Knowledge Base Materials Sustainable Science Communication on Advanced Materials

Katja Nau[1(✉)], Sara Espinoza[2], Harald F. Krug[3], Clarissa Marquardt[1], Andreas Mattern[4], Nadja Möller[2], Christoph Steinbach[2], and Dana Kühnel[4]

[1] Institute for Automation and Applied Informatics (IAI), Karlsruhe Institute of Technology (KIT), Hermann-Von-Helmholtz-Platz 1, 76344 Eggenstein-Leopoldshafen, Germany
katja.nau@kit.edu

[2] Society for Chemical Engineering and Biotechnology (DECHEMA), Theodor-Heuss-Allee 25, 60486 Frankfurt Am Main, Germany

[3] NanoCASE GmbH, St. Gallerstr. 58, CH-9032 Engelburg, Switzerland

[4] Department Bioanalytical Ecotoxicology (BIOTOX), Helmholtz Centre for Environmental Research (UFZ), Permoserstraße 15, 04318 Leipzig, Germany

Abstract. Transparent and reliable communication of the safety of advanced and nanomaterials is an issue that has become increasingly important in recent times. The German initiative DaNa got involved in this topic at an early stage. It is running the Knowledge Base Materials, a web-based information platform on nanomaterials (www.nanoobjects.info) for more than 10 years, which is constantly being expanded. Recently, due to emerging developments in materials science, the focus has been expanded from nanomaterials to the variant-rich group of advanced materials, softening the restriction to particles below the 100 m size limit in one dimension to include larger particles with more complex composition. For the Knowledge Base Materials, this broader scope presents a challenge for science communication. In this paper, the authors describe the selection of materials, the workflow, and the quality control that was performed to provide reliable knowledge about the safety of advanced materials to humans and the environment.

Keywords: Science communication · Knowledge base · Advanced materials

1 Introduction

Materials, especially advanced materials, are the backbone and source of prosperity of a modern industrial society. These advanced materials will play a decisive role in the future. Advanced materials are designed with a purpose to have novel or enhanced properties and improve performance over conventional materials, products, and processes.

Various material innovations hold great promises to tackle today's societal challenges such as energy generation and storage, building sustainable cities, mobility or even in the global fight against diseases. To keep up with this development, the scope of the existing Knowledge Base Materials was broadened to cover advanced materials with nanomaterials representing a sub-group. Similar to the usage of nanomaterials, innovations containing advanced materials should be as safe as possible, meaning not

S. G. Scholz et al. (Eds.): SDM 2022, SIST 338, pp. 33–42, 2023.
https://doi.org/10.1007/978-981-19-9205-6_4

causing any harm towards humans and the environment. At the same time, advanced materials should not generally be perceived as a cause for concern.

In any case, a clear definition of advanced materials is difficult and has not yet been established. The term material is far-reaching and stands for the basic building blocks of all physical objects. Novel as well as known materials can be optimized or tailored to fulfil specific functionalities and address different challenges. An attempt to classify advanced materials suggests that the term refers to "materials representing an advance over conventional materials either by controlling their composition and structure or through new modifications". A good basis for defining advanced materials is provided by Javier Peña's report from 2013 [1]. Advanced materials are described as a heterogeneous group that may include nanomaterials, bioactive, anisotropic materials, among others (see Table 1). Each one has different properties and varies in composition, shape, size, interactions, and charges, resulting in a wide range of functionalities and behaviors [1, 2]. They are expected to be essential for human well-being and economic security, with applications in numerous industries including those aimed at addressing affordable and clean energy and resilient infrastructure, future key challenges to cope with the consequences of climate change [3–6].

The development and commercialization of products with advanced materials requires an accurate risk assessment of such products and appropriate risk communication measures. Risk communication and public awareness are key to avoid unjustified negative public perception and a backlash of public concern [7, 8]. This perception is also influenced by existing binding principles (such as the EC precautionary principle [9]), definitions and regulations [8, 10].

In this paper, the authors illustrate how they established the Knowledge Base Materials on advanced and nanomaterials as a web-based application (www.nanoobjects.info) and how they contribute in this way to sustainable information on advanced and nanomaterials for interested stakeholders.

