as a part of advanced materials.

A broad definition of advanced materials, currently used by the EU dates back to 2013:

"An advanced material is any material that, through the precise control of its composition and internal structure, features a series of exceptional properties (mechanical, electric, optic, magnetic, etc.) or functionalities (self-repairing, shape change, decontamination, transformation of energy, etc.) that differentiate it from the rest of the universe of materials; or one that, when transformed through advanced manufacturing techniques, features these properties or functionalities." (European Commission 2013, p.25)

By investigating categorisations of advanced materials, Broomfield et al. (2016) conducted a strength and weakness analysis of four different categorizations by considering the following points: Clear classification, sufficient key characteristics, unique material categorization, internationally consistent, and future-proof. Even though none of the categorizations was able to fulfil all criteria, the categorization of the DAMADEI report (European Commission 2013) was favoured by the authors. To avoid misleading or incomplete results due to an inappropriately narrow perspective in the early steps of the investigation, all existing categorizations except DAMADEI are considered for a characterization of the field of advanced materials for the present analysis. The respective categorizations are presented in the following reports (of which TIP was not included in the meta-study by Broomfield et al. (2016)):

DAMADEI	European Comission (2013): Design and Materials As a Driver of European Innovation, European Union.
L&M	Lukassen and Meidell (2007): Advanced Materials and Structures and their Fabrication Processes. Narvik University College.
TIP	Technology Innovation Program (2010): Manufacturing and Biomanufacturing: Materials Advances and Critical Processes. National Institute of Standards and Technology. Gaithersburg, MD.
MatSEEC	Materials Science and Engineering Expert Committee (2013): Materials Science and Engineering in Europe: Challenges and Opportunities. Science Position Paper. Strasbourg, France.
TSB	Technology Strategy Board (2008): Advanced Materials Key Technology Area 2008-2011.

Despite the classifications for advanced materials differing a lot, they show some overlap by referring to similar material types, by partially using the same phrases and sometimes different

<sup>&</sup>lt;sup>3</sup> "Value added materials are products whose worth is based on their performance or functionality, rather than their composition." (Romanow and Gustafsson, 2012, p.17). According to Romanow and Gustafsson, if their worth becomes a function of the market, the material turns into a "commodity".

but closely related phrases (e.g. smart materials in L&M and active materials in DAMADEI). As identified by Broomfield et al. (2016), none of the classifications refer to unique material categories. Some categories are related to the composition of the material, some to their functionality and others to the production process of the respective material. Hence one material may fit in two or more categories (e.g. as a smart material and a nanomaterial). For the present approach, all categorizations are taken into account while overlapping categories are fused. Even though this procedure does not lead to a unique material categorization, it nonetheless supports a holistic view on the broad field of advanced materials and provides criteria for a first structuring. Based on the initial evaluation of classifications (see Table 3) a quantitative analysis of emerging materials within the research area was conducted.

# **3.1** Evaluation of classifications of advanced materials

In the first step of the literature research, previous existing classifications of advanced materials have been analysed. Table 3 represents a summary of the five different classifications. In all classifications listed in the right column, at least one of the synonyms listed in the second column or the name itself (first column) was an existing category of advanced materials. By aggregating all five classifications, six material clusters, shown in 3, were created: active materials, composites, structural materials, nanomaterials, biobased materials and advanced manufacturing.

	Synonyms	Description	Examples	Existing in classification of
Active materials	smart, functional, multifunctional, adaptive	active materials are able to modify any of their properties	alloys, coatings, electro active materials, photoactive materials, materials for targeted surface properties, which change surface functionality, self-repairing, Bio-inspired materials	DAMADEI, L&M, TIP, TSB, MatSEEC
Composites	advanced composites, composite materials,	composites represent combinations of two or more materials	Fibre + glass, polymers, Mixtures under REACH, polymer-matrix composites, natural fibres reinforcement, sandwich constructions	DAMADEI, L&M, TIP
Structural materials	structured materials, multi- structural, artificially structured	structural materials are structured in two or three dimensions	advanced textiles and fibres, cellular materials, gels and foams, light alloys, soft materials	DAMADEI, L&M, TSB, MatSEEC
Nano- materials	nanotechnology	at least one of the dimensions nanomaterials is in the range of 1 to 100 nanometres	carbon nanotubes	DAMADEI, L&M, TIP, TSB
Biobased materials	biomaterials	biobased materials either represent materials applied to a	high performance polymers reinforced with bio-fibres	TSB, MatSEEC

#### Table 3: Evaluation of classifications of advanced materials

	Synonyms	Description	Examples	Existing in classification of
		biological system or materials derived from a biological source		
Advanced manufac- turing	advanced processing	advanced manufacturing relies on adding or removing material through virtual geometry, without the use of pre-shapes and without subtracting material	shaping technologies, subtractive technologies, additive technologies	DAMADEI

Whereas the three clusters of composites, nanomaterials and biobased materials are related to the composition of the material, structural materials and active materials are related to the materials' characteristics, independent of the substances used. Advanced manufacturing, as a cluster of materials characterized by their production process, is also independent of the chemical composition of the material. These substance independent keywords related to activity (functionality), structure and additive manufacturing as well as their synonyms were used for the first quantitative literature research (Section 3.2).

In a second step of the quantitative literature research, material classes from the five classifications mentioned above are considered (Section 3.3). Next to these "new materials types", "advanced classics" are often mentioned in the classification reports. According to Lukassen and Meidell (2007) classical material types could be identified to cover glasses, ceramics, polymers, metals and elastomers.

# **3.2** Investigation of research activity with regard to the dimensions 'structure', 'functionality' and 'manufacturing'

Appropriate terms to characterise materials regarding their functionality, structure or manufacturing processes have been identified in the five classification reports of advanced materials (see Section 3.1) and the number of related publications between 2000 and 2018 was determined.

With regard to the **functionality** of advanced materials the terms, "active materials", "smart materials", "functional materials", "multifunctional materials" and "adaptive materials" have been identified and applied as keywords in a quantitative literature research. Figure 3 shows the increase in the number of publications per keyword between 2000 and 2018. The keyword "functional materials" shows the highest increase within this time period and reached 1,284 publications in 2018. "Active materials" also shows a high increase, especially after 2009, reaching 795 publications in 2018. "Smart materials" as well as "multifunctional materials" show a rather small increase until 2016. However, within the last three years the number of articles related to "smart materials" have strongly increased. The number of publications containing the keyword "adaptive materials" only increased slowly and never exceeded more than 23 publications per year.



Figure 3: Numbers of publications containing keywords on functionality in their title, abstract or keywords per year for the period of 2000-2018

Source: Own presentation, WoS Core Collection, June 2019

Regarding the **structure** of advanced materials the terms "structural materials", "structured materials", "multistructural materials" and "artificially structured materials" have been used as keywords for the bibliometric analysis. Figure 4**Fehler! Verweisquelle konnte nicht gefunden werden.** illustrates that the keyword "structural materials" is the most prominent term over the whole time period, yielding between 125 and 440 publications a year. Especially between 2016 and 2018 the number of publications containing this term increased strongly. The use of the keyword "structured materials" shows a slow, but steady increase with a maximum number of 121 publications in 2018. "Artificially structured materials" is used rather seldom and never exceeded more than 3 publications a year, whereas the keyword "multistructural materials" was never used.





Source: Own presentation, WoS Core Collection, June 2019

Focussing on the **manufacturing process**, the keywords "advanced manufacturing" and "advanced processing" could be identified from the classification reports. Figure 5 illustrates a heavy increase in the number of publications beginning in 2014 using the term "advanced manufacturing". In 2018, 160 publications contained the term in either their title, abstract or in the keywords. The term "advanced processing" in contrast, never retrieved more than 35 publications per year.



Figure 5 Numbers of publications per year containing keywords on manufacturing in their title, abstract or keywords for the period of 2000-2018

Source: Own presentation, WoS Core Collection, June 2019

As visible in Figure 3, Figure 4 and Figure 5, the numbers of publications for "active materials", "smart materials", "functional materials" as well as "structural materials" and "advanced manufacturing" show the highest increase in number of publications. Among these keywords "active materials" as well as "functional materials" show an average slope of > 20 over the period from 2000 to 2018. "Smart materials", "structural materials" and "advanced manufacturing" show an average slope of > 20 within the last four years.

As it is assumed that the increase in the number of publications indicates a presumably high relevance of these materials, in a second stage of the quantitative literature research the five keywords "active materials", "smart materials", "functional materials" as well as "structural materials" and "advanced manufacturing" are used in combination with terms related to "classical" and "new" material classes.

# **3.3** Quantitative identification of relevant material types with regard to the dimensions 'structure', 'functionality' and 'manufacturing'

In a combined search query, the selected keywords for functionality, structure and manufacturing of a material (cf. Section 3.2) were connected by "AND" with "new" materials types as well as "classical" material types (see Table 3). In advance, a search query combining the material types (classical and special) by AND with the general term "materials" was conducted. The types of classical materials are taken from literature, whereas the new material types are the ones identified in the five classification reports (cf. Section 3.1).

Type of material	Examples
Classical material types	glasses, ceramics, polymers, metals, elastomers
New material types	alloys, coatings, electro active materials, electronic materials, electric materials, photoactive materials, self-repairing materials, sandwich construction, cellular materials, gels, foams, light alloys, soft materials, nano, nanoparticle, nanomaterial, biobased, organic, biomaterial, bio-fibres, advanced textiles, advanced fibres

#### Table 4: Terms for material types used in the search query

To restrict the field of investigation to ongoing research and development activities which are relevant for advanced materials, all material classes with less than ten publications in each year between 2000 and 2018 were neglected in further screenings. As shown in Figure 6, the search query on the terms sandwich construction, light alloys, bio-fibre, advanced fibres and advanced textiles retrieved not more than ten publications per year. When the keywords "advanced fibres" and "advanced textiles" were shortened to "textile\*" and "fibre\*" for the combined search, a steep increase in the number of retrieved publications could be obtained. The keywords "sandwich construction", "light alloys" and "bio-fibre" were omitted in further steps of the analysis.

For the materials "electric\*" and "electronic\*" comparable numbers were obtained as well as a certain overlap in publications. Some 159,240 publications were found in a combined query ("electric\*" OR "electronic\*") and 173,673 if searched separately (results for "electric\*" added to results for "electronic\*"). Hence, these two types have been summed up in one type named ("electric\*" OR "electronic\*") for further searches.





Source: Own presentation, data from WoS Core Collection, June 2019

Therefore, in the combined query, five substance independent keywords and the remaining 23 material types from the preselection (Figure 6) were used for further examination. Their combination results in 115 search strings which enable a more differentiated analysis of the field (cp. Table 5).

For further examination, all combinations of material classes, with less than ten publications in every year between 2000 and 2018 were neglected. Thereby, the total number of search strings decreased from 115 to 67 combinations and its respective results. For all search strings neglected, no values (NV) are shown in Table 5.

For the remaining 67 results the average normalized slope of publications between 2000 and 2018 as well as the slope between 2015 and 2018 was calculated. The slope over the whole period from 2000 till 2018 (19 years) is shown by the first value in Table 5. The second value shows the normalized slope over the last four years from 2015-2018 (4 years). The search strings with the highest increase either in the whole time period (2000-2018) or in the last four years (2015-2018) were selected for a qualitative examination of the exact types of materials discussed in the respective papers.

# Table 5: Slopes (as percentage) of the number of publications in WoS for the combination of keywords for functionality, structure and manufacturing process (column) AND keywords for material types (row).

	"functional materials"19 yr	"functional materials"4 yr	"active materials" 19 yr	"active materials" 4 yr	"smart materials" 19 yr	"smart materials" 4 yr	"structural materials"19 yr	"structural materials"4 yr	"advanced manufacturing"19 yr	"advanced manufacturing"4 yr
"glass*"	4,8%	5,5%	4,1%	14,8%	5,2%	3,6%	2,9%	15,9%	NV	NV
"ceramic*"	3,9%	13,2%	3,3%	11,3%	2,1%	0,0%	2,5%	19,7%	NV	NV
"polymer*"	4,9%	13,6%	4,8%	10,3%	4,7%	11,3%	3,3%	15,9%	NV	NV
"metal*"	4,4%	16,6%	4,6%	13,0%	<mark>3,9</mark> %	12,7%	3,4%	7,5%	3,4%	20,4%
"elastomer*"	3,8%	27,0%	4,8%	12,7%	4,2%	<mark>24,4</mark> %	3,1%	-5,0%	NV	NV
"alloy*"	3,9%	16,8%	3,6%	-10,0%	4,2%	-0,6%	3,5%	10,2%	2,9%	10,6%
"coating*"	4,0%	18,3%	5,0%	12,2%	4,7%	5,9%	3,2%	23,4%	NV	NV
"electro active"	NV	NV	NV	NV	NV	NV	NV	NV	NV	NV
("electronic*" or "electric*")	4,4%	15,7%	4,9%	13,1%	4,1%	9,0%	3,0%	19,6%	2,2%	15,3%
"photo- active*"	4,5%	19,0%	NV	NV	NV	NV	NV	NV	NV	NV
"self-repairing"	NV	NV	NV	NV	NV	NV	NV	NV	NV	NV
"textile*"	4,6%	31,8%	3,4%	23,9%	NV	NV	NV	NV	NV	NV
"fibre*"	NV	NV	NV	NV	2,6%	-10,8%	NV	NV	NV	NV
"cellular*"	4,9%	-1,8%	NV	NV	NV	NV	2,2%	17,0%	NV	NV
"gels*"	4,7%	15,3%	NV	NV	4,8%	12,5%	NV	NV	NV	NV
"foam*"	4,2%	25,9%	4,8%	11,9%	4,2%	13,0%	3,7%	20,0%	NV	NV
"soft material*"	5,3%	1,7%	NV	NV	3,3%	23,0%	NV	NV	NV	NV
"nano*"	5,1%	13,3%	5,3%	10,0%	4,6%	12,1%	4,6%	15,0%	3,0%	10,0%
"nano- particle*"	5,6%	9,9%	5,2%	10,4%	4,9%	16,6%	5,7%	16,2%	NV	NV

	"functional materials"19 yr	"functional materials"4 yr	"active materials" 19 yr	"active materials" 4 yr	"smart materials" 19 yr	"smart materials" 4 yr	"structural materials"19 yr	"structural materials"4 yr	"advanced manufacturing"19 yr	"advanced manufacturing"4 yr
"nano- material*"	4,2%	15,1%	4,8%	10,0%	3,4%	26,7%	NV	NV	NV	NV
"biobased*"	NV	NV	NV	NV	NV	NV	NV	NV	NV	NV
"organic*"	4,9%	13,5%	4,7%	13,5%	3,6%	14,3%	3,5%	15,0%	NV	NV
"bio- material*"	5,1%	11,6%	NV	NV	5,0%	<mark>22,7</mark> %	NV	NV	NV	NV

The blue shaded backgrounds represent the normalized slope within 19 years (2000 – 2018, darker shades for higher values), the yellow shaded backgrounds represent the normalized slope within 4 years (2015 – 2018, darker shades for higher values). NV= no values for neglected combinations; data from WoS Core Collection, July 2019

Derived from the values in Table 5, regarding the **classical material classes** the combination of "smart materials" and "glass\*" shows the highest total increase in publications, followed by the combination of "functional materials" and "polymer\*". Concerning the **new material classes** the keywords "nano\*" and "nanoparticle\*" show a steep increase in nearly all combinations. Nevertheless, it was decided not to include the term in further steps of this study due to recent and ongoing efforts in risk assessment and risk management for engineered nanomaterials in the EU and Germany. For example ECHA is addressing the issue of "second generation nanomaterials" and whether they fit in REACH Regulation in a currently published report. They conclude that new methods of testing are necessary and that the development of OECD test guidelines is ongoing (ECHA 2019).

