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Final report of the research project on behalf of the Thinktank Industrial Resource Strategies

PFAS: APPLICATION, TECHNICAL FUNCTIONS AND SUBSTITUTION POSSIBILITIES IN THE INDUSTRY

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Preface

"Throwing out the baby with the bathwater"?

It is undisputed that some PFAS (per- and polyfluoroalkyl substances = PFAS) pose risks to health and the environment due to their persistent and bioaccumulative properties. At the same time, this class of substances, with over 10,000 compounds, is essential for numerous industrial applications and consumer products because of its unique features – including chemical stability, water and fat resistance, slipperiness, non-stick properties, as well as resistance to fire and heat.

Key industries crucial for future technologies such as energy transition and e-mobility, as well as core sectors like chemistry, mechanical engineering, automotive industry, and medical technology, would be particularly affected by a potential ban. In this context, the question arises: Are there already or will there be adequate substitutes that could replace PFAS without compromising performance and safety?

To address this question, a specially developed artificial intelligence was utilized, extensively trained for this task. After analyzing 35,246 scientific documents and open-source publications worldwide, our AI-based system identified 420 materials and summarized them into 32 classes for the five prominent companies involved from Baden-Württemberg, namely Carl Zeiss AG, Karl Storz SE & Co. KG, Mercedes-Benz AG, Novaliq GmbH, and Richard Wolf GmbH.

This initially promising result yielded only a very limited number of potential substitute materials upon closer analysis of the requirements of the participating companies, which could partially substitute PFAS according to current standards. It is precisely the simultaneous combination of different functions that make PFAS so unique. In one case, two to three identified materials have the potential to partially substitute PFAS according to current standards. In other cases, no adequate replacement could be found.

Given these results, the selection of PFAS based on a differentiated benefit-risk assessment is imperative. Particularly in medical technology, the use of PFAS does not pose an immediate health risk, and in other industries, they remain in closed processes without burdening the environment.

The findings provide important starting points for the future strategic direction of research and development, including funding measures, as well as for deeper investigations into the use of PFAS and the search for alternative materials.

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1 INTRODUCTION AND OBJECTIVES

Per- and polyfluoroalkyl substances (PFAS) are organic compounds consisting of carbon chains in which the hydrogen atoms are completely or partially replaced by fluorine atoms.[1]

The strong chemical bonds between carbon and fluorine atoms in PFAS lead to very stable substances with particularly useful properties such as chemical inertness, water repellency, lubricity, non-stick properties, fire resistance and heat resistance. However, they are poorly biodegradable and therefore difficult to decompose in the environment (Ye et al. 2015).

PFAS are used in many fields of application in industry and in end products, such as in industrial production, in seals, lubricants, packaging, metal coating, in medical devices, electronic devices, solar cells, fuel cells, batteries, in the construction sector and also in consumer products in textiles, cookware and cosmetics (Glüge et al. 2020, ECHA 2023).

Due to their effects on the environment and humans and their persistence in the environment, PFAS are currently the subject of much debate and the process towards possible substance bans has been initiated at EU level (ECHA 2023).

Companies from Baden-Württemberg and all over Europe are therefore looking for substitutes for the use of PFAS in order to have alternatives available in the event of a possible ban on the substances.

The aim of this meta-study is to create an overview of possible substances and groups of substances that have the potential to replace the technical functions of PFAS. This is examined in depth using selected examples from the automotive industry, semiconductor technology, medical technology and the pharmaceutical industry.

[1] see https://www.bmuv.de/faqs/per-und-polyfluorierte-chemikalien-pfas, last accessed 08. 12. 2023

The focus is on the following questions:

1. Where have PFAS been used/applied to date? What technical functions do PFAS provide?
2. By which alternative substances could PFAS be substituted?
3. What conclusions can be drawn from this for innovation development in the industry in Germany and Baden-Württemberg in particular?

Possible substitutes are identified and evaluated in a structured manner using software tools based on artificial intelligence.

The following companies from Baden-Württemberg were involved in this study:

- Carl Zeiss AG (technology company in the optical and optoelectronic industry)
- KARL STORZ SE & Co KG (medical technology manufacturer, in particular endoscopy)
- Mercedes-Benz AG (automobile manufacturer)
- Novaliq GmbH (pharmaceutical manufacturer, in particular ophthalmic therapeutics)
- Richard Wolf GmbH (medical technology manufacturer, in particular endoscopy)

These companies provided experts with application know-how and took over the evaluation of the identified substitutes.

The study is structured as follows:
First, an introduction to PFAS substances and their use in industry is given (Chap. 2). Then the methodological approach chosen to identify possible PFAS substitutes is explained (Chap. 3). The materials with PFAS substitution potential identified in this way are presented in chapter 4. Finally, the substitution potential of the identified materials is presented on the basis of use cases from cooperating companies (Chap. 5). The study then concludes with a summary and an outlook (Chap. 6).

2 INTRODUCTION TO PFAS SUBSTANCES AND THEIR USE IN INDUSTRY

PFAS are organic compounds consisting of carbon chains in which the hydrogen atoms are replaced by fluorine atoms (completely: perfluorinated, or partially: polyfluorinated). The definition of the European Chemicals Agency ECHA can be used as a more precise description. Accordingly, a PFAS is "any substance that contain at least one fully fluorinated methyl (CF_3-) or methylene (CF_2-) carbon atom (without any H/Cl/Br/I atom attached to it)." (ECHA 2023)

This comprises a very large group of substances with an estimated 10,000 compounds. Important subgroups are perfluoroalkyl acids and their precursors, fluorinated gases and PFAS polymers (ECHA 2023).

PFAS are expensive to manufacture and are therefore used where other substances cannot provide the required performance, or where they can provide the same performance as a larger quantity of non-fluorinated chemicals in much smaller quantities. Examples include applications that operate over wide temperature ranges or uses that require extremely stable and non-reactive substances (Glüge et al. 2020).