2 Methodology

2.1 Selection of Advanced Materials

For a novel material to be included in the Knowledge Base Materials (www.nanoobjects.info) two main criteria apply: market relevance and existence of relevant toxicological studies. Guiding questions are i.e. "Is the material already available in a product on the market or will it be available soon?" and "Is there sufficient scientific knowledge published on material safety?". The latter question is the most decisive factor as the DaNa project focusses on processing published research data from the scientific literature for science communication purposes and does not conduct its own laboratory research.

Javier Peña's report provides a good basis for expanding the existing knowledge base to include advanced materials [1]. Table 1 summarizes material categories with examples of possible materials / material classes.

2.2 Selection Criteria and Quality Check of Publications

Various factors contribute to a successful and objective communication of scientific findings to a broader community. Ensuring good quality, reliability and comparability

Table 1. Main categories of advanced materials and examples for each category. It follows the categorisation as suggested in [1] as well as in [11].

Material category	Examples
Fibres	PECH / PAN based carbon fibres
Bio based	DNA origami
Advanced textiles and fibres	Self-cleaning fabrics
Advanced manufacturing	3D-printing
High performance polymers	Self-healing polymers
Light alloys	Titanium-, Magnesium-based
Active materials	Micro-encapsulated phase-change materials
Gels and foams	Aerogel
Layers	Graphene
Coatings	Electrically-conductive ink
Nanomaterials	Nanowires
Advanced composites	Organic light-emitting diode

of the research studies conducted are impertinent to draw reliable conclusions from the results, whether for scientific or regulatory purposes or for the information of interested stakeholders via the Knowledge Base Materials. Due to the huge amount of nanotoxicology studies published annually, this became even more important [12]. The number of publications for advanced materials has not even been recorded yet.

To address the issue of accuracy and reliability of scientific studies, the implementation of a comprehensible procedure for study quality control is an important step: First, the most critical parameters and factors influencing (toxicological) studies on advanced materials (including nanomaterials) are identified and compiled by different experts. These cover material properties, dispersal of materials for toxicological tests, the toxicity study design itself and additional criteria such as usage of Standard Operating Procedures (SOPs) or other official test guidelines.

As a result, the literature criteria checklist "Methodology for selection of publications" was established. It is a functional and comprehensive tool for evaluating published research studies for reusage, with specific focus on science and risk communication on nanomaterials [13, 14].

At the same time, the tool makes the evaluation process objective, transparent and comprehensible. The fulfilment of mandatory and voluntary criteria allows a differentiated weighing on quality and reliability of study results (Fig. 1). Similar approaches for evaluating study quality differing in purpose and degree of details have also been developed by others, e.g. [16–20].

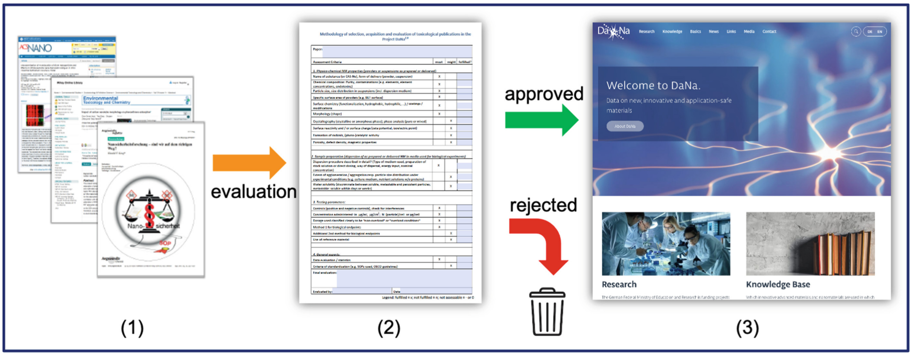

Fig. 1. DaNa writing process for article creation: (1) Bibliographic analysis of peer-reviewed scientific papers on selected advanced materials. (2) Evaluation of selected papers with the help of the DaNa literature criteria checklist "Methodology for selection of publications" [15]. (3) Approved papers serve as a source of information on the characteristics, human and environmental toxicology of advanced materials and are cited on www.nanoobjects.info.