The combination of the keyword "soft material\*" and "functional materials" also presents a strong increase between 2000 and 2018, closely followed by the keyword "biomaterial" combined with "functional materials" as well as "smart materials". Further combinations taken into account due to their total slope over the whole time period of this analysis are the combination of "coating" and "active materials" with a normalized slope of 5 % and the combinations of "organic\*" or "cellular\*" and "functional materials" as well as ("electronic\*" or "electric\*") and "active materials" with a slope of 4,9 %, respectively.

The normalized slope within the last four years (2015 – 2018) was particularly taken into account to identify the currently emerging materials. The most successful keyword combinations for 2015-2018 differed greatly from the search strings that gave the best results for the overall period of analysis (2000 -2018). In this regard the combination of "textile\*" and "functional materials" as well as "textile\*" and "active materials" is remarkable: When considering the overall normalized slope for 2000-2018, textiles did not show a strong increase. For the combination of "textile\*" with "functional materials" our query obtained not even a single publication until 2008. However, within the last four years they show the highest normalized slope of all search strings.

In the cluster of new materials, the combinations of "foam\*" and "functional materials" as well as "soft material\*" and "smart materials" also yield a high increase in publication numbers within

the last four years in contrast to a rather modest increase when considering the whole time period. For the keyword "foam\*" the query obtained a high increase in publications within the last four years in combination with the term "structural materials". The combination of "biomaterial\*" and "smart materials" is the only search string showing a vast increase considering both normalized slopes: over the total time period as well as within the last four years. Regarding classical materials, the keyword "elastomer\*" in combination with "functional materials" as well as "smart materials" obtained the highest numbers of publications within the last four years.

There was no combination of keywords without an increasing number of respective publications over the total time period of the analysis. But for the last four years decreasing publication numbers have been observed. In particular for the combinations "alloy\*" and "active material" as well as "fibre\*" and "smart materials" the numbers of articles decreased (by more than 10 %). Regarding the materials "ceramic\*", "metal\*"," alloy\*" "photoactive\*" "self-repairing" "fibre" and "gels\*" only a comparably slow increase in publication numbers could be obtained for both time periods. Therefore, these keywords were considered to be less relevant.

# 3.4 Qualitative analysis of relevant material types

Out of the results of the most relevant keyword combinations, which have been identified by the bibliometric analysis in the previous section (Section 3.3), a sample of arbitrarily chosen recent articles from each field was selected for an initial qualitative analysis of the relevant materials. In total 62 recent articles (mainly reviews) were examined for the identification of the concerned substances, products and production processes (see Appendix C).

To ensure an effective and meaningful evaluation of the qualitatively examined publications, they were grouped according to the concerned products and applications. However, an overlap of substances or material types for the respective product groups could not be avoided. In the following passages the results of this analysis are described according to the identified application fields.

Medical applications seem to be an important use area of advanced materials. Especially drug delivery, disease diagnosis, tissue engineering as well as in-body sensors and switches represent an active field of research. The identified substances consist mainly of polymers. Often nanostructures play an important role. Furthermore, with aerogels, hydrogels and sol-gels, soft materials are mentioned frequently. Considering functionality, the publications focus on the active and controllable release of substances or sensing purposes. In this regard, the field is closely connected to the area of electronic products. As a new mechanism, the ability of products to change their qualities after a certain time period or due to alternating environmental conditions is often considered for medical purposes (e.g. for controlled drug delivery).

A further frequently discussed use of advanced materials is the field of wearable electronics. In particular for the term 'textiles', publication numbers currently increase (Figure 3). Electronic applications embedded in textiles are used for power generation, sensing or communication. Some examples are heating pads or health-care monitoring devices. Within that area, supercapacitors play an important role as well as organic electronics. The latter have the advantage of being more flexible than common electronic devices. In addition, the coating of these electronic devices is frequently discussed. Supercapacitors play an important role also in applications like microelectronic devices or hybrid electric vehicles. Next to them and closely related by their functional mechanisms, other types of energy storages are frequently described (in particular Li-Ion batteries), mainly for their use in electronic vehicles. Among the substances discussed are organic substitutes and graphene or polymer coatings. Functionalities range from

an enhanced electric storage capacity to their protection from water or an improved environmental compatibility.

With regard to classic concrete as a construction material, foams seem to play an important role. Despite the fact that concrete belongs to the rather traditional materials, there are attempts to improve its structure. For this purpose, concrete is reinforced by polymers or textiles and gains new properties from cellular structures.

Foams and gels seem to play an important role also in the field of biomaterials. The term biomaterials is mainly used for materials based on regenerative biological resources. Some examples are chitin, starch or even organisms like the algae euglena. They are intended for a variety of applications ranging from scaffolds to food supplements. Important requirements for their qualities lie in a regenerative and biodegradable character.

In terms of the different manufacturing processes, a large variety is mentioned in the analysed publications. In general, additive manufacturing seems to play an important role for different substances and product categories. Here the specific advantage of additive manufacturing lies in the ability to prepare internal structures within a material. These approaches mainly concern polymers and a lot of effort is invested in copying natural cellular structures.

In general, polymers seem to play a major role in the field of advanced materials. With regard to their functionality in particular materials that tend to be small, adaptive (or even active) or flexible are frequently discussed. Nearly all materials mentioned in the analysed publications represent a combination of several different substances.

# 3.5 Network analysis of advanced materials

To further characterize the field of research and development by an assessment of the relations between functionalities, particular materials as well as key actors, a network analysis based on information retrieved from publications in the field of advanced materials was conducted. Maps were produced by visualizing co-authorships and the co-localization of terms for functionalities as well as materials in the same paper as an interconnected network of nodes. These interactive networks serve as a means to identify author groups and relevant fields of advanced materials. Thereby players, who work together closely, can be identified. This enables an interviewee selection, which covers all author groups and thereby all relevant topics. Three maps were generated using data of 13,471 publications from the WoS Core Collection related to the term "advanced materials": 1) An author map, showing the activity of the authors, as well as their connections to each other; 2) a keyword map, visualizing the main keywords as well as the combinations in which they are used and 3) an author-keyword map, illustrating the connections between used keywords and authors.

By generating the author map, it appeared that the highest number of publications (85) is authored by "anonymous", covering different disciplines, journals and document types. All of these publications are neither cited in any other article, nor available in full-text. Hence it is not possible to derive any information about authors, author connections or author-keyword connections from these publications. Therefore, these publications are not included in the author network graph.

Figure 7 illustrates the multicentric author landscape. One group of authors mainly based in the USA and China (green centre on the left-hand side) is strongly connected and is publishing the most. Some further author groups exist, which also show multiple connections, but no connection to the most publishing author group. There are also several authors showing a high

number of publications, but no connection to other authors at all (big pink dots), e.g. Froes or Kraft.



Figure 7: Author map, screenshot from Gephi. The size of words and dots show the amount of publications of an author (all cited authors are counted)

The greener the dots are, the more connections to other authors exist; the pinker the dots are, the less connections exist. A connecting line represents a co-authorship in a publication. Source: Own presentation, data from WoS Core Collection, July 2019

Figure 8 shows the keywords used within the 13,471 publications on "advanced materials". In total 7,430 keywords were used. In 132 publications "advanced material" appeared as a keyword resulting in more than 3,000 connections to other keywords. This number as well as the network graph itself illustrate a rather diverse use of keywords within these publications. The most used keywords (large size of the dots in Figure 8) appear in publications, which also belong to the group of the most cited articles (dark blue colour of dots in Figure 8). The most prominent are terms related to nanomaterials, e.g. nanoparticle, nanocomposite, graphene, carbon nanotube, nanomaterial, nanostructure and nanotechnology. Closely connected to the nano-related keywords, the term "composite" is the second most used keyword, mentioned in 77 publications. It is closely related to other prominent keywords like "mechanical properties" and "microstructure". "Polymer" and "ceramic" are the most used classical material classes. A group of closely connected keywords considering the field of biomaterials, e.g. biomaterial, tissue engineering, biocompatibility and drug delivery reflects the medical use of advanced materials as described above (Section 3.4). The frequent appearance of the term "self-assembly" in contrast was unexpected, since it was not noticed by the quantitative literature research described in Section 3.3.





The size of words and dots represent the respective number of articles. Blue indicates a high number of citations for the retrieved articles, red a small number of citations. Keywords, which occurred less than three times are neglected.

Source: Own presentation, data from WoS Core Collection, July 2019

Figure 9: Author-keywords map, screenshots from Gephi. Keywords connected to the author with the highest amount of publications (left). Authors connected to the keyword with the highest amount of publications (right).



The size of words and dots represent the amount of publications by author or keyword. Keywords are shown in green, authors in red. Bold grey lines indicate a higher number of connections (i.e. occurrence in one and the same article). In this graph, only connections between authors and keywords are shown. Connections between two authors or two keywords are omitted. Keywords and authors, which occurred less than three times are neglected.

Source: Own presentation, data from WoS Core Collection, July 2019

The leading group of authors, identified above, tends to use the same keywords. The group around the two most publishing and most cited authors John Rogers and Yonggang Huang (both at Northwest University, USA), focuses on the keywords advanced material, fatigue, 3D printing, origami, shape memory polymer and flexible electronics (Table 6). As visible in Figure 9, they are also well connected to other important authors like Yihui Zhang, Mengdi Han, Zheng Yan and Fan Zhang. Figure 9 (right) demonstrates that all of them use the keyword "advanced materials".

A group of six authors around Michael Hinds was excluded from further analysis, since these authors only appear until 2003 due to a regular report on atomic spectrometry, which includes "advanced materials" in the title, but does not seem to be relevant for the topic of this study. Froes was excluded as well since the last publication is from 2004 and therefore considered as not relevant for emerging advanced materials.

Table 6 lists the most prominent authors identified by the network analysis using the search string "advanced materials", their related keywords as well as the number of articles and citations for these authors. Many of the most used keywords are equal to the ones identified by screening all existing classification reports of advanced materials (Section 3.1), e.g. composites, polymer or nanoparticle, others are entirely new. Especially the frequent appearance of graphene and self-assembly adds new topics. Also, the keywords origami and kirigami, used by the dominant authors, were not mentioned in the classifications analysed above.

Table 6: A list of the most prominent authors of the network analysis on advanced materials (data	J
from WoS Core Collection, July 2019) <sup>4</sup>	

Name	Publications	Citations	Main keywords	Note
Rogers, John A.	22	1131	advanced material, fatigue, 3D printing, origami, shape memory polymer, flexible electronics	Central author group
Huang, Yonggang	18	1115	advanced material, 3D printing, origami, shape memory polymer, flexible electronics, metamaterials	Central author group
Zhang, Yihui	17	784	advanced material, modelling, 3D-printing, origami, shape memory polymer	Central author group
Liaw, Peter K.	14	1400	-	One paper on high- entropy alloys and bulk metallic-glass cited 1 328 times
Diederich, Francois	13	587	Nanomaterials, conjugated polymer, electrochemistry, chirality, molecular recognition	
Han, Mengdi	11	338	Advanced material, fatigue, origami, metamaterials, kirigami	Central author group
Yan, Zheng	11	742	Advanced material, kirigami	Central author group
Zhang, Fan	10	344	modelling, 3D-printing, origami, shape memory polymer, 4D printing	Central author group
Anderson, Eric	9	458	Advanced material, self-assembly, nanocomposite, microstructure, smart material	
Laurencin, Cato T.	9	387	Composite, biomaterial, bone, nanofiber, chitosan	
Zhang, Qiang	9	326	Carbon nanotube, Graphene, nanostructure, biocompatibility, Li-ion	

# 3.6 The structure of "advanced materials" as a field of research and development

The field of advanced materials is a diverse research area, dominated by materials science. The total number of 4,027 publications and 13,471 authors on the topic "advanced materials" in the WoS core collection as well as the steep slopes of the bibliometric analysis indicates high research activity. In CORDIS, the EC project database, 594 projects on advanced materials are listed under the Horizon 2020 research framework program.

<sup>&</sup>lt;sup>4</sup> Some authors are not connected to any keywords since only keywords, which are used three times at least are shown in the analysis. Some publications in WoS only show keywords Plus and no author keywords. If the network visualization includes related keywords, the top five are listed in the column 'main keywords'.

The field greatly overlaps with the research area of nanomaterials. Even though the focus in the present report was not on nanomaterials, they do appear in several areas of advanced materials.

The network analysis showed several nano-related terms within the group of most used keywords. Additionally, in the bibliometric analysis the nano-related material types, especially "nanoparticle\*", queries returned the steepest slope for the investigated time period in combination with the substance independent advanced material keywords. As confirmed by first expert interviews, nanomaterials and advanced materials can hardly be separated from each other. Nanomaterials are not one type of advanced materials, but rather seem to play a role in several advanced materials.

New material classes, which are broadly used to classify advanced materials, have been identified. Most of them are connected with a specific characteristic or application of a material, but they do not represent a unique feature which justifies the formation of a respective material class. Besides nanomaterials, the most emerging new categories of materials are coatings, electronics, textiles, cellular materials, gels and foams, soft materials, organic materials and biomaterials. The term biomaterials is used in two entirely different fields: On the one hand for active materials for implementation in biological systems, as e.g. the human body, and on the other hand materials derived from regenerative resources to reduce the environmental impact<sup>5</sup>. In both cases soft materials are discussed. Not identified within the quantitative analysis, but mentioned in an expert interview, functionally graded materials are a further emerging type of advanced materials.

With regard to the building blocks used to produce advanced materials, polymers seem to play the most important role. The network analysis showed a high use of 'polymer' as a keyword and the bibliometric analysis yielded high slopes of "polymer\*", especially in combination with the terms functional-, active- and smart materials. Surprisingly, the classical material glass showed a high increase in numbers of publications within the bibliometric analysis whereas in the network analysis glasses had only a minor role. In the latter ceramics appeared as a prominent keyword.