The wide range of possible applications of PFAS was first analyzed in a 2020 technical article by Glüge and co-authors (Glüge et al. 2020). It shows that PFAS are used in almost all branches of industry and many consumer products. More than 200 uses in 64 categories were identified for more than 1400 individual PFAS. Categories with more than 100 identified PFAS are photographic industry, semiconductor industry, coatings, paints and varnishes, sealing foams, medical devices, personal care products and printing (Glüge et al. 2020).

They are based on the special technical properties of PFAS. These can be simplified as follows and summarized in so-called benefit dimensions:

- Low surface tension
- Dielectric properties at low temperatures
- Corrosion-resistant, non-reactive materials
- Hydrophobic and oleophobic coatings
- Long-term stability of gases or materials
- Low flammability of polymers and fabrics

In 2020, between 140,000 and 310,000 tons of PFAS were placed on the market in the European Union (ECHA 2023).

From an environmental perspective, the main criticism of PFAS is the very high persistence of them and/or their degradation products: they can remain in the environment longer than any other man-made chemical. PFAS are already ubiquitous in the environment: in organisms, drinking water sources and food, as well as in remote and pristine areas. Many PFAS continue to accumulate in organisms and (eco)toxicological effects are also seen for some substances. Further release would lead to an increase in the concentration in the environment, as there is no degradation under natural conditions; as a result, negative environmental and health effects are expected. The removal of PFAS from surface water, groundwater, soil, sediment and biota is also technically extremely difficult and very costly, if possible at all (ECHA 2023).

A ban on PFAS is currently being discussed in the EU: Several European countries submitted a restriction proposal to the European Chemicals Agency (ECHA) at the beginning of 2023[2]. According to this proposal, the manufacture, placing on the market and use of PFAS is to be restricted. A broad focus was deliberately chosen to avoid the substitution of one PFAS by another PFAS (which may not even be technically manufactured yet). For most PFAS, a complete ban was proposed with an 18-month transitional period with use specific, time-limited exemptions and an additional exemption for 5 or 12 years. The classification is essentially based on the availability of possible substitutes for PFAS substances in the applications under consideration from a technical and economic perspective (ECHA 2023). However, it is unclear exactly how these possibilities were determined.

[2] Following a public consultation phase, the ban proposal is now being evaluated.

3 IDENTIFICATION OF POSSIBLE PFAS SUBSTITUTES

In the following chapter, the process of identifying possible PFAS substitutes is examined in more detail. First, the status quo of the use of PFAS in industrial applications is examined, with a particular focus on the companies involved and the applications in which PFAS currently still play a significant role. The empirical identification of alternative materials through AI-supported research is then described. An extensive data pool of material research publications is used as a basis, and a specially developed AI system is used to extract relevant information. The identified materials are evaluated for their suitability as potential substitutes for PFAS in industrial applications.

This chapter lays the foundation for understanding the methods used and the identification of the materials, which are explained in more detail in the following sections. It provides a comprehensive overview of the process of searching for PFAS substitutes and the specific criteria that play a role in the evaluation of these substances.

The previous chapter highlighted the need for a possible replacement for per- and polyfluoroalkyl substances (PFAS): this group of substances is widely used in various industrial applications and at the same time has become the focus of attention due to its potential health risks and environmental impact. The current status of the use of PFAS in industrial applications is therefore examined below. Particular attention is paid to the companies involved in this study and the applications in which PFAS play a significant role.

3.1 Identification of PFAS functionalities to be replaced

The companies involved (Carl Zeiss, Mercedes-Benz, Karl Storz, Novaliq and Richard Wolf) are players in the medical technology, semiconductor manufacturing technology, automotive and pharmaceutical industries. They are significantly affected by the planned restriction or a possible ban on PFAS, as they rely on the unique properties of these substances in their products and processes.

The applications in which per- and polyfluoroalkyl substances (PFAS) have a significant presence and are therefore considered to be particularly affected will be considered in more detail in this section. This is essential as it helps to understand the extent of the challenges associated with the potential substitution of PFAS in industrial processes and products.

The applications particularly affected were identified or developed on the basis of extensive literature research in joint workshops with the industry consortium. The economic significance and potential effects of PFAS substitution in the respective applications were also taken into account.

Per- and polyfluoroalkyl substances (PFAS) have unique functionalities. These are of crucial importance in many industrial applications. These functionalities contribute significantly to the fact that PFAS have established themselves as indispensable components in various products and processes.

In the discussion with the participating companies, the following six main dimensions of PFAS functionalities were identified:

> **Chemical stability, acid and hydrolysis resistance:** Their exceptional chemical stability makes PFAS resistant to aggressive chemicals and acids. Furthermore, their ability to withstand hydrolysis processes is of crucial importance for many applications.
> **Long-term stability:** PFAS offer remarkable long-term stability: they maintain their performance over an extended period of time without significant degradation or deterioration.
> **Temperature stability, low outgassing behavior:** The temperature stability of PFAS allows them to be used in extreme temperature environments without losing their functionality. In addition, they are known for their low outgassing behavior, which is an advantage in applications with high vacuum requirements.
> **Sliding properties (non-stick, no stick-slip, easy-to-clean, non-wetting, non-sticky, very low surface tension):** PFAS are characterized by their high anti-friction and non-stick properties, which are essential in many areas, including food processing and medical technology. They also have a very low surface tension, which makes them water and oil repellent.
> **Weather resistance, UV and light stability:** PFAS are extremely weather-resistant and have high UV and light stability. This makes them particularly suitable for outdoor use and in environments with intense sunlight.
> **Biocompatibility:** In some applications, particularly medical devices and pharmaceuticals, biocompatibility is critical. Many PFAS are known for their low toxicity, which supports their use in medical devices and drug formulations.

These PFAS functionalities served as guiding principles in the search for potential substitutes. Substitute materials should offer comparable performance characteristics in order to meet the requirements of the industry. Ultimately, it must be decided on a case-by-case basis to what extent an identified material fulfills the required functionalities and can therefore serve as a substitute from a technical perspective.

The evaluation was carried out by the experts from the participating companies on the basis of a qualitative rating scale (5: very good/high, 1: very low/poor).