3 Results

3.1 Provision of Quality-Checked Publications

Adaptions on quality criteria for advanced materials studies

As mentioned before, the term "advanced materials" includes an even broader class of different materials than the term "nanomaterials". Moreover, little is known today on toxicity-relevant properties of many advanced materials. Within the community, the current focus of the discussion is on how to identify materials of concern for human and environmental health [21–23]. As a consequence, the Knowledge Base Materials team constantly monitors the existing study quality criteria checklist for novel criteria that describe the specificities of advanced materials. As the listed criteria need to be applicable to a broad variety of different materials, the team faces the challenge to formulate as precise as possible but not too limiting for only specific criteria. So far, there are only few indications on relevant criteria that need further consideration. For example, with the expansion of the Knowledge Base Materials from nanomaterials to advanced materials, the size factor of the evaluated material is not limited to the nanoscale anymore. However, size and dimensions (shape) of the investigated particulate or fibrous materials should be clearly stated and characterised accordingly. Since a clear definition of advanced materials does not currently exist and also appears impossible in the near future due to the heterogeneity of materials, expert knowledge is indispensable, since the term is used in different contexts and the published research results must therefore also be evaluated in the respective context.

One example for the need to adjust the existing evaluation criteria for ecotoxicity testing are polymer materials, which are used for example as composite materials in 3D printing [24]. On the basis of quality criteria developed for nanotoxicity studies, it was explored if and which additional criteria need to be considered for this specific group of materials (e.g., additive content), and which criteria are not relevant (e.g., porosity).

3.2 Knowledge Base Materials Structured Writing Approach

Following the evaluation of study quality, the content of the quality-assured research data is transferred into generally understandable articles. For better clarity for the readers, all texts follow a fixed structure for which a tiered approach has been adopted: each article starts with a short and relatively simple summarizing paragraph (teaser). The scientific details are then further elaborated as the article continues ending with a reference list of the most important quality assured scientific publications for the respective material (Fig. 2).

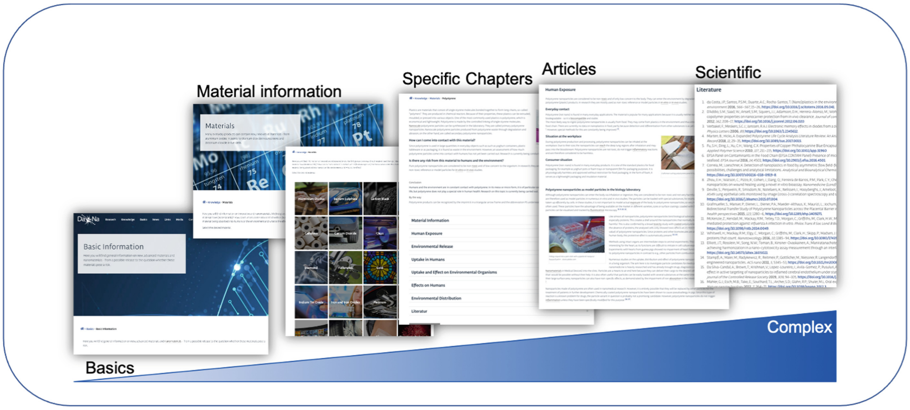

Fig. 2. A graduated complexity addresses different educational backgrounds of visitors. The complexity of the information increases from the basic articles to the material overviews and material-related information (1 subchapter) on human toxicology (3 subchapters) and ecotoxicology (3 subchapters) to the cited scientific literature.

For each material, information is provided on the material properties and applications, as well as detailed content on exposure scenarios, behaviour, and hazard assessment for humans and the environment.

The Knowledge Base Materials expert team is working according to a multi-eye principle: the scientific review of the initial article is followed by a second review conducted by a non-scientist, which focuses on the implementation of general comprehensibility. Since technical terms cannot be completely avoided, a separate glossary is provided to further improve general understandability.

If a new material fulfils the previously mentioned criteria to be added into the knowledge base, the content creation process is started. A brief fact sheet summarising the most important information is compiled, allowing the reader to get a quick overview and creating interest in reading further. This is followed by more detailed information on the material itself as well as the relevant toxicological aspects for humans and the environment.

