Advanced Materials SAFETY 2023

8 - 10 November 2023
Saarbrücken, Germany

Abstract book

Advanced Materials Safety 2023

Functionality of advanced materials, their impact on humans and the environment as well as the acceptance of the technologies are the focus of the conference. With the Advanced Materials Safety 2023, we bring together researchers with different relevant expertise and identify possible interfaces for joint research projects that allow us to investigate such complex challenges.

Organizers: Leibniz Research Alliance Advanced Materials Safety

INM – Leibniz-Institute for New Materials, Saarbrücken

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12:00	Discussion The discussion will be logged; you are invited to contribute before, during and after the discussion in this document: https://docs.google.com/document/d/14xWgwBvjc6fGbt-Sd54PK-fCO41kuzCrU0I1qNbEcx4/edit?usp=sharing Moderation: Felix Bach, FIZ Karlsruhe, Co-spokesperson NFDI4Chem, Karlsruhe, Germany
12:20	Closing session
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Abstracts

Oral presentations

End-of-life perspective for advanced energy storage, mobility and electronics technology materials: a gateway to a sustainable circular economy

Ajay B Patil, Jens Gutzmer

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The world is witnessing unprecedented advances in the field of renewable energy generation, storage, electrical mobility, and digital technologies. These developments are necessary to achieve our ambitions of becoming a green and sustainable society that retains economic prosperity. Behind the scenes this transition is enabled by a multitude of increasingly complex materials marked by impressive optoelectronic and/ magnetic properties. Not only does the complexity of materials increase, but also similar is true for the compositional architecture of machines, gadgets and installations. This is combined with an ever-increasing speed with which advanced technologies penetrate global markets and the often very limited life span / planned obsolence of many advanced technologies. Together, these factors yield a rapidly increasing volume of waste materials of complex composition. Such complex waste materials do not only contain a vast variety of valuable resources but, if left untreated, may cause great harm to humans and the environment. It is, therefore, obvious that we need no less than a paradigm shift. EoL products should be regarded not as waste but as valuable secondary resource. Technological solutions are urgently needed to drive the transition towards holistic recycling concepts.

The simple, holistic and yet sustainable answer to all these questions is the adoption of circular economy strategies. This talk will present the opportunities and challenges in management of advanced materials with end-of-life perspective. How the fundamental understanding of materials properties and quantities is necessary in viable circular economy process developments and implementation. It will be complemented by select examples of technologies developed for the recycling of relevant materials and its materials safety-related implications.

Synthesis and recycling of MXene electrodes for high performance energy storage

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3 Saarene – Saarland Center for Energy Materials and Sustainability, 66123 Saarbrücken, Germany

The field of battery research continually seeks to improve energy storage capabilities while addressing sustainability concerns. This applies in particular to the exploration and development of novel materials, such as the promising material group of MXenes.

The presentation highlights the development of high-performance sodium-ion batteries using MXene / antimony hybrid electrodes. This hybrid material exhibited a high reversible capacity of 450 mAh/g at 0.1 A/g, along with excellent cycling stability and rate capability.[1] We also explore the combination of MXenes and SnO_2, a conversion material, for enhanced lithium-ion battery performance of over 500 mAh/g for 700 cycles at 0.1 A/g.[2] The resulting nanocomposites demonstrated high-capacity retention over numerous cycles and excellent rate capability.

Additionally, we demonstrate MXene electrode recycling and upcycling. With binder- and additive-free MXene paper electrodes, we show the significance of finding sustainable and efficient approaches to recycle spent lithium-ion and sodium-ion batteries. The recycled electrodes exhibited good electrochemical performance and were easily recovered through direct recycling processes, achieving high capacity recovery rates. Moreover, the cycled MXene electrodes could be transformed into TiO_2/C hybrids with adjustable carbon content, providing opportunities for their utilization in various battery and electrocatalysis applications.[3]

Collectively, we emphasize the potential of MXenes and MXene hybrid materials for enhancing charge storage capabilities in batteries. They also underline the significance of developing sustainable recycling and upcycling approaches for MXene electrodes, contributing to the overall advancement of battery technology.

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A Multimodal Approach to Quantify Surface Functional Groups and Ligands on Amorphous Silica Nanoparticles

Isabella Tavernaro[1], Nithiya Nirmalananthan-Budau[1], Bruno Di Giacomo[1&2], Mengshu Zhu[1&2], Viktoriia Osipova[1&2], Ute Resch-Genger[1]

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Nowadays amorphous silica nanoparticles (SiO_2-NP) are one of the most abundant engineered nanomaterials, that are highly stable and can be easily produced on a large scale at low cost. Surface-functionalized SiO_2-NP are of great interest in the life and material sciences, as they can be used e.g. as drug carriers, fluorescent sensors, and multimodal labels in bioanalytical assays and imaging applications. Their performance in such applications depends not only on particle size, size distribution, and morphology, but also on surface chemistry, i.e. the total number of surface functional groups (FG) and the number of FG accessible for subsequent functionalization with ligands or biomolecules, which in turn determines surface charge, colloidal stability, biocompatibility, and toxicity.[1] Aiming at the development of simple, versatile, and multimodal tools for the quantification of many bioanalytically relevant FG and ligands, we investigated and compared various analytical methods commonly used for FG quantification (Figure 1). [2,3] This includes electrochemical titration methods, dye-based optical assays, and other instrumental analytical techniques such as nuclear magnetic resonance and thermal analysis methods.

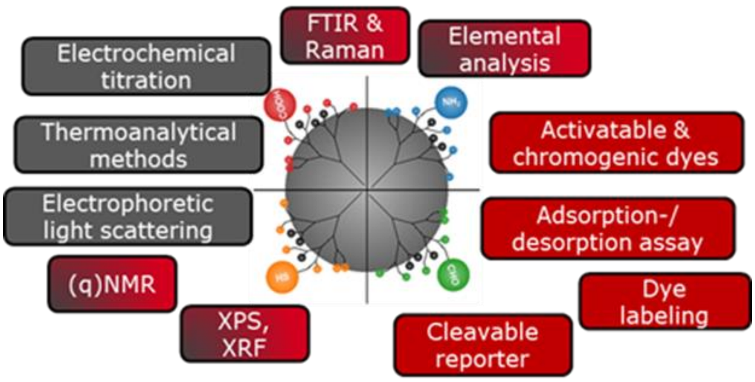

Figure 1. Analytical methods commonly used to quantify the total number of FG (grey) and accessible number of FG (red) present on the NP surface.

The potential of our multimodal approach for FG quantification was demonstrated for commercial and custom-made silica particles of varying FG, showing not only an influence of the synthesis methods on the number of FG but also on the performance. In the future, our strategy can contribute to establish multi-method characterization strategies to provide a more detailed picture of the structure-properties relationship.