3.2 Procedure for identifying and evaluating alternative materials

The following describes how the empirical identification of alternative materials was carried out. The aim was to create a comprehensive database in order to identify potential PFAS substitutes that could fulfill the criteria defined above.

The process of identifying alternative materials is based on current materials research publications and is supported by the use of artificial intelligence (AI). This enables a systematic and comprehensive exploration of the available scientific findings. As a result, potential substitutes can be identified that represent a promising basis for future research and development work.

Using an AI system developed in-house by TIM Consulting, an innovative approach is being used in the course of this study to identify a wide range of materials that could potentially be used as PFAS substitutes. The careful selection and analysis of these materials forms the basis for the subsequent evaluation of their suitability and application potential.

The identification of potential substitutes for per- and polyfluoroalkyl substances (PFAS) requires a highly precise and systematic approach. In order to meet these requirements, the AI tool "CumulusAI" developed by TIM Consulting was further developed and tailored specifically to the needs of this project.

The following section describes the process of empirically identifying alternative materials and shows how modern technologies such as artificial intelligence can help to provide a comprehensive database for the search for PFAS substitutes.

Specifically, an extensive data pool was first created. The data pool was determined on the basis of the PFAS functionalities described above. To this end, a comprehensive overview of current materials research publications was compiled, taking into account a variety of sources, including scientific journals, conference papers and research reports. The basis for this was the Clarivate database "Web of Science" (accessed in July 2023). This approach enabled a wide range of research results from different disciplines and research areas to be recorded.

This was followed by the selection of publications on the basis of predefined criteria: They were closely oriented to the identified PFAS functionalities and served to check whether the materials recorded had the required performance characteristics (see above).

A total of 35,246 individual documents were identified and included in the data pool. This forms the basis for further investigation and analysis of the identified materials with regard to their suitability as PFAS substitutes.

TIM Consulting's in-house development CumulusAI was used to analyze the data pool. CumulusAI, an advanced analysis tool for large amounts of data, uses transformer-based language models for efficient data handling and deeper insights. It supports information processing as an AI assistant, using patents and publications from Espacenet and OpenAlex as data sources. A specific search strategy extracts relevant data parts in which topic clusters and trends are automatically identified. The clustering is based on a multi-criteria vectorization that evaluates words in their specific context, resulting in more homogeneous and clearly defined clusters. In addition, metadata is used to identify trends and subject matter experts (see Figure 1).

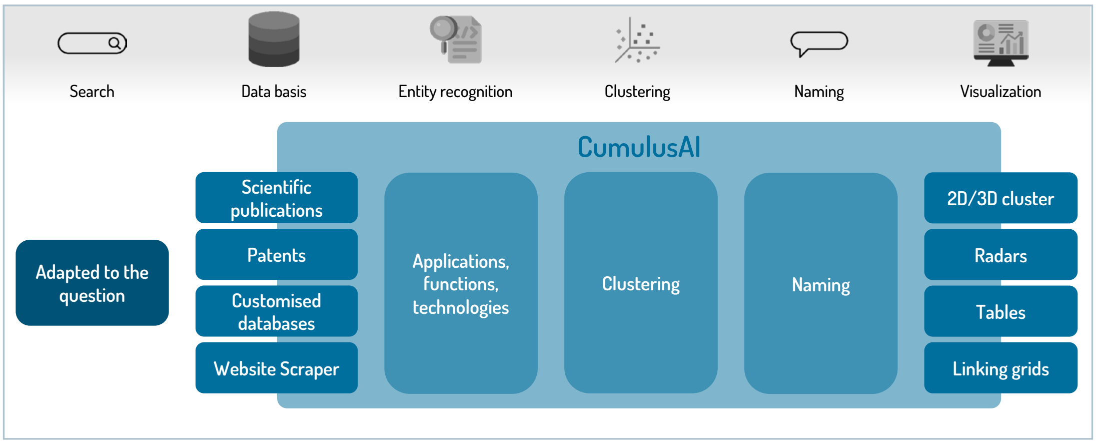

Figure 1: CumulusAI

For this study, CumulusAI was equipped with a specific material algorithm. This algorithm was developed to identify materials within the previously described data pool that could potentially be considered as substitutes for PFAS. The use of the algorithm, which is based on machine learning principles, allowed for precise and efficient sifting through the extensive data pool. Advanced text analysis and pattern recognition techniques were used to extract relevant information, especially with regard to the entity "material".

CumulusAI has been specially trained to identify materials in scientific publications, research reports and technical literature. Specific, predefined criteria and functionalities were taken into account, such as chemical stability, temperature resistance and sliding properties. This was achieved by using a Named Entity Recognition (NER) model based on extensive text data from the field of materials science. The aim was to use neural networks to learn how to recognize and classify material names and their associated properties in texts in order to precisely identify material-related entities.

An evaluation scheme was developed to assess the identified materials in terms of their suitability as potential substitutes for poly- and perfluorinated alkyl substances (PFAS). It is based on technology management evaluation systems (see e.g. [Warschat et al. 2015]) and uses criteria to determine whether the identified materials meet industry requirements and can be considered as viable alternatives.

The evaluation scheme is based on the following main criteria:

> **Technical performance:** This describes the material's ability to technically replicate the specific PFAS functionalities. It therefore includes aspects such as surface activity, water and oil repellency, temperature resistance and other performance properties relevant to the respective application. This involves determining the extent to which the substitute materials are able to effectively take over the functions of PFAS.
> **Environmental impact:** Environmental impact is a key criterion as it takes into account the ecological consequences of the materials used. Factors such as biodegradability, toxicity and the potential for environmental impact are assessed to ensure that the substitutes are more environmentally friendly than PFAS.
> **Costs:** The economic aspects play an important role in the selection of substitute materials. The costs for the production and use of the materials as well as possible effects on the overall production costs are taken into account.