So far, the qualitative investigation of the scientific literature has shown that the most emerging fields of applications of advanced materials are electronics and medical applications. Especially wearable electronics, but also other uses of flexible electronics play an important role. In addition, other uses of electronic materials like supercapacitors or batteries are emerging fields of research and development. In this context coatings are also frequently discussed. Regarding medical applications, soft materials as well as polymers play an important role. Also, nanostructures as well as the ability of a material to change its properties represent emerging fields of research.

In general, the functionality – or even activity – of a material seems to play a major role in advanced material science. This is indicated by the frequent use of the terms functional, smart and active detected by the bibliometric analysis as well as the high abundance of self-assembly in the network analysis. For new functionalities new material structures seem to be necessary. The materials are produced by new production processes indicated by the keywords advanced manufacturing or 3D. Nearly no advanced material consists of a single substance. 'Composites' is the second most prominent keyword identified in the network analysis while the qualitative analysis showed that the structure and compositions of the materials are actively investigated.

<sup>&</sup>lt;sup>5</sup> Subsequent parts of this study will therefore differentiate between both conceptions of biomaterials.

# 3.6.1 Towards a determination of advanced materials

A characterization of an emerging field of research and development can either focus on its products or try to define the prevailing principle of its practice as the common denominator for the work of the involved actors. For advanced materials some attempts to define the field have already been published. They focus on the first characterisation approach and identify the development of materials with new and outstanding functionalities as the specific criteria of the field. Broomfield et al. (2016) define advanced materials as

"[...] all new materials and modifications to existing materials to obtain superior performance in one or more critical characteristics." (Broomfield et al. 2016, p. 2)

In its report on value added materials Romanow and Gustafsson (2017) describe advanced materials as

"[...] tailored to fulfil specific functions and/or have superior structural properties." (Romanow and Gustafsson 2017, p. 9)

Unfortunately, definitions of this kind are limited in their value because it is hard to determine the beginning of the period of advanced materials given the assumption that new or specific functions have always been a driver of new developments in the field of materials (e.g. low-carbon steel by Bessemer in the mid of the 19<sup>th</sup> century). At least the "superior structural properties" might separate the era of advanced materials from a time in material development, where the structure of materials relied on the repertoire offered by nature. More beneficial is a characterization of the change of practice as a general paradigm of the field. Under that perspective Kadic et al. (2019) propose the following definition for so called metamaterials:

"[...] metamaterials are rationally designed composites made of tailored building blocks that are composed of one or more constituent bulk materials. The metamaterial properties go beyond those of the ingredient materials, qualitatively or quantitatively." (Kadic 2019, p.198)

Due to their outstanding new functionalities that partially go beyond what can be observed in nature, according to the definitions given above, metamaterials can be referred to as an advanced material. The claim of rational design in the proposed definition for metamaterials by Kadic et al. (2019) reflects a tendency of methodological turn that is also recognized in large parts of applied biology: Since the advent of synthetic biology in the beginning of this century, the implementation of rational design in areas of molecular biotechnology represents its central claim (Endy 2005). In biology the field gained its courage by the substantial growth in data on key characteristics of molecular biological elements due to the progress in high-throughput analysis and data processing. As in classical engineering, knowledge in the potential behaviour of the elementary building blocks is regarded as the prerequisite for rational design to overcome the laborious process of trial and error that still characterizes developments in the field of biology to date. The question arises, whether this change of paradigms in terms of our capabilities to perform a controlled and predictable process of design has already shaped the field of material science as well. This hypothesis would imply that metamaterials are only an example for the approach in modifying and even creating materials. Our observation is supported by the notion that rational design is recognized as a necessary precondition in definitions for the whole field of advanced materials. The DAMADEI-report defines advanced materials as:

"[...] any material that, through the precise control of its composition and internal structure, features a series of exceptional properties (mechanical, electric, optic, magnetic, etc) or functionalities (self-repairing, shape change, decontamination, transformation of energy, etc) that differentiate it from the rest of the universe of materials; or one that, when transformed

through advanced manufacturing techniques, features these properties or functionalities." (European Commission 2013, p. 25)

As already explained, "exceptional properties" and "functionalities" seem questionable in their value as a distinction between former products of material science and the current capabilities because one might ask whether that hasn't always been the main goal of material modifications. Nevertheless, by stressing the need for precise control to obtain these materials, the DAMADEI definition is in line with our hypothesis that rational design represents the core of a definition and thereby also a differentiation of advanced materials from other fields of material development. The MatSEEC report on 'Materials Science and Engineering in Europe' additionally highlights two preconditions for a rational design,

a) analytical power:

"Characterisation of advanced materials, and particularly of materials with necessarily complex structures such as bio and functional ones, requires analytical tools for observation and monitoring all relevant length scales (nano, micro, meso and macro)." (MatSEEC 2013, p. 19)

and b) modelling capabilities:

"Progress is needed in developing modelling with predictive power for the processing, structure control and function of advanced materials." (MatSEEC 2013, p. 21)

Following these demands the following iterative design process for advanced materials is assumed where the whole structure of the prototype is already defined in a model and may be optimized if necessary, as illustrated in the following scheme.

# Figure 10: Iterative design process of advanced materials



Source: Own presentation

Provided that rational design fulfils the demands of a methodological definition of the field of advanced materials, one should be able to identify relevant substances which can be processed into an advanced material with the help of current techniques for rational material design, (either by shaping it into a predefined structure or by a certain combination with other substances, mixtures, materials or articles).

From the first expert interviews and a consultation of scientific literature, two dimensions of design are possible: a predetermined arrangement of new structures and a composition of either different materials or different structures. Thereby, optical, magneto-optical, mechanical or thermodynamic properties can be affected according to the needs of specific applications. Moreover, advanced techniques to design materials in a kind of 'bottom up' approach, enables expanding the properties of condensed matter to a behaviour which goes far beyond what can be observed in nature (Singh, Rajni and Marwaha 2015).

# 4 Relevance assessment

# 4.1 Introduction to relevance assessment

A core aim of the project is to identify which advanced materials should be regarded as "relevant". The relevance assessment should allow deselecting some distinct types of advanced materials as "not a priority for (immediate) action with regard to chemical safety" and selecting others as "of concern with regard to chemical safety". Concerns regarding the circular economy should be considered but have lower priority in this study, due to the primary focus on chemical safety. In the context of this study, an advanced material is understood to be of "relevance" if:

- ▶ There are indications of potential hazards, exposures and risks and/or
- ▶ Information on hazards and risks are missing and/or
- There is a lack of legal coverage of the advanced material in its (intended) applications or its implementation, including enforcement and/or
- ▶ Hazard and risk assessment approaches and tools are not (fully) applicable and/or
- There are challenges regarding the circular economy, resource consumption or other environmental aspects.

The above aspects indicate potential challenges but may not be sufficient to substantiate an actual "concern" with regard to chemical safety. Therefore, the term "relevance" is used. It is a "flag" highlighting that an advanced materials should be prioritised for further action, in particular a more in-depth assessment of a potential concern, which may in the first instance consist of data collection and generation.

Relevance of advanced materials could, in addition, be regarded as enabling significant benefits in terms of contributing to the solution of environmental and societal challenges. Acknowledging the innovative potential and the importance of material development for technological progress, including to improve the state of human health and the environment, this aspect is not covered by the relevance assessment in this project, mainly for three reasons:

- 1. The overall project aim is to identify action needs to ensure chemical safety; it is not about unlocking innovative potentials in material sciences.
- 2. The benefits of advanced materials are very difficult to identify and/or predict as many are still in the research and development stage.
- 3. To anticipate technology governance by weighing risks against benefits is not appropriate at this stage of assessment where the primary goal is to first of all inform authorities about potentially critical areas of new and emerging materials<sup>6</sup>.

The diversity and complexity of advanced materials and their applications require taking different perspectives and addressing various aspects to identify the "relevance" of an advanced material.

<sup>&</sup>lt;sup>6</sup> Following a prioritisation, the benefits should be considered in the evaluation of potential risk management or other follow-up measures to be taken by authorities, industries or other stakeholders, such as research institutes: If a prioritised advanced material after an more in-depth assessment is identified as "of concern" regarding chemical safety (or the circular economy), the potential benefits from its application should be considered in deciding on how to further manage potential risk with as little hindrance to the further innovation processes and actual implementation in the market. This step is not part of the current project.

The relevance assessment should identify those advanced materials that should be subject to further assessment and potentially subsequent action regarding chemical safety. It is hence a first step, which supports the decision on which advanced materials to focus on. Consequently, the relevance assessment is intended for use based on easily available information and is an exercise of broad coverage rather than an in-depth assessment.

The following sections introduce a possible approach and criteria of a relevance assessment framework. It is based on, among others the discussions at the Fourth ExpertDialogue on Nanotechnologies organised by the BMU in May 2019<sup>7</sup>, the First Thematic Conference on Advanced Materials, expert interviews and the responses obtained from the participants of the online survey conducted within the present project. Further it is based on considerations of the project team related to the availability of information and the practicability of the assessment based on the literature and internet research on advanced materials.

# 4.2 Aspects of relevance

In this study, relevance is described in four dimensions, which are interrelated but can be assessed separately. The reason why an advanced material is identified as relevant would then be used to decide where to focus and what information to collect as the next step. Furthermore, the combination of perspectives enables differentiating between different advanced materials that are identified as "relevant". Figure 11 shows the four dimensions of the proposed relevance assessment approach and the core questions that can be addressed with information in this area. In the following sections the relevance of advanced materials is discussed in relation to these four dimensions and criteria and indicators of relevance are discussed.



#### Figure 11: The four dimensions distinguished in the relevance assessment

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Source: Own presentation

<sup>&</sup>lt;sup>7</sup> The stakeholder dialog focused on advanced materials. A summary of discussions and the pertaining report with suggested relevance criteria are available at: https://www.bmu.de/en/download/5th-dialogue-phase-expert-dialogue-4-opportunities-and-risks-of-advanced-materials/

# 4.3 Scientific dimension

From a science perspective the relevance of an advanced material could be indicated by the **novelty of properties** or the **novelty of scale or combination of properties** that advanced materials may have. These may, among others, consist of new ways of interaction with other materials, including biological systems. While the number of genuinely novel properties of advanced materials is comparably low, e.g. "motility" or "targeted change of state" (switching), the number of changed property scales and combinations appears to be infinite.

The (novelty of designed) properties are suggested as relevance criterion because they indicate the level of discovery and whether or not new grounds and principles are conquered. The novelty of properties has relations to the other dimensions of relevance because they may determine or influence:

- Specific behavior and effects of advanced materials (hazard and risk);
- ▶ If and how advanced materials are covered by legislation and regulated (regulation);
- ▶ The applicability of risk assessment approaches and tools (hazard and risk);
- The potential uses of the materials in products and processes (technology).

# 4.3.1 Criteria for relevance from a scientific perspective

Table 7 lists possible criteria and specific indicators to describe the scientific relevance of advanced materials that could be applied in a relevance assessment. Column 3 indicates the expected information availability, i.e. the likelihood that the indicator can actually be formed. This information is based on expert judgement and the experience from the literature research on advanced materials conducted during the project. Column 4 shows to which particular aspect of relevance the indicator provides an input and is derived logically from the nature of the indicators. The last column of the table contains general comments on the practicality of the indicators.

Criterion of relevance	Types of indicators	Expected information availability	Gives (rough) information on	Comment on practicality
Novelty of (combination of) property/- ies	Physical and chemical parameters, e.g. conductivity, hardness, activity	High: property is target of design process	Type and width of use/ application spectrum; Potential hazards	"Novelty" is a relative term
Ability to scale and/or tailor the target property/ies;	Variety of structural and combination options that influence the properties	High: Deducible from data on composition and structure; Publications	Width of use and application spectrum; Potential for (future) development of further advanced materials in the same cluster;	The indicator is likely to change over time and with scientific and technological progress; Information may be (kept) confidential; Publications exist mainly for successful developments but not for

Table 7: Potential relevance	criteria from a	scientific perspective
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Criterion of relevance	Types of indicators	Expected information availability	Gives (rough) information on	Comment on practicality
			Ability to fulfil specific requirements of applications	failures, hence limitations are challenging to determine
Ability to scale and/or tailor the target property/ies;	Ability to predict properties based on composition and structural information	Medium: Deducible from publications or experience	Width of use and application spectrum; Potential for (future) development of further advanced materials in the same cluster; Ability to fulfil specific requirements of applications	The indicator is likely to change over time and with scientific and technological progress; Information may be (kept) confidential; Publications exist mainly for successful developments but not for failures, hence limitations are challenging to determine
Ability to scale and/or tailor the target property/ies;	Ability to steer the manufacturing process to actually construct the advanced material	Medium to low: Potentially from publications and expert interviews	Width of use and application spectrum; Potential for (future) development of further advanced materials in the same cluster; Ability to fulfil specific requirements of applications	The indicator is likely to change over time and with scientific and technological progress; Information may be (kept) confidential; Publications exist mainly for successful developments but not for failures, hence limitations are challenging to determine
Novelty of manufacturing technology of advanced materials	Type of manufacturing technology and needed equipment, including analytics, to describe the materials' composition and structure	Medium: Detailed information may not be published (confidentiality, scientific interest etc.)	Innovation progress (direction of material development, abilities of manufacturing); Time required for the innovation process until market entry	"Novelty" is a relative term and will change over time; Manufacturing technologies may be alternative to existing ones or enabling production for the first time
Interest in advanced material or technology in general	Number of publications in scientific literature	High: Public information	Amount of current research and areas of potential scientific progress in the near future	No clear relation between science and market developments; Evaluation of publication is time consuming

# 4.4 Economic and technical dimension

Relevance of advanced materials could also be evaluated with a view to their potential impact on technology development. The diversity of existing and potential future uses and the types of uses would give rough indications of release potentials which, in combination with property

information on the advanced materials, would allow approximating exposure levels of humans (workers and consumers) as well as the environment. This includes both, indications on exposures from manufacturing processes but also from use phase and the disposal of products.

In addition, the economic and technological dimension would give indications on potential contributions to other aspects of sustainable development than chemical safety, which are not particularly considered in relevance assessment, but should be considered in the evaluation of consequences from an identified concern (cf. Section 4.1).

The economic and technical dimension relates to the **potential** of an advanced material **to** successfully reach the market in one or several applications or, in other words, how far can the advanced materials **trigger innovations** at process or product level in one or several sectors.