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Advanced Materials – How to handle them in Industry?

Jonas Schubert[1,2]

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2 DermaPurge GmbH

Advanced materials are increasingly applied in industry. They provide benefits for costumers, companies and the environment. However, in many cases the long-term effect of frequent usage of advanced materials cannot be foreseen. Consequently, risk management strategies are needed to ensure a safe and long-lasting implementation for these materials.

In this talk two industry branches will be displayed to show, where advanced materials constantly generate human health risks. In these cases regular soap is not suited to clean the skin effectively. Soap is not optimized for specific substances. Its cleaning performance is therefore extremely insufficient; in some cases below 5%. Furthermore, soap opens up the skin pores and thus leads to an increased uptake of the hazardous substances.[1] The talk will, however, present a solution to the problem. To mitigate the health risks, three skin cleaning agents were developed that clean the skin from hazardous substances. The presented solutions are free from so called penetration enhancers and exhibit a cleaning efficiency of more than 96%.

Take home messages:

1. The application of nano-sized powders in 3D printing processes generate health risks as the particles can easily cross the skin barrier
2. The largely increased prevalence of cancer for firefighters is (partly) caused by the polymeric materials they work with.
3. Risk Management is the key factor for a long-lasting implementation and acceptance of advanced materials.

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Design and synthesis of high Tg thermoplastic polyhydroxyurethanes by reactive extrusion

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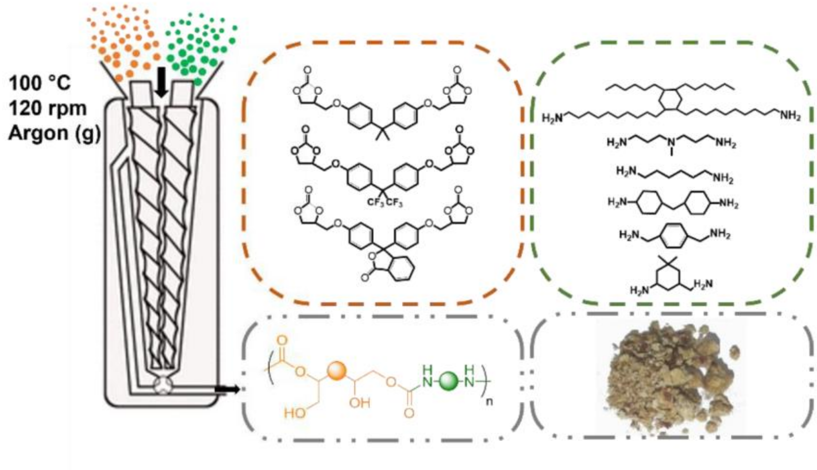
Polyurethanes (PUs) are common commodity plastics that cover a wide range of applications. However, PUs are based on isocyanates, toxic compounds that pose respiratory and dermal hazards. As a more sustainable alternative, polyhydroxyurethanes (PHUs) have gained attention as PU substitutes[1,2]. However, their utility is often limited by low molecular weights and inferior properties. To overcome these shortcomings, the present study focuses on the application of reactive extrusion to the synthesis of thermoplastic PHUs, allowing for rapid production without compromising molecular weight. Careful selection and target-oriented synthesis of monomers has enabled the production of a series of linear PHUs with high T_g (to 90 °C), high strength (to 60 MPa), and good thermal stability. Validation of this approach with a range of different monomers provides ample opportunity for the tuning of PHU performance as well.

Key words: Non-isocyanate polyurethane, reactive extrusion, polymer synthesis.



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Safe and Sustainable-by-Design and challenges for Advanced Materials

Hubert Rauscher, Carla Caldeira, Lucian Farcal, Irantzu Garmendia Aguirre, Davide Tosches, Elisabetta Abbate, Lucia Mancini, Kirsten Rasmussen, Juan Riego Sintes, Serenella Sala

European Commission, Joint Research Centre (JRC), Ispra, Italy

The EU Chemicals Strategy for Sustainability (CSS) aims at contributing to the safeguard of human health and the environment as part of an ambitious approach to move towards a zero-pollution and toxic-free environment. A key action defined in the CSS is the development of criteria for safe and sustainable by design for chemicals. SSbD aims at facilitating the industrial transition towards a safe, zero pollution, climate-neutral and resource-efficient production and consumption, addressing adverse effects on humans, ecosystems and biodiversity from a lifecycle perspective. Advanced materials are a source of prosperity of an industrial society and will also have a major in the transition towards sustainability.

To fulfil these ambitions, the European Commission (EC) developed a framework for the definition of criteria for SSbD chemicals and materials to steer innovation towards the green industrial transition, foster substitution or minimisation of the production and use of substances of concern, and minimize impact on human health, climate and the environment.

The framework encompasses both safety and sustainability assessment, conducted by means of life cycle assessment and it represents the backbone of the EC recommendation released in December 2022.[1]

The framework is composed of two components: a (re)design phase in which design guiding principles and indicators are proposed to support the design of chemicals and materials, and a safety and sustainability assessment phase in which the safety, environmental and socio-economic sustainability of the chemical/ material are assessed.

To foster the application of the SSBD framework to steer eco-innovation, innovators and the chemical industry have a pivotal role to play encompassing e.g., data availability, specific methodological development, sectorial rules, definition of benchmarks. The presentation will illustrate the framework and the specific implications and challenges for advanced materials.

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Commission Recommendation (EU) 2022/2510 of 8.12.2022 establishing a European assessment framework for 'safe and sustainable by design' chemicals and materials, https://eur-lex.europa.eu/legal-content/EN/TXT/?uri=CELEX:32022H2510

Industry session: Sustainable approaches to advanced materials

Abstract

The session follows a keynote by Hubert Rauscher: "Safe and Sustainable-by-Design and challenges for Advanced Materials". Company representatives will give short impulses introducing their companies and projects. A moderated discussion will allow the audience to interact with the speakers who will share insights from their points of view in more depth.

Mechanical recycling of polymer nanocomposites with CNT: technical and safety aspects

Carla Sottili

Nanocyl SA, Sambreville, Belgium

Carbon nanotubes have amazing properties. These can be transferred into a matrix, such as polymers, elastomers, resins, concrete, or water, to improve thermal and electrical conductivity and add mechanical strength. However, their extremely small dimensions and high surface activity raises Health Safety and Environment questions. The presentation aims to give an overview of the risks associated to the exposure to Nanomaterials such as carbon nanotubes. Moreover, recyclability of carbon nanotube enhanced materials will be discussed.