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- **Availability:** The availability of the identified materials on the market is of crucial importance, as it has an influence on practical feasibility. It is checked whether the material under consideration is available in sufficient quantity and quality to cover the expected demand.
- **Regulatory compliance:** Compliance with applicable rules and regulations is a key criterion for ensuring that the identified materials meet legal requirements. This includes compliance with environmental regulations, safety standards and other legal requirements as well as approval requirements in the medical field.

The definition of this evaluation scheme provides a structured basis for systematically analyzing the identified materials and assessing their suitability as PFAS substitutes.

4 IDENTIFIED MATERIALS WITH PFAS SUBSTITUTION POTENTIAL

The systematic exploration of the data pool with CumulusAI made it possible to identify materials that meet the previously defined requirements and can therefore be considered as promising candidates for PFAS substitutes. The approach of integrating CumulusAI with the material algorithm ensures that the search for alternative materials takes place on a data-driven and evidence-based basis. This enables a comprehensive exploration of the data pool and the identification of materials that have the potential to take over the functions of PFAS in industrial applications, ensuring high precision and efficiency in the identification of relevant materials.

By using the AI tool "CumulusAI" in conjunction with the extensive data pool, a total of 420 materials were identified that have the potential to replace poly- and perfluorinated alkyl substances (PFAS) in various industrial applications (see Figure 2). These materials were carefully an alyzed and structured into 32 material categories to better understand their diversity and range of applications.

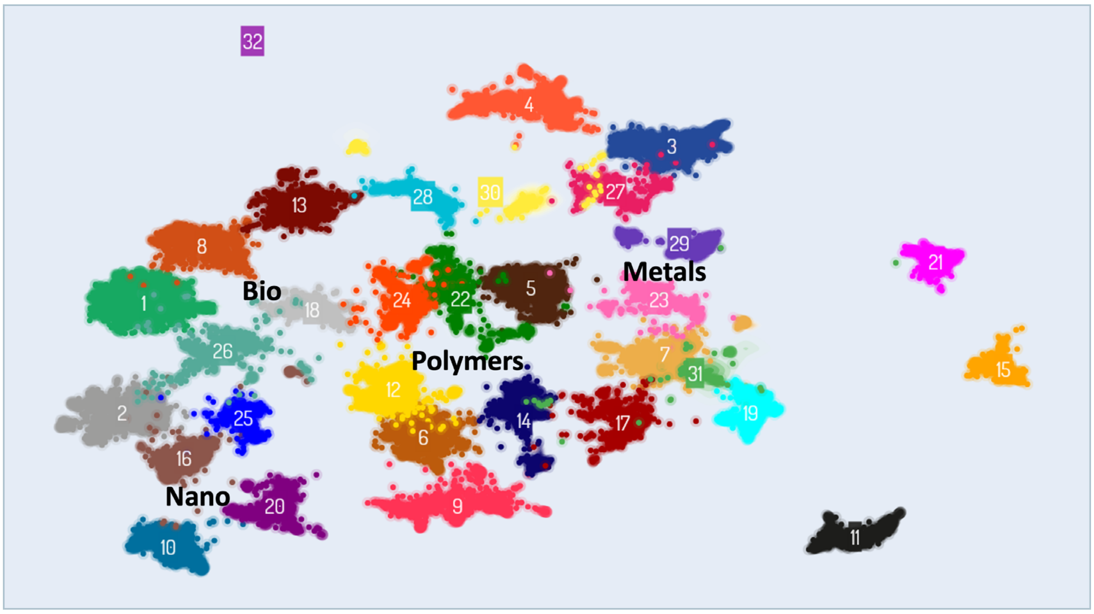

Figure 2: Overview of the 420 materials identified with CumulusAI

The materials identified cover the following classes and types:

- **Polymer-based materials:** This category includes a wide range of polymer compounds, including silicone materials and other high-performance polymers. These materials are characterized by their versatility and adaptability.
- **Ceramic materials:** Ceramic materials, including oxides and nitrides, have been identified as potential substitutes. They offer special properties such as high temperature resistance and chemical stability.
- **Metallic materials:** This category includes various metals and alloys that are considered promising substitutes due to their unique mechanical and thermal properties.
- **Biomaterials:** This group includes biocompatible materials that may be relevant in medical applications. Biomaterials may offer a safe alternative to PFAS in biological environments.
- **Nanomaterials:** Nanomaterials, including nanoparticles and nanotubes, have also been identified. These materials can be useful in various applications due to their small size and special properties.

The identification and structuring of these materials into different categories enables a targeted analysis and evaluation of their suitability as PFAS substitutes. Each material category can offer specific requirements and advantages in relation to the defined PFAS functionalities. This forms the basis for the subsequent evaluation phase, in which the performance and suitability of these materials is examined in detail.

The results of the analysis provide valuable insights into the variety of applications that could be affected by a potential PFAS ban and lay the foundation for further investigation into the challenges and opportunities associated with finding alternative materials and technologies in these areas.

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The comprehensive analysis of the materials identified with CumulusAI leads to significant findings regarding their potential as PFAS substitutes. Through the joint evaluation of all user-specific data sets, a detailed functionality profile could be created for each material and visualized using spider diagrams (see for example Figure 3 and for the complete list see appendix). These profiles or diagrams serve as a decisive basis for evaluating the suitability of specific materials in terms of their applicability and the achievable advantages compared to PFAS.