Material Information - Properties and Usage

Each material presented is characterized in the "Material Information" section. General information on properties and use as well as occurrence and production are provided. A guideline of questions is applied during article creation to provide a structured guidance for the author as well as a clear orientation for the reader to find information later on in a targeted way. In addition, for regular users a recognition effect is created.

Toxicological aspects of advanced materials for humans

The mentioned principles of the predefined writing scheme are also applied to the creation of articles for the topic of human toxicology. Evaluated scientific publications are sorted according to the main topics addressed in the Knowledge Base, namely (I) *Human exposure*, (II) *Uptake in humans* and (III) *Effects in humans*. Again, a specific set of guiding questions structures the article and guides the reader through the provided information. The catalogue of questions for the topic of exposure to humans encompasses questions such as: *Are epidemiological studies available? In which (everyday-relevant) applications do people come into contact with a (nano)material? What is the situation at the workplace? What about the release of materials at the workplace? Is the worker exposed to material at the workplace?*

Since the knowledge base is primarily aimed at citizens without scientific knowledge in toxicology, it is important to consider the situation of the consumer. Thus, relevant questions to be addressed are: *Is it possible for the materials to be released from consumer products? How likely is the exposure and what are the effects?* For this purpose, in vitro and in vivo studies are evaluated. The next stage is the uptake of released materials into the human body. Here, studies on the lung, skin and gastro-intestinal tract are being considered. In the process, the focus is on aspects such as the following: *Which absorption mechanisms are relevant for the different forms of the material (bulk/nano)? Which uptake mechanisms are relevant for the different forms of the material or are there relevant differences for the material in different forms? What happens to the material in the lung (e. g. removal from the body, inflammation or absorption into the body)?*

In addition, the effects of materials on humans after the uptake are also being covered. *How is the distribution and effect in the body? Will the material be taken up in cells and if so, in which way?* The answers to the questions on uptake and behaviour are important to draw final conclusions for the hazard and overall risk assessment of the material related to human toxicology. They ensure to cover topics of specific interests for the general public related to material safety.

Environmental impact of advanced materials

Analogous to the previous section, specific guiding questions serve as a blueprint for a uniform structure of this texts. Three individual sections inform on (I) *Environmental release & exposure* of advanced materials, their (II) *Behaviour in the environment*, and (III) *Uptake and effects in environmental organisms.*

Accordingly, the following questions are considered: *Is there a release at all? At which stage of a products life cycle? What and how much material is released into the environment? Into which compartment? How is the material behaving regarding transformation and transport processes?* And finally, *Is the material taken up by environmental organisms, is it affecting the organisms?*

Especially the last question needs attention in order to provide a balanced overview on environmental safety. For advanced materials it is important to consider toxic effects resulting from the specific form (shape, dimensions), the materials composition, or from by-products (e.g., endotoxins, additives), which are contained in the material.

4 Lessons Learnt

Scientific conferences, publications and textbooks are the usual channels for scientists to communicate their results. However, websites and social media are becoming more and more important in the present time. However, fake news and false information are also on the rise. Consumers often cannot evaluate scientific information and scientific terms and cannot distinguish them from such false information. As a scientist, however, you also strive to communicate findings to a broad audience. In order to provide validated fact-based information to a broad interested audience via a public website, the consecutive German DaNa projects were initiated with the aim of communicating data and knowledge on the safety of advanced and nanomaterials. These science communication projects were intended to avoid repeating the previous communication failures of other branches of science, such as genetic engineering or nuclear power. Scientific results on the safety of advanced and nanomaterials should be presented in a transparent and structured manner at an early stage of technology and application development. Since 2009, scientists in these initiatives have been working in the area of tension between precise scientific facts on the one hand and simplified presentations on the other. The result is the current web-based Knowledge Base Materials (via www.nanoobjects.info). From the authors perspective, the established quality assurance procedure facilitates the unbiased and transparent assessment of scientific outputs in alignment with community-validated characteristics [15]. In addition, the implementation of mandatory and voluntary criteria gives the evaluators a certain amount of freedom to individually rate and judge certain aspects of the selected studies from an expert's point of view. The template of the literature criteria catalogue is available online in order to make the process of evaluating the literature transparent. The question-guided writing scheme supports a harmonized summary of the compiled scientific information to give answers to the most relevant questions for the target groups.