Electro-transformation of CO_2 to carbon nanomaterials

Apostolos Segkos

UP Catalyst OÜ, Tallinn, Estonia

Graphite and carbon nanomaterials are widely used in energy storage applications and are an important strategic resource for the EU. UP Catalyst produces graphite, multi-walled carbon nanotubes and carbon nanofibers by electro-transforming CO_2. The technology, which will be described in this talk, coupled with green, renewable energy sources leads to a carbon negative process which can convert approximately 3.7 t of CO_2 per ton of produced nanomaterials.

Degradation and disassembly concepts for tackling plastic pollution

Seema Agarawal

Macromolecular Chemistry II, University of Bayreuth, Bayreuth (Germany)

The extreme stability of polymers has challenged society with the accumulation of plastic waste and its management worldwide. Therefore, new and refined old concepts are urgently needed for the recycling and environmental degradability of plastics reducing and avoiding the accumulation of plastic waste. In this context, one of the questions raised very often is whether biodegradable polymers can be one of the solutions to the problem of plastic waste. For some of the specific applications, the answer is yes but for many other applications new recycling concepts would be preferred.

In the talk, the present scenario of the environmental acceptability of polymers and the opportunities offered by biodegradable disassemblable composites and recyclable cross-linked polymers will be discussed.

Microfibers in the marine environment: from analytical challenges to bio-inspired solutions

Francesco Saliu

Earth and Environmental Science Department, University of Milano Bicocca, Italy

Due to the risk of external contamination, fibers were excluded from the first microplastic surveys of the ocean. Nowadays, they have become the focus of attention and they are reported as the most common type of anthropogenic particle, from subsurface waters to deep-sea sediments and even in marine organisms. This is unsurprising, considering the rapid increase in global fiber production. It's noteworthy that most of the fibers identified in the ocean are not plastic, but chemically modified cellulose, which has sparked a debate in literature regarding the need for a common analytical methodology.

Additionally, the origin of fiber pollution is under investigation: while textile washing has been identified as the major source, research is underway to identify the key factors that contribute to fiber release from textiles. Finally, the negative effects of fibers and associated contaminants on marine organisms have been less studied than those associated with spherical and fragmented particles. Given the higher proportion of fibers in the marine environment, this is a significant knowledge gap. The presentation will address the current challenges in detecting microfibers and associated contaminants, recent research findings on their fate and interaction with marine organisms, and possible bioinspired solutions.

Plastic particles as a food source and their incorporation in tests of large benthic foraminifera

JOPPIEN Marlena[1,2,3,4], CHANDRA Viswasanthi[2], DOO Steve S.[1,2], STUHR Marleen[1], WESTPHAL Hildegard[1,2,3]

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2 Physical Science and Engineering Division, King Abdullah University of Science and Technology (KAUST), Thuwal, Saudi Arabia.

3 Department of Geosciences, University of Bremen, Bremen, Germany.

4 Asian School of Environment, Nanyang Technological University (NTU), Singapore, Singapore.

Large benthic foraminifera (LBF) are essential components of tropical coral reef communities and key carbonate-producing organisms. LBF can be utilized as indicators of pollution and environmental change. Marine litter, particularly plastic debris, presents a largely unquantified stress on foraminifera. Most studies on plastic pollution have focused on physiological responses of few organism groups (e.g., fishes, corals). Previous studies showed negative effects of micro- and nanoplastics on organismal physiology and ecosystem functioning. The potential responses of foraminifera remain widely unknown.

We present some of the first feeding choice experiments on LBF, comparing plastics with common food choices. Initially, we document the impact of microplastics (150-300 µm) on heterotrophic feeding behavior of *Amphistegina gibbosa* incubated either with *Artemia sp. nauplii* only, with pristine microplastic particles only or with a choice of nauplii and pristine microplastic. In a duplicate experiment, we compared the effect of pristine microplastic vs. microplastic that was pre-conditioned in artificial seawater. Our results indicate a strong feeding selection against pristine microplastic, suggesting a selective ability of the foraminifera to discern between potential food sources. The presence of pre-conditioned microplastic caused similar feeding interaction rates as with the natural food source *Artemia*. This suggests that feeding behaviour (and subsequently energy resources) of LBF may be more severely impacted by microplastics with longer residence times in marine environments.

In a subsequent long-term study, we exposed *A. lobifera* and *A. gibbosa* to nanoplastic particles (~1 µm) and sterilized *Nannochloropsis* algae cells as a natural food source within the same size range. Here, observed the uptake of polymer nanoparticles deep into the foraminiferal test and the incorporation of plastic particles into the outer calcite walls of the tests. Despite the high degree of specialization regarding skeletal formation of LBF, in this study, abundant cases of nanoplastic encrustation into the calcite tests were observed. Nanoplastic incorporation into the test was associated with LBF growth by formation of new chambers, in conjunction with continuous nanoplastic ingestion and subsequent incomplete egestion. Microalgae presence in nanoplastic treatments significantly increased the initial feeding response after 1 day, but regardless of microalgae presence, nanoplastic ingestion was similar after 6 weeks of chronic exposure. While ~40% of ingesting LBF expelled all nanoplastic from their cytoplasm, nanoplastic was still attached to the outer test surface and subsequently encrusted by calcite. These findings highlight the need for further investigation regarding plastic pollution impacts on foraminifera, such as their function as potential plastic sinks or plastic pollution indicators, as well as the effects of alterations in the structural integrity of foraminiferal tests. Large-scale incorporation of nanoplastic into LBF tests as well as potential consequences (e.g., test instability, toxicity) could impact ecosystem functions related to LBF, such as carbonate sediment generation on coral reefs.

Predictive 3D lung models to assess the hazard of aerosolized (advanced) materials

Barbara Rothen-Rutishauser

BioNanomaterials group, Adolphe Merkle Institute, University of Fribourg, Chemin de Verdier 4, CH-1700 Fribourg, Switzerland

Abstract

In field of inhalation toxicology there is a considerable lack of predictive and pre-validated in vitro lung models, which may be considered as substitutes for animal testing. A range of realistic, reliable, and predictive 3D lung models have been established over the last few years to investigate the potential hazard of aerosolized (nano)materials. Despite this significant progress in increasing complexity and physiological relevance, the models are still restricted for use in research environments. For the regulatory acceptance of in vitro lung models, robustness, reproducibility, and predictivity need to be demonstrated. Several approaches and efforts are currently ongoing to close these gaps such as projects that address standardization by testing the transferability and reproducibility of in vitro lung cell systems via interlaboratory comparison studies. This presentation will cover the challenges of pre-validation steps in the field of 3D lung model engineering and provide an overview of how these models can be used to assess the hazard assessment of (advanced) material aerosols.