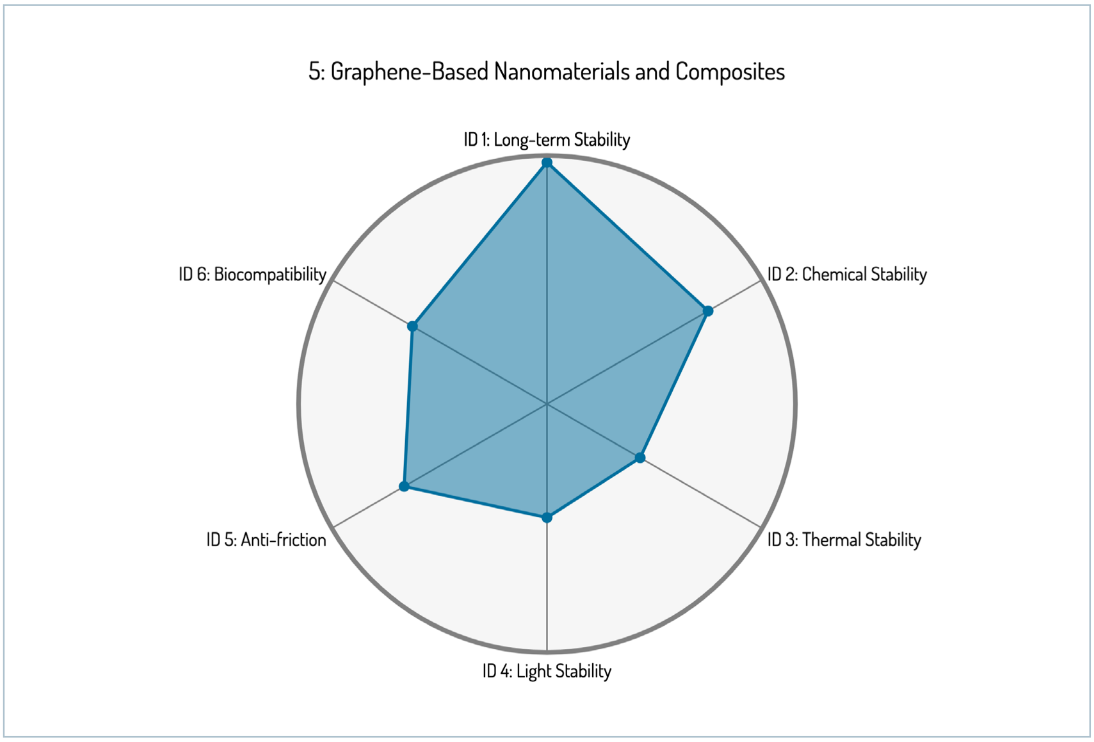

Figure 3: Exemplary functional profile for "Graphene-Based Nanomaterials and Composites"

5 EVALUATION OF THE SUBSTITUTION POTENTIAL OF THE IDENTIFIED MATERIALS BASED ON SPECIFIC USE CASES

The following chapter describes the evaluation of the substitution potential of the previously identified materials using specific examples (use cases). This is based on specific use cases in the participating industrial companies that are highly relevant to the respective companies. The case studies derived in this way were developed in close cooperation with the companies concerned in order to develop and evaluate realistic estimates of the substitution potential for the materials mentioned within the scope of the project.

After defining the use case, the list of materials identified was filtered according to the relevant use dimensions. This resulted in a specific list of possible PFAS substitutes for the respective application with a brief description and reference to descriptive technical literature.

The materials identified in this way were then evaluated by company experts using the evaluation criteria described above on the basis of a qualitative evaluation scale (5: very good/high, 1: very low/poor). The focus was initially on the technical performance in order to obtain a general classification of whether a material can be used as a PFAS substitute. The other criteria were then evaluated (where possible)[3]. The process is shown in Figure 4 for an application example from optical photolithography (see also the following chapter 5.1)

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[3] In many cases, the other criteria were not assessed because the experts had too little information available. For this reason, they are not presented in this report.

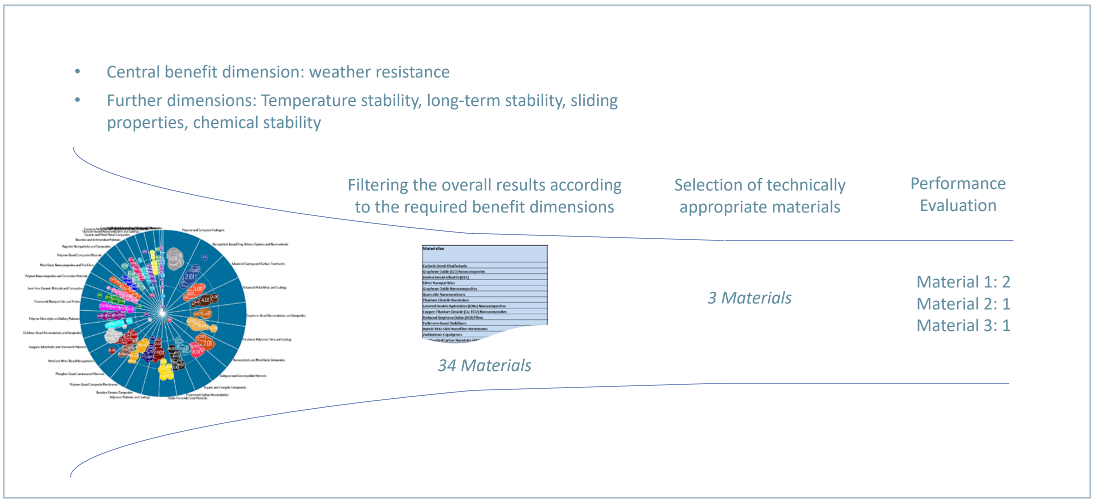

Figure 4: Filtering and evaluation of possible materials as PFAS substitutes, shown for an application example from optical photolithography (evaluation scale: 5: very good/high, 1: very low/poor)

5.1 Semiconductor technology application example: Optical photolithography for the production of microchips

5.1.1 PFAS use: status quo[4]

80% of all computer chips produced worldwide, in particular 100% of the most modern and powerful chips, are manufactured using ZEISS lithography optics.

Optical photolithography (hereinafter referred to as "lithography") is the critical production step in the manufacture of microchips. It is used to create the nanometer structures that form the transistors in the chip. Lithography optics is therefore one of the key technologies in the field of semiconductor production, in which Germany has a unique selling point worldwide for the latest optics.

This new technology of extreme ultraviolet (EUV, see Figure 5) enables the computer applications of the next decade, such as autonomous driving, 5G and artificial intelligence. Corresponding optics are manufactured in Oberkochen, Wetzlar and Jena, for example.