It can be assumed that emerging technologies do not suddenly appear on the market but a longer period of announcement exists. Due to the large amounts and diversity of advanced materials, it appears useful to focus monitoring and potential regulatory activities on those materials, which are already on the market or expected to reach the market in the mid-term. In these cases, sufficient information on the actual use may be available to assess, the market/technology impact, the potentially related exposures and risks as well as potential needs for adapting the legal framework or assessment instruments.

# 4.4.1 Criteria for economic impact and technical relevance

Table 8 lists a number of criteria that could be applied to evaluate the relevance of an advanced material in the technical and economic context. Regarding chemical safety, the technology readiness level (TRL) or degree of market penetration as well as the versatility of (potential future) applications are indications of relevance regarding exposure potentials and "urgency" to act. Column 3 of Table 8 indicates the expected information availability, i.e. the likelihood that the indicator can actually be formed. This information is based on expert judgement and the experience from the literature research on advanced materials conducted during the project. Column 4 shows to which particular aspect of relevance the indicator provides an input and is derived logically from the nature of the indicators. The last column of the table contains general comments on the practicality of the indicators.

Criterion of relevance	Types of indicators	Expected information availability	Gives (rough) information on	Comment on practicality
Potential of the material to enter one or several applications or markets	Physical and chemical properties	Medium: Property is target of design process; versatility of uses to be determined by expert judgement and/or literature	Sectors or products of (future) use; Expected use amounts and release scenarios; Potential market success	Requires some expertise in judging on potential applications; Innovative uses difficult to predict; No direct link to actual market entry of "interesting" materials; Confidentiality may hinder information collection on potential uses
Potential of the material to enter one	Functionalities enabled in	Medium to low: Indications of enabled	Sectors or products of (future) use;	Requires some expertise in judging on potential applications;

Table 8: Po	otential relevance	e criteria from a	an economic or	technical	perspective

Criterion of relevance	Types of indicators	Expected information availability	Gives (rough) information on	Comment on practicality
or several applications or markets	products and processes	functionalities from literature and expert judgement	Expected use amounts and release scenarios; Potential market success	Innovative uses difficult to predict; No direct link to actual market entry of "interesting" materials; Confidentiality may hinder information collection on potential uses
Potential of the material to enter one or several applications or markets	Products and sectors of use	Medium: Publications and expert knowledge	Sectors or products of (future) use; Expected use amounts and release scenarios; Potential market success	Requires some expertise in judging on potential applications; Innovative uses difficult to predict; No direct link to actual market entry of "interesting" materials; Confidentiality may hinder information collection on potential uses
Degree of market penetration	Known applications in products and processes	Medium/low: Publications (early: data on use types, later: product statistics, market shares, websites, sector publications; Publications likely to decrease when use becomes common; No precise information	Application areas to be used to derive exposure levels (in combination with use amounts)	Same challenges to gather use information as for chemicals as such; use amounts and specific applications are most likely not available
Degree of market penetration	Number of patents involving use of advanced materials	High: Patent applications are publicly available	Potential occurrence on the market and types of uses; Expectations of market success	Indicator may not be useful as a patent is only an indication of an intent to enter the market but not of actual market presence
Research on concrete, marketable products	Number of funding programmes and/or specific research calls	High: Public information	Research interest of funding institutions; Possible future direction of R&D	Funding programmes may give a wrong impression, as there are (also) political reasons behind their priorities
Use amounts	Production and/or use amounts	Low: No publicly available information on use amounts; Information from manufacturers may be confidential	Over time: Market success; Potential exposure levels (in combination with use information)	An increase in production and use indicates increasing market relevance but information is likely to be missing

# 4.5 Hazard and risk dimension

Chemical safety of substances, mixtures and articles is assessed in the regulatory context by dividing **effect thresholds** of different endpoints by **exposure levels** (measured and/or predicted). If the resulting risk characterisation ratio exceeds the value of "1" an unacceptable risk is demonstrated. Hence, both the hazardousness of an advanced material and the potential exposure levels need to be considered in a risk assessment, including the (conditions of the) use(s) and related emissions as well as the waste stage.

An advanced material would be considered relevant due to hazard and/or risk aspects if:

- 1. There are indications of a potential hazard, e.g. based on the functionality of the advanced material and/or available information on hazards;
- 2. There are indications of critical exposures of humans and/or the environment from the expected use contexts;
- 3. There is insufficient information to determine either the hazards or the exposure levels (need for information gathering or generation).

Each of these aspects could as such be a reason for identifying an advanced material as relevant.<sup>8</sup>

As the aspects and criteria should support a screening for relevance, a demonstrated risk (i.e. risk characterisation ratio > 1) is not currently regarded as a useful indicator.

# 4.5.1 Criteria for the identification of potential hazards and risks

Several criteria, which could indicate a relevance because they point to the existence of either hazards or significant exposure levels of humans or the environment, are described in the <u>report</u> prepared in the context of the German ExpertDialogue on advanced materials organised by the BMU in May 2019. The following table lists these and additional potential relevance criteria. It provides further details on potential indicators for these criteria, whether or not related data is expected to be available and issues on the criteria's practicality. The lack of information on the criteria may also be a reason to identify an advanced material as relevant. Hence, viewing the information availability for these criteria as a whole may give another reason for "concern".

Criterion of relevance	Types of indicators	Expected information availability	Gives (rough) information on	Comment on practicality
(Indication of) adverse effects	Data for material and/or building blocks indicates SVHC properties <sup>9</sup> and/or other hazards to human health or the environment	Medium to low: For building blocks: depends substance types; For entire materials: low	Potential to cause adverse effects	Criterion has to be applied case-by-case for each individual advanced material

Table 9: Potential re	levance criteria	from a hazard	and risk perspec	tive

<sup>&</sup>lt;sup>8</sup> The extent of potential risk and the amount of evidence supporting an expectation of risk may differ for different types of advanced materials. These differences could be used to differentiate an urgency of potential action as well as the type of needed action.

<sup>&</sup>lt;sup>9</sup> Carcinogenicity, mutagenicity, reprotoxicity (CMR), persistent, bioaccumulative and toxic/very persistent, very bioaccumulative substances (PBT/vPvB) as well as substances of equivalent concern, such as endocrine disrupters (EDs), persistent, mobile toxic substances (PMTs), respiratory sensitisers.

Criterion of relevance	Types of indicators	Expected information availability	Gives (rough) information on	Comment on practicality
(Indication of) adverse effects	Structural similarity (of building blocks and/or their degradation products) to substances with adverse effects	Medium to low: Composition data available; Data on entire material: less available	Potential to cause adverse effects,	May be used also in conjunction with information on stability of material and/or use
(Indication of) adverse effects	"Critical properties <sup>10</sup> " (of building blocks), e.g. high reactivity	High to medium: Properties partly design target; Physical chemical characterisation	Potential types of interaction with organisms; Stability during use and in environment	Deducing adverse effects from physical-chemical properties likely to require expert judgement
Critical morphology and/or structure(s) <sup>11</sup>	Content of fibres or structures that are or could break into WHO fibres <sup>12</sup> ; Granular, biopersistent dusts (GBD)	High to medium: Structural info on fibres/GBS should be available; Breaking into fibres not available	Potential inhalation effects (cancer, inflammation, sensitisation)	Breaking of fibres/structures into WHO fibres may be predictable but more likely has to be measured
Content of critical building blocks <sup>13</sup>	Content of biological structures (DNA, proteins etc.) or biologically active structures.	High to low: Composition information should be available Information on (eco- )toxic properties of building blocks may vary	Potential kind of interaction with living organisms on the level of cells and biological materials	More information on adverse effects of biological structures is needed
Content of critical building blocks	Content of building blocks / components with known (eco- )toxicity, e.g. Pb, Cd	High to low: Composition information should be available Information on (eco- )toxic properties of building blocks may vary	Potential kind of interaction with living organisms on the level of cells and biological materials	Partly doubling the first criterion
Emission potential	Production and use amount	Low: No publicly available data on use amounts;	Exposure levels via amount that could theoretically be emitted (in	Only rough proxy for release potential; data on types and

<sup>&</sup>lt;sup>10</sup> Several properties of the materials and their building blocks could be used. Which physical-chemical properties are useful depends on the type of advanced material checked for relevance. Therefore, no detailed list of potential indicators is included here.

<sup>&</sup>lt;sup>11</sup> Currently, only the here explicitly addressed fibres are identified as potentially causing hazardous effects. However, this may change in the future and further criteria / morphologies could be added under this heading.

<sup>&</sup>lt;sup>12</sup> The World Health Organization (WHO) characterised the properties of bio persistent fibers. This refers to inorganic fiber dusts (except asbestos fibers) with a length > 5 <u>microns</u>, a diameter < 3 microns and a length-to-diameter ratio of > 3:1; taken from: https://www.nanopartikel.info/en/glossary/266-who-fibers

<sup>&</sup>lt;sup>13</sup> Not only the building blocks as such may be critical, but concerns may relate also to their degradation products.

Criterion of relevance	Types of indicators	Expected information availability	Gives (rough) information on	Comment on practicality
		Manufacturers' data may be confidential	combination with use information)	use conditions also needed; Information may be collectable "case-by- case"
Emission potential	Type of use and use conditions via "classical" emission parameters <sup>14</sup>	Medium: Generic data available; Use conditions in principle deducible	Release and exposure potential from application; Type of expected waste stream after end of service-life	Information may support targeting hazard information collection; Combines with regulatory information
Persistence during use and in the environment	Stability of the materials during use; Persistence and (biological) degradation; Composition	Medium; Stability of material part of technical specification; Persistence and degradation may be deductible. Data on building blocks depends	Release potential of the individual building blocks and/or other substances and components Potential occurrence of the material in the environment and in wastes	Persistence is key characteristic for hazard and risk
Persistence during use and in the environment	Conditions of and functionality for intended use	High: Properties and/or uses are a design target	Potential stability during use and in the environment	Uncertainty from deducing stability in the environment from conditions of use
Behaviour	Bioaccumulation	Low: Data for building blocks may be available	Potential exposure levels in the environment and/or organisms	Uncertainty from deducing accumulation potential from properties
Behaviour	Translocation in the body	Low: Kinetic information on material unlikely to be available; Data on building blocks may exist	Potential exposure levels in organisms	Very specific endpoint for which data is not normally available
Behaviour	Critical degradation products	High to low: May be deducible from stability and type of building blocks	Potential formation of and exposure levels to (hazardous) degradation products	Combined information on stability of material and building blocks and adverse effects;

<sup>&</sup>lt;sup>14</sup> User groups (consumers, workers), formation of dusts/aerosols, use in mixtures and/or articles, intended or non-intended release, indoor/outdoor use, wide disperse or narrow use, use in/on the human body etc.

Criterion of relevance	Types of indicators	Expected information availability	Gives (rough) information on	Comment on practicality
Behaviour	Carrier effects	High to medium: Carrier activity may be design target; information on unintended mobilisation usually not available	Influence on translocation in organisms Interaction with other molecules and (certain) cells	Unintended effects on other compounds can hardly be assessed.
Lack of information	View on availability of information for on any of the criteria in this table	Medium to low: Data gaps likely for most advanced materials For building blocks: data availability mostly depends on applicable legal requirements	Level of (un- )certainty with which hazard and risks could be deduced	If no or very little information is available, priority may be given to the generation and collection of that information

# 4.6 Regulatory dimension

Chemicals legislation is divided into several regulations, with REACH being the core regulation applying to industrial chemicals. Each legislation defines which types of substances and mixtures are covered, and may include requirements for the generation and assessment of information on hazards and exposures as well as for the assessment of risks. Generally, the extent of requirements increases with increasing risk potential of the chemicals that are regulated.

From the regulatory perspective an advanced material could be considered relevant if:

- ▶ There are indications of an unacceptable hazard and/or risk;
- It is not possible to conduct a hazard and/or risk assessment. There are two main reasons, why a risk assessment could be impossible:
  - Insufficient information on an advanced materials' hazards and exposures due to:
    - the material not falling under the scope of existing legislation;
    - the material being covered by legislation, but with data requirements that are not sufficient for hazard and/or risks assessment;
    - generally missing data and experiences with the hazards or risks of the material.
  - The existing hazard and/or risk assessment approaches and tools are not applicable to advanced materials.

In general, full and partial risk assessment requirements, which include the obligation to generate hazard data, exist in legislation on pharmaceuticals (substances and mixtures) and medicinal products (substances, mixtures, articles), biocides (substances and mixtures, partly articles), plant protection products (substances and mixtures), industrial chemicals (substances and their uses in mixtures and articles) as well as consumer protection legislation, such as the regulation on food contact materials or the cosmetics regulation. Some of the requirements in

these legislations have been adapted to nanomaterials but may not be sufficient to identify hazards and/or risks from advanced materials.

# 4.6.1 Criteria for the identification of regulatory relevance

Table 10 is based on the criteria related to regulatory relevance identified at the ExpertDialogue on Advanced Materials organised by the German Environment Ministry in 2019. Further criteria were added to the proposals of that dialogue and the use of potential indicators and their practicality are discussed.

Table 10 lists potential criteria of relevance and the pertaining possible indicators. The column "Gives (rough) information on..." indicates the consequences of whether or not a definition applies and/or if tools are available and/or applicable. The last column contains practicality aspects. In contrast to the above tables, it does not specify the expected information availability, because this is not the main challenge of applying the criteria: the interpretation of the definitions and how exactly it applies to advanced materials is the most difficult issue, which may be exacerbated by an (additional) lack of information.

Also, regarding the applicability of existing hazard and exposure assessment tools it is not so much a question of availability but more of applicability. The applicability has not yet been systematically evaluated; however, for individual clusters of advanced materials it may be possible to assume or logically deduce the applicability in the frame of a screening for relevance.

Criterion of relevance	Types of indicators	Gives (rough) information on	Comment on practicality
Applicability of existing definitions in REACH Art. 3 <sup>15</sup>	Substance definition applies (lower relevance)	Information availability under REACH	Basis for assessing regulatory coverage; Proxy for information availability; Ambiguity for many materials → may require formal clarification
Applicability of existing definitions in REACH Art. 3	The definition of a nanoform according to REACH Annex VI applies (lower relevance)	Potential "particle" hazards; Data availability to characterise the particularities of nanoforms	Basis for assessing regulatory coverage; Proxy for information availability; Ambiguity for many materials → may require formal clarification
Applicability of existing definitions in REACH Art. 3	Polymer definition applies (higher relevance)	Information availability under REACH	Basis for assessing regulatory coverage; Proxy for information availability; Ambiguity for many materials → may require formal clarification
Applicability of existing definitions in REACH Art. 3	Mixture definition applies (higher relevance)	Legal coverage and applicable requirements; Potential challenges from deriving hazards of the material as such	Basis for assessing regulatory coverage; Proxy for information availability; Ambiguity for many materials → may require formal clarification

	Table 10: Potentia	l relevance	criteria	from a	regulatory	perspective
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<sup>&</sup>lt;sup>15</sup> In this table, the core reference is REACH Art. 3, which defines a substance, a substance in nanoform, a mixture, article and polymer. Advanced materials that are substances may fulfil the definitions of active substances under further legislation (e.g. medicinal products or biocides) or may have uses/functionalities that are relevant e.g. under the Cosmetics Regulation or legislation on Food Contact Materials. In this context, the fulfilment of a more detailed elaboration of criteria for relevance assessment, relevant definitions from other legislation than REACH could be added, e.g. of "active substances", "pharmaceuticals" or "medicinal products".