About Barbara Rothen-Rutishauser

Prof. Dr. Barbara Rothen-Rutishauser received her Ph.D. in 1996 in cell biology at the Swiss Federal Institute of Technology in Zurich (ETHZ). She worked as a postdoc and group leader at ETH Zürich and University of Bern, Switzerland. She is an expert in the field of cell-nanoparticle interactions, with a particular focus on 3D human lung tissue models. Since 2011, she is the co-chair of BioNanomaterials at the Adolphe Merkle Institute, University of Fribourg, Switzerland, the position is shared equally with Prof. Alke Fink. Prof. Rothen-Rutishauser has published more than 300 peer-reviewed papers, is an associate editor of “Particle and Fibre Toxicology” and is currently president of the International Society of Aerosols in Medicine (ISAM).

Impact and mechanisms of action of metal-based nanomaterials on bioavailability and cell toxicity in advanced lung cell systems

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Abstract

Metal-based nanomaterials are increasingly applied as catalysts or antimicrobial additives, including nanoparticles of different metals, but also so-called nanowires of the same materials. This increases the risk of adverse health effects, since toxic metals may be released, and even essential trace elements may be toxic under overload conditions. To assess and compare toxic effects and to identify decisive factors leading to respective toxicity, we applied submers and advanced cell culture models combined with bioavailability studies and gene expression analysis via high throughput-RT qPCR related to genomic stability including epigenetic alterations as well as other relevant endpoints to establish toxicity profiles.

Different examples will be presented, such as chromium(III)oxide particles as compared to water soluble chromium(VI) or chromium(III) as well as the impact of copper- and silver-based nanoparticles and nanowire on genomic stability, demonstrating the role of intracellular bioavailability. Altogether, the applied cell systems and methods provide valuable tools to assess nanomaterial toxicity and, besides new mechanistic insights, the results are of major importance for risk assessment and read-across for metal-based nanomaterials.

Specific toxicity of CeO_2-nanoparticles

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Since CeO_2-nanoparticles induces specific toxicological effects, they do not belong to the group of so-called granular bio-persistent dusts (GBS). Inhalation exposure to CeO_2 elicits inflammatory and fibrotic effects in the lungs of humans and rats. Data in humans as well as in animals indicate individually varying health effects due to inhalation of CeO_2. In a long-term inhalation study with nanoscale CeO_2-particles, cerium phosphate was clearly detected in rat bone tissue.

In an extensive 2-year-inhalationstudy using nanoscale CeO_2-particles in rats, exposure concentrations as low as 0.1 mg/m^3 elicited statistically significant granulomatous inflammation and interstitial fibrosis of the lung. With decreasing particle size, the proportion of the two stable cerium valence states increases in favor of the Ce^{3+} proportion. This leads to altered chemical-physical properties, including an increased redox potential (Ce^{3+}/Ce^{4+}) and higher solubility. In the biological system, the toxicity of CeO2-particles is primarily due to their redox potential at the particle surface. However, a toxic effect due to soluble parts of the CeO_2 cannot be excluded.

Workshop – Communicating materials safety

Abstract

Communicating current scientific research and research results to the public is always a challenge. With the topic of Advanced Materials Safety, we find ourselves at the interface of three fields at once:

- the structures of the materials are usually extremely small and thus difficult to imagine for people outside the field
- the effects of the materials can usually only be determined indirectly – measurable, but rarely directly visible
- the perception of opportunities and, above all, of risks is very differently shaped individually.

The aim of the workshop is to present basic principles and communication formats relevant to the topic of Advanced Materials Safety in theory and in practice. The focus will be on the communication of opportunities and risks as well as the format of 360° videos. The makers of the DaNa platform will share their experiences from 14 years of communicating properties and potential risks of Advanced Materials. During the lunch break following the workshop, everyone is invited to try out selected communication activities from the Leibniz Research Alliance Advanced Materials Safety. A poster on the DaNa knowledge base will invite further discussion during the poster session and after the workshop.

Communicating nanotechnology in museums – insights from experience

Lorenz Kampschulte

Deutsches Museum, Munich, Germany

DaNa4 – Facts on Advanced Materials for interested persons

Dana Kühnel

Helmholtz-Zentrum für Umweltforschung (UFZ), Leipzig, Germany

Communication format 360° videos

Robin Wagner

Leibniz-Institut für Wissensmedien (IWM), Tübingen, Germany

Elucidating biological response in vitro of two-dimensional $Ti_3C_2T_x$ MXene

Agnieszka Maria Jastrzębska, Anita Rozmysłowska-Wojciechowska, Aleksandra Szuplewska

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Despite intensive research on the application of MXenes in medicine, the knowledge concerning their mechanisms of bio-action is still not fully clear. In recent years, we have been analyzing the most explored MXene and the influence of its surface chemistry on various interactions with biological matter. Current results point to the conclusion that surface oxidation of 2D $Ti_3C_2T_x$ MXene into Ti_xO_y oxides is responsible for the observed bio-action. As material's surface is responsible for its first impression on a mammalian cell in vitro, such an event must have a tremendous impact on further cell behavior. Therefore, by carefully studying the 2D $Ti_3C_2T_x$ MXene etching and delamination pathway and allowing for oxidation, we were able to elucidate its underlying mechanisms of biological action.

Our findings give evidence that the synthesis, processing, and oxidative instability of 2D $Ti_3C_2T_x$ MXene are responsible for the specific biological response in vitro. This knowledge is an essential tool for materials design and should be rationally used to develop future biotechnological applications of MXenes and related materials.

$Ag@TiO_2$ nanoparticles as photoacoustic contrast agent

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Titanium dioxide nanoparticles are promising candidates for applications in the biomedical field on the production of contrast images due to their photocatalytic properties [1]. However, it just absorbs light in the UV region. Deposition of noble metals as dopants is one way to overcome this. But generally, this synthesis involves the use of common strong reducing agents. This material can also be applied as a contrast agent in a promising imaging technique called Photoacoustic Microscopy (PAM)[2]. In this work, silver nanoparticles were deposited in TiO2 surface by a green sol-gel route. To study the influence of dopant, samples with 5 and 10% of silver, with calcination times of 2, 5, and 24 hours were prepared. The samples are characterized by IR, XRD, MEV, UV/Vis, and PAM. The infrared spectrum showed wide bands of stretching vibration of OH groups and flexion of Ti-O bonds. Diffraction peaks related to the anatase phase were predominant. The presence of silver was well distributed in titania surface. The deposition of silver improved the absorption profile of all samples to visible region, reaching NIR, in comparison with pure TiO_2. This improvement has a direct influence on the PAM analysis, where all the samples excited with 532nm showed uniform images with good contrast. On the other hand, excitation at 808nm generated greater variability in signal intensity. Samples with a higher concentration of silver (10%) were able to generate more intense signals when compared to samples with 5% silver. This is directly correlated to the light absorption capacity. These results demonstrate good potential for the application of the material as a contrast agent in photoacoustic imaging systems since the generated signal was also detected within the first biological window.