This general article structure implemented on the website for all listed materials within the knowledge base creates an expert-guided user experience with high recognition value. Complex information derived from scientific publications on the safe handling of advanced and nanomaterials is presented in a structured, comprehensible and comparable way. The increase of content complexity from basic articles to material-specific descriptions of safety-relevant aspects with the corresponding scientific literature caters to the background and needs of the different stakeholder groups such as interested citizens, journalists or scientists.

This information is supplemented by a FAQ collection and a glossary. If the website visitors still have unanswered questions, they can directly interact with the expert team behind the knowledge base via a contact form. Thus, an open discussion on the safety of advanced materials and nanomaterials is facilitated.

5 Conclusion

Today, science has an even greater responsibility to provide fact-based answers and to develop solutions to most urgent issues of current times, such as climate change, health research or digitalisation. This responsibility also encompasses the major task of science communication. A dialog with the public must be conducted, current debates must be presented in a factual manner, and the challenges and opportunities of new scientific developments must be highlighted. Both funding agencies and EU wide policy put currently big emphasis on the importance of science communication [25–27]. Science communication needs to be driven by the scientists and has to become a constant part of the science system. Besides the sharing of scientific outputs, the processes and methods used to achieve these results need to be shared with the public to create more transparency, explain the complex and provisional nature of scientific results and thus strengthen trust in the scientific community. To initiate this transformation of science communication becoming an integral part of the science system, e.g., in Germany the initiative "#FactoryWisskomm" was set up in 2021. Within this think tank exchange format, representatives from politics, science communication and science journalisms have formed working groups around the most important topics to create recommendations and strategic next steps for the field of science communication [28]. These cover e.g., science journalism in the digital age, public engagement formats for science communication or quality assessment & quality management in science communication.

As presented in this paper, the concept of the web-based Knowledge Base Materials provides processed fact-based structured results on the safety of advanced and nanomaterials (www.nanoobjects.info). This approach generated by an expert team of different research disciplines (biology, chemistry, material sciences, toxicology) has successfully set up this objective information source with easy online access for different stakeholder groups. This processing of scientific findings is also transferrable to the novel developments in material science and the team is currently working on the generation of new content for the novel classes of advanced materials. As with any scientific field, the process is constantly monitored and adjusted accordingly upon recent updates from the scientific community.

Taken together, the overall science communication activities of the team have strongly contributed to the science and risk communication for nano- and now advanced materials as part of risk assessment, thus promoting a sustainable and responsible use of these materials in future.

Acknowledgments. The authors would like to thank the Federal Ministry of Education and Research (BMBF) for funding (DaNa4.0 Information on the safety of new, innovative materials and nanomaterials, FKZ 03XP0282).

References

1. EU: DAMADEI Design and Advanced Materials As a Driver of European Innovation (2013)
2. Kennedy, A., et al.: A definition and categorization system for advanced materials: the foundation for risk-informed environmental health and safety testing. Risk Anal. **39**(8), 1783–1795 (2019)
3. Goel, P., et al.: Perovskite materials as superior and powerful platforms for energy conversion and storage applications. Nano Energy **80**, 105552 (2021)
4. Lee, G.-H., et al.: Multifunctional materials for implantable and wearable photonic healthcare devices. Nat. Rev. Mater. **5**(2), 149–165 (2020)