Criterion of relevance	Types of indicators	Gives (rough) information on	Comment on practicality
Applicability of existing definitions in REACH Art. 3	Article definition applies (higher relevance)	Legal coverage and information availability under REACH	Decision if form, design or structure of advanced materials are more important for their function than the chemical composition may be a principle decision/interpretation for authorities to make
Applicability of hazard assessment approaches and tools	Availability of appropriate test methods and guidance; Availability of suitable modelling tools (QSARs etc.)	Potential to generate hazard information in time; Need to adapt or develop tools to generate hazard information; Uncertainty regarding hazards	May differ across materials whether the building blocks could/should be assessed or the material as such or both
Applicability of exposure assessment approaches and tools	Availability of approaches, tests and modelling tools to determine exposure levels for the material as such	Potential to generate exposure information in time; Need to adapt or develop tools to generate exposure data; Level of uncertainty regarding exposure levels	This includes generation of data on persistence and accumulation, as well as exposure models or measurements in the environment.
Lack of use and release information	Availability of information on uses and release	Potential exposure levels	

# 4.7 Further criteria that could be considered in the relevance assessment

Apart from the above discussed dimensions of relevance, additional criteria may be considered, which concern environmental and societal impacts of the use of advanced materials but do not fit into the four dimensions discussed above. These could, among others, relate to the suitability of advanced materials for a circular economy, their impacts on different environmental pressures, such as the use of resources and the emission of greenhouse gases, or to ethical aspects, such as whether or not equal access to innovations exist or if benefits are achieved for one group of people at the cost of others. Some of these criteria are contained in the report of the ExpertDialogue, others have been added to the table based on learnings of the current project. Social and ethical aspects have not been addressed in the list because they would need much more information on the applications and its economic context which is not achievable with the limited resources of this study.

Criterion of relevance	Types of indicators	Expected information availability	Gives (rough) information on	Comment on practicality
Separability from the waste stream	Possibility to separate products (and/or their components) that contain advanced materials from the waste streams	Medium: Based on information on advanced materials' containing products collection system and separability can be deduced	Whether or not advanced materials could be separated (for recovery and recycling) from the general waste stream within the products they are contained in, at least in theory.	Indicator is based on use information; i.e. the type of product and not the material as such
Recyclability	Recoverability of an advanced material with an intact (meta) structure	Medium to low: Stability of (meta) structure may be known as well as the Product; Conditions of waste treatment to be deduced based on (likely) product and/or material	Whether or not the value/resource input for the structure of an advanced material could be maintained over the waste stage	Criterion is relevant only if products with advanced materials are separable from the overall waste stream (cf above); Influences the economic incentive for waste sorting and separation
Recyclability	Contamination of material cycles; (Eco-)toxicity and/or content of (eco-)toxic building blocks	Medium to low: For building blocks: depends substance types; For entire materials: low	Potential of material to introduce hazards into existing material flows	Relevance of contamination depends among others on type of materials / conditions of recycling
Recyclability	Disturbance of the recycling process and / or decrease in the quality of recyclates	Low: Different possibilities how an advanced could influence existing recycling processes and/or the obtained material quality	Whether or not advanced materials could be an additional/new challenge to the circular economy	Requires information from recycling industry to identify which materials could cause technical or quality problems
Resource consumption	Resource consumption per amount of advanced material	Low to medium: Information on resource use may be available in general but is unlikely to be published	Potential environmental burdens/relief due to the use of an advanced material	Resource consump- tion should be related to functional units. This requires assessing a particular use
Resource consumption	Difference in resource consumption to achieve a particular functionality	Low: Information requires LCA to compare differences in resource uses	Impacts on the environment comparing advanced materials and (conventional) technologies	Existence of LCAs or similar, potentially more focussed assessments only likely for research projects

# Table 11: Other potential relevance criteria

Criterion of relevance	Types of indicators	Expected information availability	Gives (rough) information on	Comment on practicality
Consumption of critical raw materials	Amount and type of critical resources used per kg of advanced material	Low: Information on production inputs are normally not published	Potential environmental and social burdens from the production and use	Information could be obtained from manufacturing on request but may be confidential

# 4.8 Proposed indicator set for screening relevance of advanced materials

Due to the versatility of advanced materials, there is a need to identify those materials, for which a potential need for action by the authorities is regarded more likely than for others. Setting priorities on which materials to focus (first), can be supported by the set of relevance criteria proposed in Table 12. There may be additional priorities that could influence whether or not an advanced material, which is identified as relevant, could be evaluated as more urgent/important for further work than others.

Potential activities or further work on advanced materials identified as relevant could be, among others, the collection of (further) hazard, use or exposure information, determine in detail which of the regulatory definitions applies and hence, how a material is covered by legislation, conducting market surveys to substantiate information on (future) uses or conducting a detailed assessment of potential risks, or determining adaptation needs of hazard and/or risk assessment tools. Consequently, a screening should, in the best case, not only indicate the relevance of an advanced material, but also the potential action needs regarding chemical safety.

The following demands were considered in selecting criteria and indicators from Table 7 to Table 11 to develop an indicator set for relevance screening:

- The screening should be possible with the available information<sup>16</sup> (i.e. no need to generate new data). Indicators for which the information availability is currently identified as "low" in the previous tables of this section do not therefore qualify as a screening criterion.
- The screening assessment should allow evaluating types of advanced materials at a medium level of aggregation, i.e. it should neither target individual materials nor very large clusters, which include many, different variants. In the context of this project, the categorisation of types of advanced materials described in the factsheets was used for guidance in this regard.
- The criteria should include indicators of potential hazards and risks as well as of current legal coverage.
- In order to avoid working on advanced materials that are very far from being on the market or that are likely to be applied in niche markets and low amounts, criteria reflecting the current or future market relevance should be included.

Table 12 lists the proposed criteria and indicators for a screening relevance assessment. The criteria and indicators are directly taken from Table 7 to Table 11.

<sup>&</sup>lt;sup>16</sup> Although being "available", data from publicly accessible information sources, such as databases or scientific (review) articles may have to be compiled and evaluated. However, no generation of data should have to be performed if these publicly accessible sources do not provide sufficient data to define an indicator for a particular advanced material.

Criterion of relevance	Types of indicators	Data source / interpretation	Type of conclusion: Advanced material
(Indication of) adverse effects	Data on (eco)toxicity: CMR, PBT/vPvB; EDC, PMT properties as well as other hazards to human health and the environment	Databases / review articles on hazardous properties of the material and its building blocks	has been demonstrated to have hazardous properties has/has not been assessed respectively
(Indication of) adverse effects	"Critical properties" (of building blocks) e.g. high reactivity	Databases, review articles, public knowledge	has been demonstrated to have hazardous properties has/has not been assessed respectively
Critical morphology and/or structure(s)	Content of fibres or structures that are or could break into WHO fibres; Granular, biopersistent dusts (GBD)	Databases, review articles, public knowledge, expert judgement	may/may not be hazardous to human health has/has not been assessed respectively
Content of critical building blocks	Content of biological structures (DNA, proteins etc.) or biologically active structures.	Databases, review articles, public knowledge, expert judgement	contains/does not contain biological materials/structures that could cause adverse effects
Persistence during use and in the environment	Stability of materials during use; Persistence and (biolo- gical) degradation; Composition	Databases, review articles, public knowledge, expert judgement	could/could not degrade into its building blocks could persist in the environment and in biota
Persistence during use and in the environment	Conditions of and functionality for intended use	Databases, review articles, public knowledge, expert judgement	could/could not degrade into its building blocks could persist in the environment and in biota
Degree of market penetration	Known applications in products and processes	Literature review, market analyses, expert interviews	is on the market/about to enter markets/in product specific R&D/in scientific development
Research on concrete, marketable products	Number of related funding programmes and/or specific research calls	Monitoring of funding programs	is/is not in the focus of funders and may be developed for specific applications
Applicability of hazard assessment approaches and tools	Availability of appropriate test methods and guidance; Availability of suitable modelling tools (QSARs etc.)	Information on the composition and structure, expert judgement	could be subjected to in-depth risk assessment immediately/after adaptation of methods/after development of new methods (and data generation)
Applicability of exposure assessment	Availability of approaches, tests and modelling tools to	Information on the composition and	could be subjected to in-depth risk assessment immediately/after adaptation of methods/after

# Table 12: Overview of proposed relevance screening criteria

Criterion of relevance	Types of indicators	Data source / interpretation	Type of conclusion: Advanced material
approaches and tools	determine exposure levels for the material as such	structure, expert judgement	development of new methods (and data generation)
Emission potential	Type of use and use conditions via "classical" emission parameters	Literature review, public knowledge expert judgement	could be emitted to a large/medium/low extent to the human/natural environment and/or during waste treatment
Applicability of existing definitions in EU-legislation	Substance Nanoform Polymer Mixture Article	Information on the composition and structure, expert judgement	is considered a (nanoform of a) substance, a polymer, a mixture or an article the advanced material is/is not covered by [] legislation
Ability to scale/tailor the target property/ies	Ability to predict properties based on composition/structural information	Expert judgement / literature review	may be successful in many/some/few markets may/may not allow adjusting the design, including regarding hazardous/adverse properties
Ability to scale and/or tailor the target property/ies	Variety of structural and combination options that influence the properties	Expert judgement / literature review	as high/medium/low innovation potential may conquer many/some/few different applications and markets may have many/some/few variants may/may not allow adjusting the design, including regarding hazardous/adverse properties
Novelty of (combination of) property/-ies	Physical-chemical parameters, e.g. conductivity, hardness, activity	Expert judgement / literature review	has high/medium/low innovation potential may conquer many/some/few different applications and markets
Interest in advanced material or technology in general	Number of publications in scientific literature	Search and analysis of literature	may/may not be developed further in the (near) future
Separability from the waste stream	Possibility to separate products (and/or their components) that contain advanced materials from the waste streams	Literature research on uses, (waste) expert judgement	may/may not be recovered from the waste streams (with the products / components they are contained in)
Recyclability	Ability to recover the advanced material with an intact (meta) structure	Literature on uses; (Waste) Expert judgement; Information on stability of the structure	may/may not be recovered with a high/low value from waste

Criterion of relevance	Types of indicators	Data source / interpretation	Type of conclusion: Advanced material
Recyclability	Contamination of material cycles; (Eco-)toxicity and/or content of (eco-)toxic building blocks	Literature and databases on hazards (of building blocks) Information on waste processing conditions based on product and/or material data	may/may not contaminate material flows due to being hazardous/containing hazardous building blocks are likely/unlikely to contaminate material flows as hazards/hazardous building blocks are likely to be destroyed(/separated during recycling processes.
Recyclability	Disturbance of the recycling process and / or decrease in the quality of recyclates	Literature and (waste) expert judgement	may/may not be suitable for recycling

The prioritised materials will most likely have to undergo a more in-depth assessment, potentially involving further data collection, for more robust conclusions on the different relevance areas. This may concern the potential hazards or risks, legal coverage of a material or the market occurrence and future uses, including volumes. In addition, benefits of the advanced materials' uses, which are not taken into account for the relevance assessment may be considered.
# 5 Clustering and characterising selected advanced materials (factsheets)

The aim of clustering advanced materials and describing them in a structured way in form of factsheet<sup>17</sup>s is to provide information on various advanced material types that the project team proposes to distinguish from each other. Each factsheet addresses one type of advanced material and is structured into several sections:

- Characterisation of the advanced material type, including
  - a working definition and frequently used synonyms
  - commonalities of materials belonging to the cluster
  - main building blocks/composition, structure, properties and functionalities and
  - the applicability of definitions under REACH<sup>18</sup>;
- Exemplary information on applications of the materials in the material cluster, including an indication of their state of development;
- ▶ Information on risks, i.e. hazards, safety concerns and exposure potentials;
- ▶ Indications of possible challenges regarding resource use and recyclability.

It was neither intended nor possible (cf. below) to conduct a thorough and complete scientific analysis of the available literature to derive information for the factsheets. Instead the factsheets should allow a rough screening and structuring of advanced materials as well as giving an initial overview of their main characteristics and aspects on chemical safety. This should be input to the further discussions in the project and the thematic conferences as well as any other actors working on chemical safety of advanced materials.

### 5.1 Limitations of the factsheet approach

The literature research, the online survey and the discussions at the first thematic conference supported the overall finding that until now it has proven impossible to unambiguously structure the field of advanced materials. In contrast, several overlaps between the clusters formed and exist because of the two determining elements of advanced materials (composition and structure), as well as the (related) functionalities and application areas. Furthermore, criteria to cluster advanced materials may also depend on the context within which the clustering should be applied.

As a consequence, it should be acknowledged that the approach to form clusters of advanced materials within this project is limited by:

1. The existence and availability of information to form and differentiate advanced material types;

<sup>&</sup>lt;sup>17</sup> The factsheets are provided as separate background document but not as UBA Texte. It is available for download at <u>https://oekopol.de/archiv/material/756 AdMa Factsheets final.pdf</u>

<sup>&</sup>lt;sup>18</sup> As the team found little information in the literature and was not able to decide whether or not and which definition is actually fulfilled, a respective statement is given only, if an evaluation was unambiguous or mentioned in existing documents.

- 2. The challenges posed by the range of possible combinations of structure and substance composition of advanced materials;
- 3. The need to strike a balance between a manageable number of advanced material clusters (e.g. to identify regulatory action needs) and a level of detail that actually allows the identification of differences between two or more given clusters;
- 4. The fact that certain, already partly established "definitions" of advanced materials cannot be ignored in any clustering approach;
- 5. The limited resources available to elaborate the core characteristics, potential risks and application areas for all possibly distinguishable clusters of advanced materials.

Despite the above limitations, the approach of elaborating factsheets and thereby defining clusters of advanced materials was chosen in order to give all stakeholders some (debatable) structure for their work and fix the starting point for further discussions. In this regard, the factsheets should be regarded as living documents.