Keywords: Photoacoustic Microscopy, Titanium dioxide doped with silver, contrast agent.

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3D in vitro models of the intestine for safety testing of advanced materials

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Advanced materials are hoped to help us solve many pressing modern-day issues, e.g. regarding sustainable energy production, digitalisation and medical care. As previously experienced with manufactured nanomaterials, their increasing synthesis and potential incorporation into consumer products raises questions concerning their harmlessness.

As advanced materials can be taken up to the human body via intentional or incidental ingestion, we have developed complex in vitro testing approaches for the intestine [1,2]. We have advanced these methods to model different exposure scenarios, to test low-density materials (e.g. plastics) as well as to explore potential susceptibility differences in the healthy versus the inflamed intestine.

The models have been applied for the safety testing of various engineered nanomaterials and have been partially validated against intestinal tissue of exposed mice [1,3]. We could demonstrate pronounced material-specific effects in relation to the complexity [1,4] as well as the health status of the applied model [2]. The applicability of these models can be extended to the safety testing of advanced materials that may reach the intestine upon intentional as well as incidental oral exposures.

Parts of this work have received funding from the European Union's Horizon 2020 research and innovation program under grant agreement number 760813 (PATROLS), the Jürgen Manchot Foundation and the Leibniz Research Alliance Advanced Materials Safety.

Key messages:

1. Model complexity is a key factor for the experimental outcome.
2. Inflammatory processes can affect the models' susceptibility to exposures.

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Seeing is more than believing: How bioimaging contributes to understand advanced materials-cell interactions

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In the field of biomedicine, advanced materials, comprising nanomaterials, are already used and continuously developed, e.g. as diagnostic tools or delivery vehicles. In order to support safe applications of such materials, their efficacy, but also their safety has to be proven, ideally at an early stage of the development. The same applies to advanced materials used for technical applications. However, one main difference between these two areas is that biomedical applications include intended administration of specific materials, whereas for technical applications, exposure might occur unintentionally.

Bioimaging includes methods used to detect advanced materials and to monitor their distribution in the body as well as their interactions with single cells in vitro and in vivo. The presentation highlights techniques based on optical imaging used to determine the localisation, cellular uptake, and intracellular accumulation of advanced materials. The significance and limitations of these imaging approaches are discussed in the context of safety and efficacy assessment.

Polymer/inorganic core-satellite nanoclusters as model systems to understand the fate of nanohybrid materials in biological media

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Key message 1

Structurally precise nanoarchitectures with specific functionalities are represented by core-satellite polymer-inorganic nanohybrids[1]. The inorganic components of the nanohybrids contribute distinct size, shape, and composition-dependent properties such as optical effects[2], while soft polymeric component is responsible for structural flexibility and facilitates interactions with the surrounding environment. These properties combined enable the generation of nanotheranostic agents[3]. Here, we integrate distinct patterns of behavior into those polymer-inorganic nanoclusters to generate model system for establishing the fate of such nanomaterials in biological environments.

Key message 2

The NIPAM-co-DMAM (poly(*N*-isopropylacrylamide-co-*N,N*-dimethylacrylamide)) random copolymers with lower critical solution temperature (LCST) close to the normal human body temperature were synthesized *via* reversible Addition-Fragmentation chain Transfer (RAFT) polymerization using difunctional pH-labile RAFT agent bearing ketal moiety. Hybrid AuNP-core/random-copolymer-shell particles were obtained according to a “grafting-to” approach. The study of colloidal stability in a buffer solution (0.1 M PBS) of gold nanoparticles was carried out using light scattering techniques. Core-satellite nanostructures were assembled by adding smaller AuNPs to the precursor core-shell particles.

Key message 3

This work highlights the versatility of the RAFT polymerization technique in constructing hierarchical nanostructures with tunable degradation profiles that can adapt to various physiological conditions, such as lysosomal pH. Observation of aggregation due to the detachment of polymer chains from the surface of modified gold nanoparticles in a buffer solution, as evidenced by a gradual increase in the hydrodynamic volume, is also of particular importance to establish the stability under biologically relevant conditions. The reported modular assembly strategy toward stimulus-responsive clusters opens up systematic investigations of structure-effect relationships for assessing toxicity, biodistribution, and ultimately optimized design criteria toward a new generation of nanotheranostic agents.

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Mechanisms of cellular uptake and toxicity of micro and nanofibers in intestine and lung cell models

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2 Institute of Technical and Macromolecular Chemistry in RWTH Aachen University

Due to their unique properties, advanced fibrous materials are increasingly envisaged for innovative medical applications. It is also pivotal to assess the safety of such high aspect ratio materials. In this study, poly(lactic-co-glycolic acid) (PLGA) 85:15 (Sigma, 430471) and Twaron fibers (Teijin Aramid) are utilized to better understand the mechanisms whereby fibrous particles may cause toxicity in relation to their physicochemical properties, upon inhalation or oral exposure.

5 wt% PLGA is dissolved in hexafluoroisopropanol (HFIP), resulting in electrospun fibers, thus optimizing their suitability for cellular growth. In a second attempt, PEG-mRNA is added to the PLGA solution to explore potential applications as a drug delivery system. The assessment of mRNA loaded into the fibers remains difficult since both the PLGA and mRNA absorb light at 260 nm, while the acidic solvent quenches the signal of intercalating dyes. PEG-mRNA was not also detectable by using gel electrophoresis technique.

Cutting is achieved by ultrasonication with a working frequency of 20 kHz, an amplitude of 80% with the total run time up to 8 min.

A streamlined process is employed to transform Twaron into aramid fibers. Ball milling is made for varying durations: 40 min, 4 h, and 8 h, resulting in short fibers measuring between 0.1 mm and 1 mm in length after a 40 min period. Another endeavor is made to cut Aramid fibers using cryotome, however this technique yields significantly lower product quantities.

As the next step, the mechanisms of cellular uptake by macrophage cells will be investigated.

The unraveling of the toxicity mechanisms triggered by fibrous particles will contribute valuable insights, guiding the development of strategies to mitigate potential health hazards.