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[4] The following text is taken from Mutter and Mayer 2023 and has been slightly shortened

The special optics required for the lithography systems weigh up to ten tons. They consist of up to 100,000 parts and have to be manufactured with a precision that is unparalleled in the world. In addition to this precision, extreme cleanliness is also required; less than a billionth of a gram of contamination in the wrong place destroys the function of the entire system. The combination of UV light, precision and this cleanliness makes it necessary to use PFAS materials at various points in the lithography system, for example as a sealing material, damping element, insulation and lubricant.

Conventional materials and plastics, e.g. based on pure hydrocarbons or silicones, are much less resistant to UV light and degrade quickly under the influence of UV radiation. They also outgas chemical substances (contamination), which are deposited on the optics and adversely affect the optical function of the system.

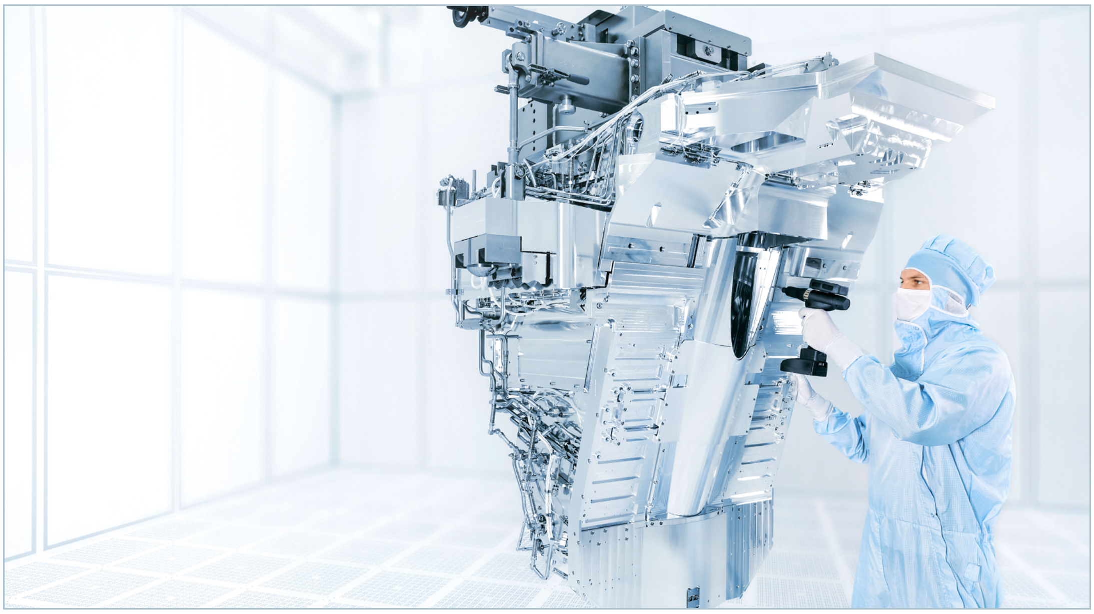

Figure 5: Optical photolithography via extreme ultraviolet (Photo: Carl Zeiss)

5.1.2 PFAS substitution potential

After filtering the overall results according to the required benefit dimensions, a list of 34 materials emerged. These were reviewed by the company experts and 3 technically useful materials were identified . Material 1 was rated with a technical performance of 2, materials 2 and 3 with a rating of 1. The feedback from the experts was that it is unclear whether material 1 has sufficient UV stability as an elastomer material for PFAS. An initial literature search on UV absorption spectra shows possible significant absorption below a certain wavelength range, which could possibly lead to photochemical downstream processes. For material 2, it is still unclear whether it also works in a very thin layer, but this is absolutely necessary for it to be useful in the application. There is no experience with material 3 so far, so the assessment here was initially "skeptical" and further detailed investigations are necessary in order to arrive at a valid assessment.

5.2 Application example automotive industry

5.2.1 PFAS use: status quo[5]

Fluoropolymer applications play an important role in the automotive industry, particularly in seals and hoses:

- Seals are used in many areas of vehicles, such as the engine and drivetrain. Fluoropolymer materials such as PTFE (polytetrafluoroethylene) and FKM (fluoro rubber) are used there due to their high chemical resistance, temperature resistance and low friction properties. They ensure reliable sealing even at high temperatures, aggressive chemicals and pressure fluctuations.
- Plastic hoses are used in cars, particularly in hydraulic brake lines, cooling systems and fuel lines. Fluoropolymer hoses offer high temperature resistance and are highly resistant to chemicals.

Overall, fluoropolymer applications in seals and hoses contribute to the reliability, efficiency and safety of vehicles. This application was the focus of the research.

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[5] The text in the following section is based, among other things, on information provided by Mercedes-Benz AG

It should also be mentioned that PFAS chemicals also play an important role in other areas of the automotive industry: For example, they are used in lithium-ion batteries, technical textiles, electrical engineering and electronic components (including in semiconductor manufacturing). They are used as lubricants/release agents and refrigerants in products in all drive technologies (for both combustion and electric vehicles) as well as in production.

5.2.2 PFAS substitution potential

After filtering the overall results according to the required utility dimensions, a list of 16 materials emerged. These were reviewed by material experts in the company and 2 technically useful materials were identified. Although the use of both materials would be conceivable, it does not relate to the base material to be replaced. In this respect, no suitable alternatives or only alternatives with qualitative losses could be identified for the "fluoropolymers" application example under consideration.

5.3 Medical technology application example: resectoscope for minimally invasive prostate operations

5.3.1 PFAS use: status quo[6]

The prostate is located below the bladder in the male body and is arranged in a ring around the urethra. It can enlarge, especially with age, narrowing the urethra and causing discomfort. Surgical intervention may be necessary to remove this enlargement. A common procedure is transurethral resection of the prostate: the resection technique is minimally invasive and an instrument, the resectoscope, is inserted into the body via the urethra up to the enlarged prostate (see Figure 6). The resectoscope is a medical instrument with a resection loop that removes tissue using high-frequency current. An image of the prostate is transmitted via a camera. The resected tissue is then removed via the urethra.