### 5.2 Regulatory information

The legal definition that an advanced material fulfils determines how it is covered by legislation and which specific requirements apply. The most important information deduced from the applicability of definitions is whether or not the substance definition under REACH is fulfilled. If this is the case, registration may be required if a manufacturing or import volume of 1 t/a and per actor is exceeded. If a registration is required, information on hazards, uses, exposures and risks may be available according to the tiered requirements defined in the annexes of REACH. Hence, if it is clear which legal definition is fulfilled, at least a "theoretical data availability" at present and in the future (with increasing volumes) can be deduced. Additionally, the applicable definition also indicates the possible implications on its risk management, e.g. which (legal) instruments could be used.

The REACH regulation includes definitions of the terms, substance, polymer, mixture and articles.<sup>19</sup> It also includes a description of the term "nanoform of a substance" in its Annex VI, which is based on the Commission's Communication (COM 2011) on a definition of nanomaterials. These definitions apply to any product placed on the market.

If substances or mixtures are used in particular applications, namely pharmaceuticals, biocidal products or plant protection products, additional definitions may apply, such as "active substance" or "co-formulant". These, and further definitions included in EU legislation were not considered in the evaluation of the regulatory situation of an advanced material. Table 13 provides a brief overview of the definitions under REACH Article 3 and its Annex VI (nanoform) and the implications on data availability and risk management.

Regulatory status	Definition according to REACH	Implication on data availability	Implications on risk management
Substance	means a chemical element and its compounds in the natural state or obtained by any manufacturing process, including any additive necessary to preserve its stability and any impurity deriving from the process used, but excluding any solvent which may be separated without affecting the	If placed on the market above 1 t/a per actor, hazard, use, exposure and risk information available,	Classified and labelled according to existing data under C&L regulation

#### Table 13: REACH definitions and implications on data availability and risk management

<sup>19</sup> The definition of intermediates is not discussed and analysed in relation to advanced materials as only those materials reaching the market (i.e. the "final product") is of interest.

Regulatory status	Definition according to REACH	Implication on data availability	Implications on risk management
	stability of the substance or changing its composition;	depending on the applicable Annex of REACH. If below 1 t/a per actor, no particular data requirements	May be subjected to REACH risks management procedures (evaluation, authorisation, restriction)
Nanoform of a substance	is a form of a natural or manufactured substance containing particles, in an unbound state or as an aggregate or as an agglomerate and where, for 50 % or more of the particles in the number size distribution, one or more external dimensions is in the size range 1 nm-100 nm, including also by derogation fullerenes, graphene flakes and single wall carbon nanotubes with one or more external dimensions below 1 nm. 20	As for "substances" with additional requirements for nanoforms	As for "substances" classification may differ for nanoform
Polymer	means a substance consisting of molecules characterised by the sequence of one or more types of monomer units. Such molecules must be distributed over a range of molecular weights wherein differences in the molecular weight are primarily attributable to differences in the number of monomer units. A polymer comprises the following: (a) a simple weight majority of molecules containing at least three monomer units which are covalently bound to at least one other monomer unit or other reactant; (b) less than a simple weight majority of molecules of the same molecular weight. In the context of this definition a 'monomer unit' means the reacted form of a monomer substance in a polymer;	Polymers do not have to be registered. Hence, little hazard, use and exposure information are publicly available	Classification and labelling based on available data May be subject to authorisation or restrictions
Mixture	means a mixture or solution composed of two or more substances;	No specific data collection required. Hazard assessment part of C&L Safety assessment only for substances in mixtures and REACH CSR is required	Classification and labelling based on ingredient information and/or mixture testing; certain hazards may be overlooked
Article	means an object which during production is given a special shape, surface or design which determines its function to a greater degree than does its chemical composition;	No registration or classification.	Communication of SVHC content if above 0.1% to article recipient

<sup>&</sup>lt;sup>20</sup> For this purpose, "particle" means a minute piece of matter with defined physical boundaries; "agglomerate" means a collection of weakly bound particles or aggregates where the resulting external surface area is similar to the sum of the surface areas of the individual components and "aggregate" means a particle comprising of strongly bound or fused particles. (REACH Annex VI)

The assessment and decision of which definition an advanced material fulfils may be challenging because of several reasons, among others that:

- the structure of an object is not (yet) well reflected in the definitions but is an important feature of advanced materials that determines their properties;
- it is not always obvious which type of bonds exist between components of an advanced material, i.e. if their production is to be regarded as synthesis or a mixing resulting in a structured particle;
- the decision whether the function of an advanced material is determined more by the chemical composition or its structure and, if advanced materials could be regarded articles as the original intention behind that definition was to capture "macro-size" objects rather than materials;
- some advanced materials are active, i.e. change their structure or energy level during use, which may result in a change of identity;
- the polymer definition as such is already challenging to apply to non-advanced materials and information may not (yet) be available to assess, if it applies. In addition, the term polymer is used in the scientific context with another meaning than in the regulatory definition.

Depending on the use of advanced materials, different product legislation may apply, which may concern substances, mixtures or articles/complex objects. For uses as substances and/or mixtures, legislation on pharmaceuticals and medicinal products, cosmetics, biocidal products and plant protection products, as well as detergents may be relevant. These legislations include, to a different degree, data generation, collection and assessment requirements for manufacturers, importers and/or placers on the market which are (partly) evaluated by authority decisions (e.g. substance or product authorisation).

Furthermore, food safety and food contact materials legislation may apply to respective uses. Requirements may also exist here that concern the assessment and/or use of advanced materials in this type of products.

Uses in some further (consumer) products, which may be articles or complex objects (consisting of several articles or complex objects), such as electrical and electronic devices, vehicles or toys have separate legislation. However, no data has to be generated and assessed just the restrictions have to be implemented. Currently, these legislations either refer to particular substances or to substances with a particular classification. Substances with a particular classification may also be advanced materials.

In the factsheets for the various advanced materials it is specified, which regulatory definition the advance materials fulfil albeit only if this is unambiguous and/or stated in reliable information sources. However, in most cases it is not clear, which of the definitions apply, and this may also differ within a cluster (potential case-by-case decision). In this case, a list of potentially applicable definitions is provided in the factsheets.

The applicability of product legislation to an advanced material depends on their fields of application. Therefore, no list of legislation is provided.

## 5.3 Use of the factsheets in the project

The factsheets supported certain aims and tasks in the project, including to:

- Derive specific questions on advanced materials and/or specific clusters of advanced materials for the online survey, i.e. aiming at filling the "major gaps" and/or verifying initial conclusions on commonalities or applications in the class;
- Provide structured and understandable information to the general public and the authorities on advanced materials in form of factsheets, which are provided as separate document;
- Initiate a discussion on the types of discrete advanced materials clusters that the (national/EU) authorities agree to focus on in their monitoring and relevance assessment;
- > Provide an information basis for a first relevance assessment of selected advanced materials;
- Highlight areas of information gaps and lack of knowledge and hence provide a basis for priority setting regarding information collection and/or selection of types of advanced materials for regulatory scrutiny and further work.

## 5.4 Extent of elaboration

The factsheets are elaborated for different types of advanced materials (cf. separate document with factsheets). It is highlighted that the factsheets are only the starting point for describing the various advanced materials and neither claim to be complete nor final with a view to the selection of described clusters. Furthermore, for some material classes, sub-groups are mentioned but no factsheets exist for these, partly due to resource constraints, partly it was not obvious whether differentiation is necessary or not. The information sources used to compile the factsheets are:

- 1. A literature research on the topic "advanced materials";
- 2. Expert interviews;
- 3. Presentations and discussions at the first thematic conference;
- 4. Additional targeted information collection from literature and an online survey.

### 5.5 Structure of the factsheets

The factsheets are separated into several sections:

General information

Under this section, a working definition of the materials is provided as well as common synonyms and a description of the main building blocks and the main structural characteristics within the cluster. Obvious and potentially confusing overlaps with other material clusters are pointed out and sub-groups are listed. Differences between the subgroups are particularly highlighted in the subsequent sections, where relevant and known to the authors. Furthermore, their specific functionalities are described.

Applications

In this section known application areas are listed (for specific sub-groups where relevant) and the development stage of the advanced materials is indicated. This information is

anecdotal due to the large number of (potential) applications already on the market and/or still in the research phase.

Regulatory information

This section only includes information on the legal status of an advanced material type; i.e. which definition it fulfils, if it is either obvious and could be assessed by the team or if it was stated so by authorities. A discussion of implications of the regulatory status and potentially applicable legislation is not provided in the factsheets (cf. Section 5.2).

Information on potential risks

In this section, general information on factors influencing the hazard, exposure and risk from the advanced materials cluster are compiled in a table. A detailed assessment could only be performed here for specifically defined materials and the more generic information in this section is only an approximation. In general, it is assumed that little information is available on the adverse (eco-)toxic effects of advanced materials and their behaviour in organisms/humans and the environment. This is confirmed by the overall impression from the literature analysis, which mainly focuses on the functionalities and design of materials.

Information on environmental impacts and material circularity With regard to the increasing discussions on the circular economy and the assessment of life cycle impacts (e.g. on critical resources and energy consumption), in this section respective information is compiled. As little data are published in this regard, the section is usually very short.

## 5.6 Initial list of advanced materials covered by individual factsheets

The following (partly overlapping) clusters of advanced materials were described via <u>factsheets</u> in this project.

- 1. Biopolymers (Materials based on naturally occurring polymers, which are designed for a specific functionality)
  - a. DNA-based Biopolymers
  - b. RNA-based Biopolymers
  - c. Protein-based Biopolymers
  - d. Sugar-based Biopolymers
  - e. Lipid-based Biopolymers
- 2. Composites (combination of two or more materials)
  - a. Macroscopic Composites
  - b. Hybrid Materials (Materials that are a combination of organic and inorganic materials)
  - c. Fibre-reinforced Composites
  - d. Particle-reinforced Composites
- 3. Porous materials (Materials which show a porous structure, differentiated by pore size)
  - a. Microporous Materials

- b. Mesoporous Materials
- c. Macroporous Materials
- 4. Metamaterials (Materials with properties that go beyond the naturally occurring properties of their components)
  - a. Electromagnetic Metamaterials
  - b. Acoustic Metamaterials
- 5. Particle systems (properties of the materials are related to their particles' structure)
  - a. Quantum Dots
  - b. Supraparticle
  - c. Nanoflowers
  - d. Graphene
- 6. Advanced Fibres (fibres several  $\mu m$  or smaller in diameter with an intended functionality)
  - a. Organic Fibres
  - b. Carbon-based Fibres (incl. CNTs)
  - c. Inorganic Fibres (e.g. silica)
- 7. Advanced Polymers (Polymers with an intended functionality)
  - a. Electro-active Polymers
  - b. Magneto-active Polymers
  - c. Self-repairing Polymers
  - d. Co-polymers
- 8. Advanced Alloys (Alloys, which comprise more than two components; at least two components have a large share in the final material)
  - a. Advanced Alloys

The factsheets are provided as a separate document<sup>21</sup> pertaining to this report. It is again stressed that these should be considered as living documents that compile information collected by the project team on the different materials. They neither claim to be comprehensive or complete, nor are they based on a systematic and comprehensive literature research.

<sup>&</sup>lt;sup>21</sup> https://oekopol.de/archiv/material/756\_AdMa\_Factsheets\_final.pdf

# 6 Findings and conclusions on the field of advanced materials and its critical areas

### 6.1 Identified definitions and classifications of advanced materials

Regarding advanced materials some attempts to define or delimit the field do exist. These concepts mainly focus on the applications of the advanced materials and identify the development of materials with new and outstanding functionalities as the specific criteria of the field. Definitions of this kind were considered to be limited in their value because new or specific functions have always been a driver of new developments in the field of materials. A characterization of a change of design and the manufacturing practice as a general paradigm is proposed to be more beneficial for delimiting the field. Therefore, a delimitation of advanced material as **materials that are rationally designed in order to fulfil the functional requirements of a certain application** is suggested. It was used to delimit "advanced materials" from those that are regarded as "non-advanced" and thereby guiding the work in this project.

Approaches to structure the field of advanced materials also differ a lot. Some classes of advanced materials are related to the composition of the material, some to their functionality and others to their production process. Table 14 summarizes all identified classifications in six thematic clusters to illustrate the main focus areas of advanced materials.

Cluster of advanced materials	Synonyms	Description	Existing in classification of
Active materials	smart, functional, multifunctional, adaptive	active materials are able to modify any of their properties	DAMADEI, L&M, TIP, TSB, MatSEEC
Composites	advanced composites, composite materials,	composites represent combinations of two or more materials	DAMADEI, L&M, TIP
Structural materials	structured materials, multi-structural, artificially structured	structural materials are structured in two or three dimensions	DAMADEI, L&M, TSB, MatSEEC
Nanomaterials	nanotechnology	at least one of the dimensions nanomaterials is in the range of 1 to 100 nanometres	DAMADEI, L&M, TIP, TSB
Biobased materials	biomaterials	biobased materials either represent materials applied to a biological system or materials derived from a biological source	TSB, MatSEEC
Advanced manufacturing	advanced processing	advanced manufacturing relies on adding or removing material through virtual geometry, without the use of pre- shapes and without subtracting material	DAMADEI

Table 14: Six identified clusters from the evaluation of classifications on advanced materials

### 6.2 Scientific activity on advanced materials

The expert survey on advanced materials revealed that around 25 % of the respondents think that scientific interest in an advanced material is an indicator of its relevance (see Annex B). The scientific activity (number of publications) on advanced materials was diverse, but dominated by material science. A steady increase in scientific activity, especially in the last decade, could be detected. The author landscape is multi-centric, comprising few bigger author groups and a lot of little independent author groups. The most active group of authors is a group of material sciential scientials and China.

In general, the functionality or activity of a material seems to play a major role in advanced materials science. The terms *functional, smart* and *active* were detected to be used often in the context of advanced materials. New types of manufacturing and processing, like e.g. 3D-printing, are also discussed heavily in scientific literature. Nearly no advanced material consists of a single substance. In the expert survey, more than 50 % of the respondents consider the potential future applications and the inherent properties of an advanced material as an indication of relevance.

The field of advanced materials greatly overlaps with the research area of *nanomaterials*. As confirmed by expert interviews, nanomaterials and advanced materials can hardly be separated from each other. *Polymers* seem to play an important role for several advanced materials. Nearly all materials discussed as advanced materials are *composites*. Most materials show complex structures and comprise at least two different building blocks. The type of binding varies a lot between different advanced materials, ranging from loose particles in a matrix to strongly connected hybrid materials. From comparatively weak binding by e.g. Van der Waals Force to tight covalent bonds, a broad variety is used meanwhile. The strong focus on composites as well as the prominent role of polymers was already present in early studies (OTA 1988).