Impact of Advanced Materials on Human Health: Dissolution Control of Copper Oxide Nanoparticles for Therapeutic Applications

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Copper is an essential micronutrient that is required as a cofactor for numerous copper-containing enzymes and transcription factors and thereby contributes to several physiological processes. However, due to the toxic potential of copper, its homeostasis is tightly regulated through copper-binding importers, chaperones, and exporters [1]. Copper oxide nanoparticles (CuO NPs) are known to release Cu^{2+} ions. However, the excessive release of these ions can cause a series of downstream effects, ultimately leading to cell death [1,2]. Using a safe-by-design approach, Naatz et al. [2] prepared CuO NPs that were doped with different degrees of iron. Thereby, they were able to attenuate the dissolution of Cu^{2+} ions and reduce the cytotoxicity of the particles. Moreover, they achieved a selective targeting of cancer cells with the iron-doped NPs [3]. However, the exact mechanism behind these observations needs to be further elucidated. The goal of this project is to further investigate the responses of relevant cell types to the different, iron doped CuO NPs and to study how they are absorbed, distributed, metabolized, and eliminated in human cells. The cytotoxicity of the NPs will be studied *in vitro* using a range of human (cancer) cell lines. Using Raman-Spectroscopy, the uptake and distribution will be investigated. To identify particle-induced cell responses and molecular signatures of the different treatments, RNA-sequencing will be performed. Since copper dyshomeostasis is also known to be associated with several neurodegenerative diseases, models assessing the neurotoxicity of the NPs will be included as well. Last, we want to identify further model systems to simulate the routes of exposure and thereby predict the safety of other advanced materials in the future.

Key messages:

1. Copper contributes to several physiological processes but can have toxic effects.
2. Iron-doping changes the dissolution kinetics and thereby the toxicity of CuO NPs.
3. Our first results indicate a lowered toxicity of the higher doped CuO NPs *in vitro*.

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The Power of Metabolomics in Advanced Materials Research

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Nanotechnology plays a significant role in the development of advanced materials. Nanomaterials exhibit exceptional properties due to the size and high surface-to-volume ratio. However, their presence in the environment and potential impacts are a subject of concern. Also, it is important to consider that the breakdown of polymer materials like plastics can lead to the formation of nanoparticles (NPs). They can be found in water, soil, and in the air, with yet largely unexplored potential risks to both terrestrial and aquatic organisms [1]. The ingestion and absorption of NPs by marine life are of particular concern. However, it is still largely enigmatic how those particles act on the functioning of organisms, e.g. when particles incorporate into the skeleton [2]. Ongoing research is crucial to assess and manage the risks associated with NPs and to develop safe and sustainable nanotechnologies.

Metabolomics is a cutting-edge analytical technique and plays a crucial role in assessing complex biochemical processes in response to environmental challenges (in contrast to the genome, largely independent of external influences). Methods like nuclear magnetic resonance (NMR) spectroscopy and mass spectrometry (MS) enable the identification of a wide range of metabolites in complex biological systems, and their alterations induced by environment and developmental state. This information aids in understanding the effect of NPs on organism fitness, and it can help biomarker discovery.

In this context, we will address specific challenges metabolomics faces with studies of corals and the techniques employed in our research. Additionally, we illustrate how analytical methods can contribute to an understanding of the safety and biological implications of newly developed materials.

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Using immersive 360° videos for science communication on the safety of advanced materials

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Today's technologies enable highly immersive experiences, such as with 360° videos. Currently, there are many technical advances in the virtual reality field, so these viewing formats are gaining more and more attention[1]. Particularly immersive 360° videos raise the hope of bringing great benefits, as they can convey authentic experiences and activities[2], e.g., in realistic scientific environments. Therefore, these forms of visualization might help to positively change perceptions and attitudes about the relevance of science[3], making them an exciting tool for science communication, for instance, regarding the safety of advanced materials. However, the effects of immersive technologies are not yet fully understood, and complete immersion seems not always to be the best approach to delivering contents[4]. To address this issue, part of the research project is to investigate the most appropriate degree of immersion for 360° videos as a science communication tool.

A common way of influencing attitudes with immersive interventions involves virtually putting people in the role of another person (Virtual Reality Perspective Taking) so that scenarios are experienced from that person's perspective[5]. However, there is scarce research on the change of different points of view within a 360° video. In this regard, there have been studies using conventional videos: Beege et al. found that a frontal view of a lecturer produced significantly stronger perceived parasocial interactions and better learning outcomes than looking at a lecturer laterally[6,7]. Whether this is also applicable to immersive 360° videos and how different points of view have an impact on variables, such as trust in scientists, remains to be proven and is thus another research aspect of the project.

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The future of materials science and engineering: How to participate and get the most out of the digital transformation

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The digital transformation in materials science & engineering will lead to a profound change in how data, information and knowledge can be shared as well as represented. In the near future, data, information and knowledge will be available through structured knowledge graphs, allowing to use materials data as well as apps (data analytics, simulations, AI-modelling) in a seamless fashion. Collaborations within and across disciplines will be just a click away and semantic interfaces will allow us to establish complex data workflows which will be fed automatically by data from experiments and simulation tools as well as from open data repositories. Altogether, the changes will enable us to accelerate scientific discovery, which gives us and the coming generations a chance to solve the pressing challenges concerning climate change, resource scarcity and give us a realistic chance to implement a circular economy.

In the first part of this talk, the goals and realistic possibilities of ongoing initiatives will be introduced. The role of the Nationale Forschungdaten Infrastruktur NFDI, and specifically the NFDI-MatWerk, as well as the BMBF MaterialDigital initiative shall be introduced and discussed.

In the second part, an introduction to practical examples from within the Fraunhofer IWM will be used to show various aspects of digitalization and their use and how it might be implemented:

- The selection and technical implementation of necessary database(s),
- Digitization of manual and (partially) automated processes in metallography,
- Structuring of a continuous data space through material ontology-based knowledge graphs,
- Use of artificial intelligence models for automated identification and representation of complex microstructures as input to material models, and
- Fusion and interpretation of data from metallography, mechanical properties experiments, and simulations.

Based on these examples, the opportunities and ToDos in establishing a common MSE data space will be discussed. Furthermore, the impact of these changes shall be discussed concerning future proposals, especially for longer lasting collaborative projects as well as proposals for the Excellence Initiative.

Autonomous decision support for nanosafety

Robert Rallo

Advanced Computing, Mathematics, and Data; Pacific Northwest National Laboratory, Richland, WA (USA)

The emergence of generative artificial intelligence (genAI) provides new opportunities to accelerate nanoEHS research. In particular, autonomous experimentation offers new possibilities to accelerate the discovery of linkages between the structure, properties and bioactivity of chemicals and nanomaterials.

In this talk we will provide an overview of the challenges and opportunities of the application of modern AI techniques in nanosafety. The talk will cover aspects related to data, latent space representation, physics-embedding, as well as the mapping of AI models to specific hardware accelerators for the autonomous operation of characterization and synthesis instruments.