Resectoscopes are also used for other indications: for the removal of bladder tumors, for interventions in the uterus or for the surgical treatment of uterine malformations. In 2021, more than 290,000 procedures were performed with minimally invasive resectoscopes in Germany alone.

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[6] The text in the following section is a summarized presentation of information from the companies Karl Storz SE & Co. KG and Richard Wolf GmbH

Fluoropolymer components (i.e. PFAS) are used in five different functions in resectoscopes: one of these is the use of PTFE sleeves for the electrical insulation of the electrodes: they ensure a very high dielectric strength of 20 kV/mm and must be thermally stable, chemically resistant, non-sticky, relatively flexible and also biocompatible (see yellow component on the left-hand edge in Figure 6).

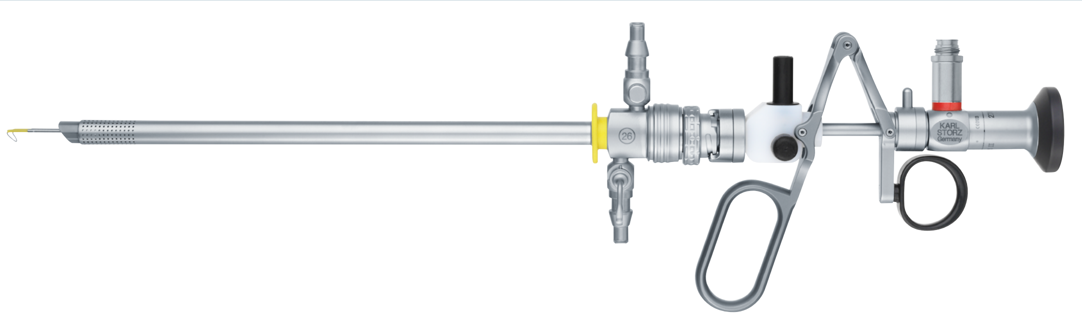

Figure 6: Resectoscope (Photo: KARL STORZ SE & Co. KG)

5.3.2 PFAS substitution potential

After filtering the overall results according to the required benefit dimensions, a list of 36 materials resulted for company 1. These were reviewed by the company experts, who initially identified 5 technically useful materials. However, after closer examination, these were not classified as possible PFAS substitutes.

A list of 20 materials was produced for company 2, none of which were considered technically feasible.

Both companies stated that use could not be ruled out after possibly longer R&D activities, but that this could only be determined after further time-consuming examination.

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5.4 Pharmaceutical industry application example: treatment of severe dry eyes

5.4.1 PFAS use: status quo[7]

Conjunctivitis sicca, or "dry eye", is one of the most common surface diseases of the eye, affecting 5%-30% of people over the age of 50. Symptoms range from mild discomfort to pain and visual impairment, significantly reducing quality of life and productivity at work (Kassumeh et al. 2022).

There are already many eye drops that are approved as medical devices for dry eye in Europe. They are based on water (eye drops) or paraffin (ointments) with various additives. However, they usually only have a short-term effect and alleviate only the symptoms, but cannot show any statistically significant clinical effects over time (Pucker et al. 2016).

The company Novaliq has developed eye drops containing perfluorohexyloctane (F6H8) (sold in Europe under the trade names Evotears, Hycosan Shield or Hylo Lipid).

Perfluorohexyloctane reduces the excessive drying caused by evaporation of the aqueous tear film and helps to restore the natural tear film. Unlike aqueous eye drops, it even penetrates the Meibomian glands in the eyelids and can improve the secretion of the lipids there. The lipids in the Meibomian glands are the sole natural source of the lipid film of the tear film, which protects the eye from evaporation.

Perfluorohexyloctane has been shown to relieve patient symptoms and at the same time have a clinically meaningful effect in the indication (Ballesteros-Sánchez et al. 2023)which the eye drops currently available cannot achieve.

In the USA, perfluorohexyloctane was recently approved by the FDA as a drug (Miebo) for the treatment of the clinical signs and patient symptoms of dry eye after extensive testing.

5.4.2 PFAS substitution potential

After filtering the overall results according to the required benefit dimensions, a list of 33 materials emerged. These were reviewed by the company experts and 2 technically useful materials were identified, which were rated with a technical performance of 2. However, their usability in practice was classified as unlikely to date.

[7] The text in the following section is based on information provided by Novaliq GmbH

6 CONCLUSION AND OUTLOOK

In this study, artificial intelligence was used to search for substances that could replace the PFASs used to date and fulfill the same functions in industrial applications.
The companies involved in the project were Carl Zeiss AG, Mercedes-Benz AG, KARL STORZ SE & Co. KG, Richard Wolf GmbH and Novaliq GmbH. The application examples examined were from the fields of optical system technology, the automotive industry, endoscopes / medical technology and pharmaceuticals / ophthalmic therapeutics. This shows that the use of PFAS offers great benefits for society.

Substitutes were determined:

1. The PFAS technology functionalities used in the companies were identified and six top PFAS technology functionalities were prioritized,
2. trained an AI system with approx. 2,000 samples (scientific literature) for the question,
3. over 35,000 articles worldwide analyzed with the AI system

From these, the AI software identified 420 known and established substances as well as substances currently undergoing research and development and structured them into 32 clusters. Material-specific functional profiles were created for the companies and the application-specific substitution potential of the identified materials was assessed by the participating company experts using a qualitative evaluation.

The research approach chosen in this study enabled a very broad, worldwide analysis of available specialist literature. This allowed extensive information to be gathered in order to identify possible substitutes.

The key findings are:

> The properties of PFAS used in the applications under consideration (as a combination of benefit dimensions) are unique: they are used where a special combination of different benefit dimensions is required.
> For the companies involved, none or only 2 to 3 identified materials have the potential to replace PFAS in the future. An adequate substitute that could be used immediately or in the near future was not found in any of the cases examined.
> These potential substitutes are currently all at an early R&D stage and still require extensive research and development work, which will very likely be significantly longer than the transition periods of up to 13.5 years currently being discussed.
> The project results can provide new starting points for their strategic focus and for the direction of their research and developments.