In the expert survey the majority of the respondents have the opinion that increasing abilities to tailor and design advanced materials' properties correlate with an increase in the number of different application areas. Advanced materials comprising of macroscopic structures belong to the most developed classes with already a number of applications. Materials with comparably small structures or subunits as well as biological materials are rather still in a research stage with only a few products that entered the market up to now. The qualitative investigation of the scientific literature has shown that in regards to applications the most emerging sectors are *electronics* and *medical applications*. Especially wearable electronics, but also other uses of flexible electronics play an important role. In addition, uses of electronic materials like supercapacitors or batteries are emerging fields of research and development. In this context coatings are also frequently discussed. Regarding medical applications, soft materials as well as polymers play an important role. Also, nanostructures as well as the ability of a material to change its properties represent emerging fields of research. Following this, assessment frameworks in the area of pharmaceuticals and medical products, in particular respective legislation, may have to be assessed with regard to their ability to deal with advanced materials. The area of electronics is vast and through electrical and electronic equipment, advanced materials may enter consumer products and various different markets. This indicates a widespread use with related exposure potentials, in particular from the waste stage of these products.

### 6.3 Relevance of advanced materials

An assessment framework was developed during the project to support assessing the relevance of advanced materials. Relevance is understood as either giving rise to concerns for chemical safety or with regard to the circular economy, with a clear focus on the former aspects. The assessment framework consists of several criteria and pertaining indicators that would allow a systematic relevance screening. The criteria cover the areas:

- 1. Science properties and functionalities
- 2. Technology and markets potential exposure levels
- 3. Hazard and risk hazardous properties and critical exposures
- 4. Regulatory challenges coverage of legislation and applicability of assessment approaches
- 5. Circular economy hindering recycling of (advanced) materials

While for each of these several indicators could be defined, only some of these actually qualified for the screening assessment framework. This is due to the fact that many indicators in the area of science, technology and markets are ambiguous and difficult to interpret with regard to chemical risks.<sup>22</sup> Secondly, for many of the potential indicators no or too little data is available to use it for screening. Hence, although it is highly valuable to evaluate the relevance of an advanced material, these indicators are unlikely to be actually used in a screening assessment. The lack of information as such or for specific (very important) relevance criteria may also indicate a relevance, as they show a need to generate more/new data.

The desk work undertaken to develop the screening level assessment framework, the related discussions, the results from the online survey and the literature research confirmed the starting hypothesis that assessing potential hazards and risks from advanced materials is more complex than for "non-advanced" ones. This is mainly due to:

- the high variability of materials and technologies that fall under the concept of advanced materials and which makes it impossible to develop a generic assessment strategy; this means the screening concept is unlikely to derive fully comparable results regarding the identified "level of relevance"
- the composition of advanced materials frequently being a mixture of building blocks which may themselves be a combination of different substances
- many advanced materials containing nanomaterials, which require additional considerations than substances at larger scales to identify hazards and physical-chemical properties, like the reactivity
- the need to consider whether or not the building blocks of an advanced material could be released and in which form (degradation products) during use or the waste stage in determining hazards
- the lack of information on the actual applications of advanced materials, including conditions of use and the extent of market penetration and market volumes

<sup>&</sup>lt;sup>22</sup> For example, a high number of research calls on a particular advanced material may indicate that (pilot) applications may enter the market soon (with the related exposure potential increasing) or may be due to a perceived need for fostering a particular technology without any direct output in terms of marketable products. The number of patents cannot be related to an actual market success. The types of properties of an advanced material may indicate potential areas of application but whether or not these actually become reality can hardly be predicted.

 lack of information and experience on the persistence/stability of advanced materials during use, disposal and in the environment or the human body.

Therefore, also the screening level assessment is more challenging and may have to rely on a few number of indications of concern regarding chemical safety or the circular economy and/or use the "overall lack of information" for an advanced material as an indicator of relevance.

The information in the factsheets could be used to do a screening level relevance assessment of the respective advanced material class. The factsheets may be used as starting point for such relevance assessments.

### 6.4 Identified material classes and their critical aspects

From first expert interviews and a consultation of scientific literature three dimensions of the design of an advanced material were identified. A new functionality is achieved by:

- manufacturing a material with a pre-determined arrangement of an entirely new structure of one or several substances
- ▶ the interaction of two or more substances and/or
- the combination of different structures of one or several substances.

This was taken as a prerequisite for the identification and structuring of potentially relevant material classes. Guided by the aim of rational design (see Section 3), the authors identified 26 classes of advanced materials comprised in 8 clusters without a claim to completeness. Besides a short characterization of the classes, easily available information on existing or planned applications, potential hazards and risks, environmental impacts and the regulatory status were compiled in the factsheets, which are provided as separate background document<sup>23</sup>.

When viewing these classes it is obvious that the new functionalities require the existence of (highly organised) and designed structures. Furthermore, there are only few classes of advanced materials with only one type of building block or consisting of only one substance like some porous materials or fibres. This confirms that also the composition of materials is an important parameter for the new functionalities. It is reflected by the frequent occurrence of the term "composite". Nanomaterials are not included in the developed list of advanced materials classes because they appear to be an important building block of many different materials rather than being a class in themselves.

As visible in Table 14 as well as from the factsheets, the field of advanced materials is very divers. Especially regarding substances and building blocks as parts of composites a large number of combinations is possible. Even so most of the building blocks are not new, new structures, combinations of substances as well as manufacturing techniques may change their risk relevant properties. However, the participants of the expert survey had mixed opinions when asked, if the ability to predict the target (technical) properties of advanced materials correlates with the ability to predict its hazardous properties<sup>24</sup>. But information on the toxicity and ecotoxicity of either the building blocks and/or the advanced material as such are regarded as crucial for risk assessment, while potential carrier effects and the future uses are of lower relevance. Reliable hazard data are frequently missing and statements on their potential risk are

<sup>&</sup>lt;sup>23</sup> https://oekopol.de/archiv/material/756 AdMa Factsheets final.pdf

<sup>&</sup>lt;sup>24</sup> Approximately 42 % do and 25 % do not see a correlation. 25 % answered they do not know. The remaining participants did not provide an answered or had no specific opinion.

complicated by vague knowledge of the application contexts and possible release rates (and potential hotspots of release). They can only be roughly based on indications that are derived from morphology, physicochemical parameters or experience with materials that are already in use.

In the following passages, the most relevant hazards and risks that have been identified for the advanced materials classes investigated in this study (see separate document with the compilation of factsheets) are summarized.

Materials can be characterized as critical due to two factors:

(a) their hazard potential (caused by e.g. a critical morphology, high reactivity)

(b) their exposure potential due to properties supporting spread, persistence and accumulation or applications with high release into the environment.

For *biopolymers* based on DNA, RNA, proteins, sugar or lipids it cannot be excluded that they may have immunogenic potential in humans or animals. Since the development of corresponding products is not yet close to the market, only preliminary information is available on their uptake by the human body as well as their immunogenic impact (Ige et al. 2012). But as they shall be directly applied in the human body (e.g. as drug carriers) already small exposure rates can be expected to have great impacts. Besides this, the degradability of synthetic biopolymers is unclear. Not all synthetic structures may be accessible for enzymatic digestion or other processes of decomposition. In particular biopolymers made of xenobiotic monomers could contribute to enhanced exposure by prolonged persistence in natural compartments.

The identified advanced material class of *hybrids* is hard to assess in terms of risk as a whole, since hybrid materials differ largely with regard to their building blocks and material structure. Due to the fact that all hybrids share the ability to incorporate different substances to achieve new properties, an improved stability and in some cases, possibly also a specific reactivity of the material might lead to new risks. Moreover, when these composites are processed during manufacture or degrade during use or by weathering, it cannot be excluded that constituent particles or parts of the matrix are released.<sup>25</sup>

Next to several applications in other sectors, *porous materials* are discussed to be used in biomedical applications. At present, there is a lack of clinical trials and in vivo screening. A reason for concern common for all porous materials as entities with low density e.g. aerogels is that their impact may be underestimated at mass-based thresholds e.g. for effects on the respiratory tract. Here, a volume-based consideration is more appropriate.<sup>26</sup>

Two further identified advanced material classes are *fibre-reinforced and particle-reinforced nanocomposites*. In relation to their combination of structure and size (or size of building blocks) spread, uptake and exposure in case of a degradation of the material (Wohlleben and Neubauer 2016) are unclear. The related risk might differ significantly between different materials within these classes. The release of fibres or particles by weathering or abrasion cannot be excluded and are particularly relevant for the use as food-contact materials or when indoor applications lead to increased exposure by respirable dust.

*Quantum dots* may affect cell growth and viability and can be cytotoxic. Some constituent substances are highly toxic and therefore potentially increase health risks, especially in combination with unintentional uptake as an aerosol or solution. In relation to the planned

<sup>&</sup>lt;sup>25</sup> Cf. 1st Thematic Conference "Rational Design of Advanced Materials", results of the working group on potential risks, December 5-6, 2019, German Environment Agency (UBA), Dessau, Germany

<sup>&</sup>lt;sup>26</sup> Ibid.

medical use of quantum dots, uncertainties about kinetic behaviour and a probably high mobility (depending on size and coatings) exist. In addition, their potentially high persistence leads to prolonged exposure when released into the environment or taken up by organisms.

The preparation of *nanoflowers* is sometimes carried out under extreme conditions where toxic by-products may form. Nanoflowers are described as highly stable, depending on the synthesis process. Increased persistence may therefore contribute to exposure. But their structural stability in intended applications and the environment is currently unknown. However, the high surface area of nanoflowers may cause unintended effects such as enhanced catalytic activity or immunogenicity. Furthermore, recuperation with intact surface structures is technically challenging and a practical realization appears unlikely, even for high value materials.

*Graphene* has already been discussed a lot and covered by REACH since it is a nanomaterial. Nevertheless, some applications of graphene may lead to further risk relevant aspects. Graphene sheets, for example, may harm cells due to sharp edges which may induce direct physical damage to the cellular membranes (Li et al. 2013). Depending on the exposure concentration Graphene can be considered as phytotoxic and as inhibiting plant growth (Wang et al. 2019). Graphene oxide, a derivative of graphene may induce pulmonary thromboembolism, act cytotoxic or lead to an inflammatory response (Singh et al. 2012, Shi and Fang 2018, Bussy et al. 2015). Furthermore, since graphene is a rather persistent material, it may lead to long term effects in tissues and organs (Shi and Fang 2018).

Advanced fibres are another class of advanced materials that was identified as risk relevant. Fibres with asbestos-like dimensions (WHO fibres) are considered carcinogenic by inhalation. Fibres may break during use and/or disposal and hence become WHO fibres. Large releases of short carbon fibres and CF dust from fires in CF reinforced structures (e.g. aircrafts, cars) is possible. Short fibres which may be produced intentionally or due to abrasion during use are respirable. A reason for concern in terms of exposure potential is their chemically inert character that leads to high persistence.

Regarding polymers a number of critical aspects are already well known but still represent a reason for concern: Although some *co-polymers* have already been used for a long time, some critical issues have to be considered. During use, nanoparticles may be formed by abrasion and might be inhaled or ingested. Abrasion resistance varies between different co-polymers. Many copolymers emit toxic fumes upon decomposition. Additionally, in terms of exposure potentials, high persistence in environmental compartments has to be expected and needs to be considered for applications where release may occur. For the class of *self-repairing polymers* it is important to consider that some of the chemical substances used are classified as hazardous and also some of the gels used to create *electro-active polymers* are toxic.

For *supraparticles* it can only be speculated that destabilization may cause the formation of nanoparticles with respective hazardous properties.

Next to the toxicological aspects, in opposition to the background of the guiding principle of a circular economy, the recyclability of materials is an important feature that should be considered when developing new materials for emerging technologies and the improvement of already used processes and products. In this regard, three questions are relevant:

- 1. Could advanced materials, due to potentially hazardous substances contained in them, contaminate waste and recycled secondary materials (toxicological challenges)?
- 2. May advanced materials disturb recycling processes (technological challenges)

3. Will advanced materials be used in products from which they can be recovered; i.e. will the products containing advanced materials be collected and sorted and will the valuable structure of the advanced materials be conserved during a potential recovery and recycling (organisational and technological challenges)?

In several classes of advanced materials, different building blocks are connected to the nano- or microscale (cf. Drisko and Sanchez 2012). In the light of the current problems with composite materials at higher scale (e.g. blades of wind turbines, see Naqvi et al. 2018) the constituents of the new fine structured composites like hybrid materials, nanocomposites and metamaterials will most probably not be separated after their use.<sup>27</sup> Regarding carbon-based fibres for example, recycling is not performed, because in most (currently known) applications, the fibres cannot be efficiently separated from the surrounding polymer. Research on pyrolysis as an option to successfully separate carbon fibres is ongoing (Naqvi et al. 2018). Hybrid materials also cannot be disassembled with reasonable effort until now (Knappich et al. 2017). All in all regarding the majority of complex composite materials, reuse (or even recycling) is currently unlikely, even though, research is ongoing.

In the course of this analysis recovery and recycling (maintaining the integrity of the materials' structures) of a number of advanced materials was identified as critical due to managerial, technical and economic reasons. In any case, the separation of advanced material containing components from those, which do not contain them appears a crucial pre-condition for the extraction from the overall waste streams.

The relevance of an advanced material for a closer assessment may also result from a lack of current legal coverage or an (assumed) lack of possibilities to adequately address and control any possibly existing risks. The first step in determining the legal coverage is an assessment of which definition applies to an advanced material. This step requires information on its composition as well as on how the building blocks are physically interlinked. However, due to the novelty of advanced materials and the importance of the structure of the building blocks, the existing definitions cannot be easily applied and different interpretations are frequently possible. For example, the article definition under REACH requires that the form, structure or design of an object are more important for its function than the chemical composition. Deciding whether or not this definition applies (and hence, no registration is required of the advanced material but possibly its building blocks) is not always possible with high certainty. Two of the advanced materials clusters identified in this study are called "polymers": biopolymers and advanced polymers. However, it is unclear if these substances actually fulfil the polymer definition.

Secondly, the legal coverage also depends on the application of an advanced material: uses as active substances, such as in pharmaceuticals, biocides or plant protection products would require a thorough safety assessment by the placer on the market and the authorities, including the need to generate respective information. Uses in other applications, such as cosmetics, may also involve a certain safety assessment process. As many advanced materials are still in the development process, the possibilities for (later) risk management cannot be fully determined.

<sup>&</sup>lt;sup>27</sup> From 1st Thematic Conference "Rational Design of Advanced Materials", results of the working group on potential risks, December 5-6, 2019, German Environment Agency (UBA), Dessau, Germany

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# A Appendix: Questions of the online survey

### A.1 Opening page

The current online survey aims at collecting expert opinions and input on different issues regarding advanced materials, the possible benefits, e.g. for the environment and resource protection, energy and climate protection, mobility and health from their application in different types of products and processes as well as the potentially related risks.