Computing infrastructure for the definition, performance testing and implementation of safe-by-design approaches in nanotechnology supply chains

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A major challenge for the global nanotechnology sector is the development of safe and functional engineered nanomaterials (ENMs) and nano-enabled products (NEPs). In order to minimize the risks to human and environmental health during the engineering of NEPs the goal of the Safe-by-Design for Nano (SbD4Nano [1]) project is to create a novel e-infrastructure for the definition, performance testing and implementation of Safe-by-Design (SbD) approaches in the nanotechnology supply chains.

SbD4Nano will overcome all the barriers to promote the implementation of SbD approaches in the nanotechnology industry, providing SMEs with a set of web-based applications and tools.

The tool integrates a number of models to predict the toxicity of ENMs, being designed to be used by SMEs and non expert users. New approaches to predict the functionality of advanced materials have been implemented to support the design of safer products without compromising the performance.

Key messages learned from the project are:

1. FAIR data is essential to overcome current barriers to develop predictive models
2. New models shall consider the functionality to support industrial uptake
3. A new knowledge infrastructure compiling models and tools have been developed

References:

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Workshop – Digital infrastructure: documenting and publishing materials safety data

Abstract

The Advanced Materials Safety community is composed of researchers from different scientific fields, each with unique information requirements, methodologies, terminologies and levels of digitization expertise. As a result, data interpretation is hampered by the existence of different data types and a lack of standardized descriptions and quality criteria, which can lead to misinterpretation. eNanoMapper represents a state-of-the-art database for this community.

While data management and sharing tools such as Electronic Lab Notebooks (ELNs) are widely used in industry, analogue workflows are still dominant in academia. This approach might lead to errors in data generation which are later difficult to trace back. During the workshop we will therefore discuss the error culture in science and how errors are managed in the academic environment and beyond: We will explore how errors can be minimized – and how they can positively impact the research process.

The BMBF project DaNa has established a web-based knowledge base to share data on the safety of advanced materials with both the scientific community and the public. The project curates data from scientific publications according to a catalogue of criteria to ensure the validity of the information. SOPs are playing an increasingly important role. Therefore, the project provides a template and a listing of such work instructions for download online. Nevertheless, in many databases data upload processes are not currently automated, making seamless data findability and accessibility extremely difficult and frustrating for researchers.

In this workshop we want to share some of our experiences made so far in NFDI4Chem and transfer our knowledge to the multidisciplinary community dealing with aspects of the safety of advanced materials. Our aim is to provide ideas and best-practice examples to generate an RDM approach towards a FAIR infrastructure also in this multidisciplinary sector.

Moderation and introduction

Felix Bach

FIZ Karlsruhe, Co-spokesperson NFDI4Chem, Karlsruhe, Germany

What do chemistry and advanced material safety data have in common?

Christian Bonatto Minella

FIZ Karlsruhe, Karlsruhe, Germany

Error culture in science

John Jolliffe

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From ELNs to Smart Labs and interconnected repositories

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Evaluation and quality of data on the safety of advanced materials

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About NFDI4Chem

NFDI4Chem envisions the complete digitalisation of all key steps in chemical research to help scientists collect, store, process, analyse, share and re-use research data. The primary goal of the consortium is to promote open science and research data management in line with the FAIR data principles. This vision and the developed architecture as well as some of the services and tools can be reused by other scientific communities like Advanced Material Safety.

Poster abstracts

In alphabetical order by last name of first author

Towards marine sustainability in textile production: disentangling the contribution of the polymer photo-degradation to microfiber release and impacts

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Current studies on the impact of plastic on marine ecosystems mainly focus on how micro/nano fragments physically interact with various marine organisms and on how plastic additives contaminate the environment [1]. However, the potential reactivity of plastic is not considered enough in the literature. As highlighted in the microplastic genesis, synthetic polymers undergo chemical and physical degradation processes that lead to both mechanical and molecular fragmentation [2]. This can result in the release of new contaminants that require proper risk assessment [3]. To assist the development of new textiles that release fewer microfibers, we optimized a testing procedure that involves controlled artificial weathering conditions and chemical characterization using advanced mass spectrometry. We then conducted ecotoxicological tests on leachates and micro fragments with marine microalgae and soft corals.

1. Textile fibers were submitted to photo-degradation and leaching tests.
2. The released photo-degradation products were fingerprinted by means of advanced mass spectrometry. Different profiles were highlighted.
3. Ecotoxicological assays were carried out. No mortality was observed but stress, with dependency on polymers and released chemicals.

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A novel miRNA nanocarrier for local device-based pharmacotherapy

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Device-based therapies have been developed as adjunct treatment approaches in cardiovascular disease, e.g., renal denervation or drug coated balloons as local therapy for the treatment of vulnerable plaques and atherosclerosis. As previously shown, miR29b inhibition may result in vessel wall stabilization by regulation of the ECM (extracellular matrix). Targeted drug delivery by the use of a carrier can improve the safety and efficiency of drug administration. In our in vitro studies we tested the use of Silica nanoparticles (SiO_2-NP) as a potential carrier.

Methods

Smooth muscle cells were exposed to various concentrations of fluorescently labeled SiO_2-NP. Subsequently, cells were treated with LNA-linked nanoparticles. Presence and localization of LNA and NP were examined via confocal laser scanning microscopy and fluorescence spectroscopy. Expression of ECM associated genes and inflammatory markers were determined by real time PCR.

Results

SiO_2-NP were rapidly internalized and uptake of the NP was observed already after 1 min. After 24 hours, inflammatory genes remained at the control level after exposure to up to 50µg/ml SiO_2-NP (Neg/Pos SiO_2-NP, n=4, MCP1: 15.86 ±0.44, p<0,001/ 0.09±0.02, n.s.; V-CAM: 25.81±4.91, p<0,05/ 0.42±0.21, n.s.; I-CAM: 20.25±5.24, p<0,05/ 6.04±0.24, p<0.001). No remarkable changes of miR29b expression as well as of miR-29b associated genes were detected. After 24h incubation with anti-miR29b LNA (20nm, 40nm) coated SiO_2-NP miR-29b LNA and NP could be detected in the cytoplasm. After 48h, gene expression of associated genes was equally regulated as in former transfection experiments. Col1: (n=4, NPneg-0=1.00±0.27, NPneg-20=1.16±0.18, n.s.; NPneg-40=1.21±0.16, n.s.; NPpos-0=1.00±0.21; NPpos-20=1.07±0.19, n.s.; NPpos-40=1.26±0.19, n.s).; Col3: (n=4, NPneg-0=1.00±0.44, NPneg-20=1.20±0.39, n.s.; NPneg-40=1.52±0.31, n.s.; NPpos-0=1.00±0.35; NPpos-20=1.33±0.34, n.s.; NPpos-40=1.77±0.33, p<0.01).Positively charged NP seemed to associate with the cells at higher amounts compared with negatively charged.