5. Fernandez, C.A., et al.: Progress and challenges in self-healing cementitious materials. J. Mater. Sci. **56**(1), 201–230 (2020). https://doi.org/10.1007/s10853-020-05164-7
6. Li, X., et al.: Metal–organic frameworks as a platform for clean energy applications. EnergyChem **2**(2), 100027 (2020)
7. Siegrist, M., Hartmann, C.: Consumer acceptance of novel food technologies. Nat. Food **1**(6), 343–350 (2020)
8. Joubert, I.A., et al.: Public perception and knowledge on nanotechnology: a study based on a citizen science approach. NanoImpact **17**, 100201 (2020)
9. Precautionary principle (April 2022). https://eur-lex.europa.eu/legal-content/EN/TXT/?uri=LEGISSUM:precautionary_principle
10. EC, E.C.: Commission Recommendation of 18 October 2011 on the definition of nanomaterial. (2011/696/EU) (2011). http://data.europa.eu/eli/reco/2011/696/oj
11. Giese, B., et al.: Advanced materials: overview of the field and screening criteria for relevance assessment. In: Dessau-Roßlau, G., ed., p. 106 (2020)
12. Hristozov, D.R., et al.: Risk assessment of engineered nanomaterials: a review of available data and approaches from a regulatory perspective. Nanotoxicology **6**(8), 880–898 (2012)
13. DaNa-Project-Consortium: Literature Criteria Checklist (9 November 2021). https://nanopartikel.info/en/knowledge/literature-criteria-checklist/
14. Nau, K., et al.: The Dana2.0 knowledge base on nanomaterials – communicating current nanosafety research based on evaluated literature data. J. Mater. Educ. **38**(3–4), pp. 93–109 2016
15. DaNa Project-Consortium. Literature criteria checklist - a methodology of selection, acquisition and evaluation of toxicological publications in the Project DaNa. nanopartikel.info 2021 2016 (April 2022). https://nanopartikel.info/en/knowledge/literature-criteria-checklist/
16. Fernández-Cruz, M.L., et al.: Quality evaluation of human and environmental toxicity studies performed with nanomaterials – the GUIDEnano approach. Environ. Sci. Nano **5**(2), 381–397 (2018)
17. Card, J., Magnuson, B.: A method to assess the quality of studies that examine the toxicity of engineered nanomaterials. Int. J. Toxicol. **29**, 402–410 (2010)
18. Faria, M., et al.: Minimum information reporting in bio–nano experimental literature. Nat. Nanotechnol. **13**(9), 777–785 (2018)
19. Schneider, K., et al.: "ToxRTool", a new tool to assess the reliability of toxicological data. Toxicol Lett **189**(2), 138–144 (2009)
20. Segal, D., et al.: Evaluation of the ToxRTool's ability to rate the reliability of toxicological data for human health hazard assessments. Regul. Toxicol. Pharmacol. **72**(1), 94–101 (2015)
21. Peijnenburg, W., et al.: Identification of emerging safety and sustainability issues of advanced materials: proposal for a systematic approach. Nanoimpact **23**, 100342 (2021)
22. Giese, B., et al.: Advanced Materials: Overview of the Field and Screening Criteria for Relevance Assessment. Umweltbundesamt (Publisher). 132/2020 (2020)
23. Reihlen, A., et al.: Advanced Materials: Overview of the Field and Screening Criteria for Relevance Assessment. UBA-Texte (2022). **Texte | 09/2022**(Final report): p. FKZ 3719 66 402 0
24. Kokalj, A.J., et al.: Quality of nanoplastics and microplastics ecotoxicity studies: refining quality criteria for nanomaterial studies. J. Hazard. Mater. **415**, 125751 (2021)
25. German Federal Ministry of Education and Research (BMBF): Grundsatzpapier des Bundesministeriums für Bildung und Forschung zur Wissenschaftskommunikation, p. 7. Berlin, Germany (2019)
26. European Research Executive Agency: Towards clearer and more accessible science communication. rea.ec.europa.eu 2022 12.01.2022 (April 2022). https://rea.ec.europa.eu/news/towards-clearer-and-more-accessible-science-communication-2022-01-12-0_en

27. SIS.net Network: Science communication - policy brief. Ref. Ares(2020)1297156 - 02/03/2020, p. 12 (2020)
28. Bundesministerium für Bildung und Forschung (BMBF): HANDLUNGSPERSPEKTIVEN FÜR DIE WISSENSCHAFTSKOMMUNIKATION (2021). https://www.bmbf.de/bmbf/shareddocs/downloads/files/factory_wisskomm_publikation.pdf?__blob=publicationFile&v=2