The survey takes place in the context of the research project "Advanced Materials – Thematic Conferences: Assessment of the need to act on chemical safety" funded by German Federal Ministry for the Environment, Nature Conservation and Nuclear safety and commissioned by the German Environment Agency. For further details, please find a brief description of the project <u>here</u>.

The survey addresses researchers in academia, industries and authorities working on/with advanced materials. It is divided into a section with questions relevant for any type of advanced materials and questions that should be answered for particular types of materials (e.g. metamaterials etc.).

#### A.2 General questions about the Responder and affiliation

Name of the institution (obligatory)

Website of the institution (voluntary)

Name and e-mail address of the responder (obligatory)

Please fill in your name and e-mail address. This is only for internal purposes and, in case we have questions about your answers, to approach you for clarification.

#### Assign yourself to one of the following stakeholder groups:

- Academia
- Private research
- ► Industry
- Consulting
- Public authorities
- Other (please specify)

#### Free text field to specify other institutions

CONSENT TO PRIVACY POLICY	CLICK_1
I AGREE TO BE CONTACTED BY ÖKOPOL GMBH FOR THE PURPOSE OF FURTHER QUESTIONS REGARDING MY ANSWERS	CLICK_2
I AGREE TO BE CONTACTED BY ÖKOPOL GMBH FOR THE PURPOSE OF REQUESTS FOR A POSSIBLE LECTURE AT ONE OF THE PROJECT'S THEMATIC CONFERENCES	CLICK_3

#### A.3 Questions on relevance of advanced materials

It is one aim of the project to identify advanced materials that are relevant for chemical safety. An advanced material could be regarded as relevant due to several reasons, in particular if:

- ▶ There are indications that risks for human health and/or the environment could occur
- The existing approaches to hazard identification, exposure and risk assessment (including e.g. modelling or testing approaches) cannot be applied
- There are indications that a material is not (sufficiently) addressed under current (chemical) legislation
- Its use may cause or be related to other significant unwanted impacts on the environment, such as high energy consumption or resource use
- A material might hinder waste processing, in particular recycling and the circular economy.

It is one aim of the project to identify criteria that support an initial screening of relevance, based on which advanced materials could be prioritised for further action. Please indicate your agreement with the following statements (1 = fully agree, 2 = agree, 3 = neutral, 4 not agree, 5 don't know)

# To what extent could the "scientific interest in" and the "novelty" of an advanced material be an indication of potential relevance?

- The novel (combination(s) of) properties allow deducing potential future uses and the functionalities advanced materials enable or support
- The more an advanced material's properties can be tailored, the more different applications they may be used in
- With an increasing ability to predict the technical (target) properties of an advanced material also the information basis on potentially hazardous properties will increase
- The number of scientific publications are an indication of relevance
- The relevance of advanced materials is more determined by the future application than by their inherent properties obtained by targeted design

#### If I had to assess risks from an advanced material I would focus on gathering ...

- hazard information on the advanced material as such
- hazard information on the building blocks of the advanced material and its potential to release these building blocks
- ▶ information on the (future) applications of the material
- don't know

# Please rank the following information types according to their ability to indicate risks from advanced materials

If you had to identify those (clusters of) advanced materials that pose the highest (eco-)toxic risks to human health or the environment, which information would you need the most?

- Acute or chronic toxicity to human or environmental organism by the advanced materials' building blocks: carcinogenicity, reprotoxicity, mortality, or endocrine disruption.
- Behaviour in the environment, in particular persistence / biodegradation and bioaccumulation potential
- Particle properties (surface area, zeta potential etc.)
- Production and use amounts
- ► Types of (intended future) uses
- ▶ Behaviour in the human body and/or the environment
- > Potential to act as carrier (intended (e.g. medical applications) or unintended)

#### A.4 Question on Clustering of advanced materials

In the scope of the UBA project, it was decided to cluster advanced materials in order to facilitate monitoring their occurrence of the market and structure the assessment of potential benefits and risks. Being aware that there are many different ways of clustering and that there are always overlaps and "grey zones", the following clusters were formed, of which several have sub-groups (indicated in brackets):

- Biopolymers (DNA-based, RNA-based, Protein-based and Sugar-based)
- Hybrid Materials
- Porous materials (microporous, mesoporous, macroporous)
- Nanocomposites (fibre-reinforced, particle-reinforced)
- Metamaterials (photonic, acoustic, electromagnetic)
- Particle systems (Quantum Dots, supraparticles, graphene, nano flowers)
- Advanced Fibres (carbon-based fibres (incl. CNTs), non-carbon based fibres (e.g. silica))

- Advanced Polymers (electro-active polymers, magneto-active polymers, electro-rheological fluids, self-repairing polymers, co-polymers)
- Advanced alloys (High entropy alloys)

#### Please comment on this clustering approach

- One or several clusters are missing (please specify)
- One or several clusters are superfluous (please specify)
- One or several clusters could be combined
- One or several clusters should be further differentiated
- No comment

Free text field for specifications

#### A.5 Specific expertise

# Please specify your main area of expertise with regard to types of advanced materials (maximum two)

This information will be used to select about which clusters of advanced materials specific questions will be posed to you in this online survey

- Biopolymers
- Hybrid Materials
- Porous materials
- Nanocomposites
- Metamaterials
- Particle systems
- Advanced Fibres
- Advanced Polymers
- Advanced Alloys
- ► No specific expertise
- ► Other

### A.6 AdMa specific questions

The following questions were asked for each of the following clusters of advanced materials. Biopolymers, Hybrid Materials, Porous materials, Nanocomposites, Metamaterials, Particle systems, Advanced Fibres, Advanced Polymers, Advanced Alloys

#### A.6.1 Characterisation of the Cluster [## Name of the cluster]

#### Which sub-groups would you define for the cluster of [##Name of the cluster]?

The following sub-groups are proposed by the project team

- ▶ I think the most relevant sub-groups are covered by that list
- ▶ I would delete certain sub-groups (please specify)
- ► I would add certain sub-groups (please specify)
- ▶ I would merge certain sub-groups (please specify)
- ▶ I would further differentiate certain sub-groups (please specify)
- ▶ I have no particular opinion on this

Free text: please specify which sub-groups you would delete/add

#### Please provide comments on our working definition of [## Name of the sub-group]

- ▶ I agree with the working definition
- ► I suggest amending the working definition (please specify)
- I cannot comment

Free text: please specify how you would define the sub-group

# Is it possible to assign a certain functionality as a common feature to cluster of [## Name of the cluster]?

- Yes (please specify)
- No
- Don't know

Free text: please specify which functionality

### A.6.2 Application(s)

#### Please characterise the state of economic development of the [## Name of the cluster]

- ► Basic scientific research
- Research on specific applications
- Introduced to the market
- ► Use is common
- ► Other

# Please name the 3 most important (future) applications of advanced materials belonging to the cluster [Name of the cluster] you are aware of

3 Free text fields

# How would you estimate the role of [Name of the cluster] in technological innovations in the future?

- very important
- ▶ important
- niche applications
- don't know

#### A.6.3 Regulation and risk assessment

# Which regulatory definition as provided by the EU REACH regulation do [##Name of the cluster] fulfil (most likely)?

- Substance
- Mixture
- Polymer
- Article
- None of these
- ► Other
- Don't know

Free text field: Please specify why you think that the specific definition is applicable

# Which information do you have about the adverse effects (toxicity, carcinogenicity etc.) of [## Name of the cluster]?

#### Free text

Which information do you have about the behaviour of [## Name of the cluster] in the environment or in organisms (e.g. stability/persistence, bioaccumulation, release of substances etc.)?

#### Free text

# What do you regard as the two core challenges for hazard assessment of [##Name of the cluster]?

- Information on hazards of building blocks/constituents of the advanced materials are missing
- Hazards cannot be deduced based on information from the building blocks/constituents
- > Appropriate test methods to identify hazards are missing
- Lack of (applicable) computational and alternative testing methods to determine hazards, e.g. QSARs
- Lack of requirements to make hazard assessments
- Lack of certainty whether or not advanced materials will enter the market and hence, whether any testing will pay off
- ► Other

Free text field: please comment and potentially specify your answer with regard to the sub-types

# What do you regard as core challenges for exposure and risk assessment of [##Name of the cluster]?

- Information on uses and related emissions of advanced materials is missing
- Information on the stability/persistence (during use and disposal and/or in the environment) is missing
- Exposure and risk assessment tools cannot be applied
- Lack of requirements to make exposure/risk assessment
- ► Other

Free text field: please comment and potentially specify your answer with regard to the sub-types

#### A.6.4 Information on environmental impacts and material circularity

# Which types of environmental impacts do you associate with the production and use of [## Name of the cluster]

#### Positive = net benefit for society and environment Neutral = no effect Negative = net deficit for society and environment

Impact	Positive	Neutral	Negative	Don't know
Raw material use (positive = overall saving resources)				
Energy use (positive = overall saving energy)				
Durability / longevity of products (positive = longer lifetime)				
Substitution of hazardous substances or materials (positive = overall less hazardous substances used)				
Replacing the use of critical resources (positive = overall less critical resources needed)				
Improvements in medical diagnostics and treatment				
Circularity of material flows in general (positive = advanced materials could increase recycling or collection of materials; negative = advanced material is likely to hinder recycling or contaminate material streams)				
Potential to recover and recycle the advanced material from products at the end of their service life				

### A.7 Specific questions according to the material groups

#### A.7.1 Biopolymers

Do you see deficits in the provisions of EU pharmaceutical and biocides/pesticides legislation that might cause potential risks from biopolymers being overlooked?

Free text

Would you consider biobased polymers as fully biodegradable in the environment?

- ► Yes
- No (please specify)
- Don't know

Free text

### **Are you aware of any close-to-market applications of RNA-based Biopolymers? Which?** Free text

#### A.7.2 Hybrid Materials

#### How would you differentiate hybrids from composites?

- ▶ Hybrids are a subgroup of Composites.
- There are some overlaps between Composites and Hybrids.
- Hybrids and Composites can be clearly differentiated from each other.

#### **Please specify**

Free text

# From a regulatory or scientific/technical perspective, which sub-groups of hybrids would you form?

- Based on (combinations) of building blocks
- Based on scale
- ► Based on functionality
- Based on scale and functionality
- ► Others

Free text: Please explain how and why

#### How do you estimate the market potential of hybrids in the future?

- ▶ Hybrids will be used in many applications, they will be produced cost-efficiently soon
- ▶ Hybrids will be used in niche-markets for very particular applications
- > No general statement is possible as there are so many hybrids
- Don't know

#### What do you consider the most promising application of hybrids?

Free text

# Do you generally consider the decomposition of hybrids into their building blocks as reason for concern?

- ▶ No, because hybrids are so firmly bound that the components can hardly be separated
- ▶ No, because this will prevent any problems during waste treatment
- Yes, because hazardous building blocks may be released causing risks to the environment or human health
- > Yes, because it is unclear if hybrids will perform during use, e.g. in construction applications
- Other (please specify)

Free text

#### A.7.3 Porous materials

Do you think that structure of porous materials could in any regard pose potential risks to human health or the environment?

- No
- Yes (please specify)
- Don't know

Free text

#### A.7.4 Nanocomposites

On a scale from 1 (very likely) to 5 (very unlikely), how likely do you consider the release of fibres or particles from reinforced nanocomposites during use and in the environment?

#### How would you differentiate composites from hybrids?

- A) Hybrids are a subgroup of Composites.
- B) There are some overlaps between Composites and Hybrids.
- C) Hybrids and Composites can be clearly differentiated from each other.

#### Please give a reason for your answer

Free text

#### A.7.5 Metamaterials

#### Do you regard photonic materials as individual sub-group of metamaterials?

- Yes
- No
- Don't know

#### Please specify your answer

Fee text

#### How would you characterise the persistence of metamaterials in the environment?

- > Metamaterials are not degraded in the environment and are hence very persistent
- Metamaterials are degraded due to oxidation, sunlight etc. they are not persistent
- Depends on the building blocks of the metamaterial
- Depends on the structure of the material

- > Persistence in the environment is specific for each metamaterial
- Don't know
- Other (please specify)

#### A.7.6 Particle systems

How stable do you regard the following particle systems during use and in the environment on a scale from 1 (very stable) to 5 (very unstable leading to release of building blocks)?

- Quantum dots
- Supra particles
- Nanoflowers

What do you regard as the most important property or functionality of particle systems in processes or/products that could create environmental/societal benefits?

Free text

#### What do you regard as biggest challenge of using particle systems?

Free text

#### A.7.7 Advanced Fibres

No additional specific questions

#### A.7.8 Advanced Polymers

No additional specific questions

#### A.7.9 Advanced Alloys

#### Which types of alloys would you consider advanced and why?

Free text

# From a regulatory perspective, what could be reasons to prioritise them for further assessing action needs on chemical safety?

- ▶ Specific hazards exist due to the substance combinations in advanced alloys
- ▶ Risk assessment tools cannot be applied
- Advanced alloys should legally be considered as substances rather than mixtures to stimulate information generation

- Advanced alloys have such high benefit potentials that particular support and funding would be important to leverage respective applications
- Other (please specify)

Free text

### **B** Appendix: Summary of survey results

Thirty-one persons answered to the survey. The majority of answers was provided by public authorities (45 %) followed by industry and academia (both around 20 % of the answers). Answers were received from 6 EU Member States, the UK, the US and EU institutions.





Source: Own presentation

More than 42% of the survey participants believe that an improved ability to predict the technical properties of advanced materials will also lead to an improved ability to predict their hazards to human health and the environment. Around 25% of the respondents think that the number of scientific publications is a good indicator of relevance, whereas 40% do not see a correlation between two. The relevance of advanced materials is determined more by their future applications than by their inherent properties, according to the opinions of more than 50% of the respondents.

Figure 13 shows the importance given to different information types on advanced materials for conducting a screening level risk assessment. A high column represents a high importance.





Source: Own presentation

The graph shows that information on the toxicity and ecotoxicity of either the building blocks and/or the advanced material as such are regarded as crucial for risk assessment, while potential carrier effects and the future uses are of lower relevance. The clustering of advanced materials proposed in this report was introduced to the survey participants and feedback was collected on the types and number of different clusters. Overall, most participants found some type of change to that system useful with suggestions, both to merge and to further differentiate several clusters. Many comments concerned nanomaterials and hybrid materials as well as the question of whether or not a material should be considered advanced or not.

As the survey was then provided only for the area of expertise the respondents indicated, only few answers were received per material cluster, in many cases only one. Hence, these answers are not evaluated in general but any factual information or opinions on specific types of advanced materials are included directly in the factsheets.

### **C** Appendix: Literature examined in the qualitative literature analysis

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