Direct substitution does not appear to be possible today, as there are currently no alternatives available for the applications that are the focus of this project. Although there are a few possible alternatives in individual cases, they are still at the R&D stage. This means that their applicability and suitability for the specific application must be investigated in more detail. This sometimes requires extensive technical, safety and regulatory analyses (which could not be carried out as part of this study). Only then will it finally become clear whether they can really be used as a fully-fledged substitute.

The current situation poses major challenges for the industry. The experts involved see the following in particular:

1. Identification, substitution and risk assessment of PFAS: The challenge is to identify all PFAS-containing materials and components and to look for technically suitable alternatives that can completely replace the current PFAS-based solutions in terms of form, fit, processability and function. At the same time, the risk of PFAS substitutes must be determined in order to avoid replacing PFAS with materials that are considered problematic from a regulatory or toxicological point of view. This requires intensive research into alternative, suitable materials or technologies.
2. Supply chain management: It is crucial to secure the supply chains for PFAS and other critical materials. In addition, recording of the entire supply chain for complex products is an important aspect.
3. Ecological and regulatory aspects: The increasing importance of ecotoxicological issues requires proactive action from the industry. In the experts' view, it is necessary to establish the concept of essential use and return to a risk-based approach. It should also be discussed whether PFAS should be seen as a precedent for future regulations and how regulatory authorities incorporate technical realities into their decisions.

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If no substitution options are found in the near future, industry in Baden-Württemberg, but also society, will suffer disadvantages, as certain high-tech applications, many of which are essential, will no longer be possible (at least at the usual level of performance).

The results obtained can serve as a basis for the further decision-making process on possible substance restrictions. A balance must be struck here between the benefits for industry and society on the one hand and the risks to the environment and health on the other. A differentiated consideration should individually address the possible risks of the respective substance in the environment, but also the disadvantages and risks that could arise from a ban on an application that makes sense for society, e.g. in the health sector.

7 LITERATURE

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APPENDIX: THE 32 IDENTIFIED MATERIAL CATEGORIES

The material categories identified in the project are shown in the following table.

Table: Identified material categories

ID	Material category	Description of the
1	Polymer and Composite Hydrogels	Water-swollen, cross-linked polymer networks with reactive and adjustable mechanical properties
2	Nanoparticle-based Drug Delivery Systems and Nanomaterials	Nanoscale carriers developed for targeted drug delivery and versatile material applications
3	Advanced Coatings and Surface Treatments	Innovative protective coatings that improve the surface properties against wear, corrosion or environmental influences
4	Advanced Metal Alloys and Coatings	High-performance metal combinations that offer superior strength, durability or specific functions
5	Graphene-Based Nanomaterials and Composites	Atomically thick carbon layers promise high electrical conductivity and mechanical strength
6	Functional Polymeric Films and Coatings	Polymer layers that offer certain functionalities such as barrier properties, conductivity or reactivity
7	Nanocatalysts and Metal Oxide Composites	Improved nanoscale catalysts in combination with metal oxides for improved reaction efficiency
8	Biological and Biocompatible Materials	Materials that are designed to interact with biological systems without harm and are suitable for medical applications
9	Organic and Energetic Compounds	Chemically produced molecules that release energy on decomposition and are used in propellants and explosives
10	Fluorescent Carbon Nanomaterials	Nanoscale carbon structures that can emit light when excited
11	Halide Perovskite Solar Materials	Crystalline materials that offer improved solar conversion efficiency in photovoltaic devices
12	Polymeric Materials and Coatings	Wide range of macromolecular materials and coatings for different applications
13	Bioactive Ceramic Composites	Ceramics that cause specific biological reactions, useful for applications such as bone implants
14	Polymer-Based Composite Membranes	Developed membranes that integrate polymers for filtration, separation or controlled release applications
15	Phosphor-Based Luminescent Materials	Materials that are capable of absorbing and re-emitting light and are important in display and lighting technology
16	Metal and Metal-Based Nanoparticles	Nanoscale metal particles with unique electronic, optical or magnetic properties
17	Inorganic Adsorbents and Framework Materials	Solid materials that can capture molecules from gases or liquids by adsorption
18	Cellulose-Based Nanomaterials and Composites	These nanomaterials are derived from natural cellulose and offer strength, biodegradability and functionality

19	Polymer Electrolyte and Battery Materials	Materials for efficient charge transfer in battery systems
20	Fluorescent Nanoparticles and Probes	Nanoscale particles that emit light and are suitable for applications in the fields of imaging, sensor technology and diagnostics
21	Lead-Free Ceramic Materials and Composites	Ceramics without lead content, with a focus on environmental safety while retaining essential properties
22	Polymer Nanocomposites and Conductive Materials	Polymers with integrated nanoscale fillers that improve conductivity or mechanical properties
23	Metal Oxide Nanocomposites and Thin Films	Nanocomposite materials and thin films that utilise the diverse functions of metal oxides
24	Polymer-Based Composite Materials	Composite materials that utilise the properties of polymers and other fillers or reinforcing materials
25	Magnetic Nanoparticles and Composites	Nanoscale particles with magnetic properties that are crucial for data storage and medical applications
26	Bioactive and Antimicrobial Materials	Materials designed to interact with or inhibit the growth of microorganisms
27	Ceramic and Metal Matrix Composites	Composite materials that combine the advantages of ceramics and metals, e.g. high temperature resistance and strength
28	Titanium-based Nanocomposites and Coatings	Compositions that utilise the strength and corrosion resistance of titanium on a nanoscale or as a coating
29	Transition Metal Dichalcogenide (TMD) Nanomaterials	Layered nanomaterials with potential applications in electronics and optics
30	Functional Coatings and Surface Modifications	Coatings intended to impart or modify certain functionalities to surfaces
31	Advanced Ceramic and Composite Materials	Ceramic materials or composites developed for high-performance applications
32	Modified Asphalt and Bitumen Composites	Conventional road construction materials that have been improved in terms of durability, flexibility or other desired properties

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