Conclusion

SiO_2-NP were a suitable carrier for miRNAs and therefore a potential new target for device based local delivery of miRNA therapeutics.

Use of THP-1 cells as a promising tool to assess NLRP3 inflammasome activation by particulate polymers

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Due to the environmental pollution with polymeric particles (micro- and nanoplastics, MNPs), inhalation and ingestion by humans is very likely, but human health effects remain largely unknown. The NLRP3 inflammasome is a key player of the innate immune system and is involved in responses towards foreign particulate matter and the development of chronic intestinal and respiratory inflammatory diseases [1,2]. We established NLRP3-proficient and deficient THP-1 cells as an alternative in vitro screening tool to assess the potential of MNPs to activate the NLRP3 inflammasome. By investigating cytokine release (IL-1β and IL-8) and cytotoxicity after treatment with engineered nanomaterials, this in vitro approach was compared to earlier published ex vivo murine bone marrow-derived macrophages and in vivo data [3,4]. This approach showed a strong correlation with previously published data, verifying that THP-1 cells are a suitable model to investigate NLRP3 inflammasome activation. We then investigated the proinflammatory potential of eight polymeric particles of different size, shape, and chemical composition. Only amine-modified polystyrene (PS-NH2) acted as a direct NLRP3 activator. However, polyacrylonitrile (PAN) and nylon (PA6) induced a significant increase in IL-8 release in NLRP3−/− cells. Our results suggest that most polymers are not direct activators of the NLRP3 inflammasome, but specific particle types might still possess pro-inflammatory potential via other pathways. We propose to use our approach as an early in vitro screening tool when assessing the hazard of advanced materials in a hierarchical testing strategy.

1. THP-1 cells are a promising tool to assess the NLRP3 activating potential of advanced materials in vitro.
2. Most polymers do not appear to be direct NLRP3 activators.
3. Some polymers induce pro-inflammatory reactions via NLRP3-independent pathways.

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Plasma functionalized TiO_2 nanoparticles immobilised on naturally recyclable cellulose fibres for enhanced photocatalytic performance

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A great number of water pollutants are quite stable to light and oxidation, which makes them challenging to degrade. Cellulose and its derivatives have gained increasing attention as functional materials for wastewater (WW) treatment.

In this study photocatalytic membrane materials were successfully fabricated using plasma-assisted spraying (PAS) of titanium dioxide nanoparticles (TiO_2) functionalized and deposited onto naturally recyclable cellulose fibres (CF). The single step innovative PAS technique provided strong chemical bonding between CF and TiO_2 by introducing the electron-rich oxygen functionalities as well as oxygen vacancies.

5min plasma exposure (*p*C05) on CF led to polymorphic changes of naturally occurring cellulose I to cellulose III indicating alterations on the cellulose crystallinity index, further confirmed by Raman spectroscopy and FTIR. In addition, XPS confirmed the presence of Ti-O-C bond formed. T_pC05, which exhibited a decrease in bandgap of TiO_2, resulted in increasing photocatalytic degradation (PCD).

Synthesized TiO_2/CF were deployed for the degradation of methylene blue (MB) and indigo carmine (IC) from industrial WW. T_pC05 showed a PCD efficiency of 71% for MB and 100% for IC, under UV-light irradiation of 180min and 90min, which is 2x higher compared to T_pC01 nanocomposites.

Biocompatibility studies of natural CF, TiO_2 and TiO_2/CF nanocomposites showed cytotoxicity of the natural CF mainly due to the presence of saponins, which are known toxic natural plant components. However, washing procedures prevent the cytotoxicity. In addition, TiO_2 immobilized on the cellulose did not induce any cytotoxicity effect up to 2mg/mL. These findings verify that oxygen plasma functionalized TiO_2/CF is a biocompatible and sustainable material for industrial PCD in WW treatment.

Key messages

1. Synthesized TiO_2/CF showed a PCD of MB and IC from industrial WW.
2. Improved photocatalytic activity could be attributed to the presence of Ti-O-C chemical bond and electron transfer.
3. TiO_2/CF is a biocompatible and sustainable material for PCD in WW treatment.

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Developing an advanced materials of a free-standing composite solid-state electrolyte incorporating Al-doped LLZO (Al-LLZO) in NCM811 for solid state lithium- metal batteries

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The development of advanced materials for energy storage devices has been of utmost importance for the transition towards clean and renewable sources of energy. In this context, solid-state lithium metal batteries have shown promising features such as high energy density, good ionic conductivity, and safer performance than conventional batteries. The primary aim of this research work is to develop a free-standing composite solid-state electrolyte (CSEs) that incorporates Al-doped Lithium Lanthanum Zirconium Oxide (LLZO) into NCM811 for solid state lithium-metal batteries followed by solution casting method. The researcher used various characterization techniques such as XRD, FT-IR, EIS and SEM to analyze the structural and morphological properties as well as the impedance of the solid state composite electrolyte. This material gives 4.9 x 10^{-4} Scm^{-1} ionic conductivity at room temperature. The NCM811/CSEs/Li exhibited after 100 cycles specific capacity 125.35 $mAhg^{-1}$ and the capacity retention 98.08 % at ambient temperature and with the rate of 0.5C.

Kew words:

1. advanced materials 2. solid state 3. Al-LLZO 4. solution casting 5. ionic conductivity

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Pro-inflammatory effects of carbon nanoparticles by reduction of neutrophil apoptosis rates

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Neutrophilic inflammation is a very effective pathogen defense mechanism of the innate immune system. However, in situations of chronic inflammation the neutrophil defense mechanisms, including oxidative burst and secretion of proteolytic enzymes, can cause tissue damage. Therefore, duration and strength of neutrophilic inflammation are mainly regulated by the restricted life span of this terminally differentiated cells [1]. Advanced materials like poorly soluble nanoparticles might come into contact with neutrophils either when applied intentionally or accidentally, when humans are exposed at the working place or in the environment. Our earlier studies indicated that the exposure of human peripheral neutrophils *ex vivo* but also of lung neutrophils from rats *in vivo* to carbon nanoparticles leads to prolonged life span of these cells by a delay in natural apoptosis [2,3].

In the current study we investigated mechanisms of apoptosis in human neutrophil from blood of healthy volunteers and in neutrophilic differentiated HL-60 cells. In both cell types exposure to carbon nanoparticles (but not to bigger carbon particles) dose-dependently reduced natural apoptosis rates, while intracellular reactive oxygen species (ROS) increased. Intervention experiments demonstrated the causal link between ROS and reduced apoptosis. In depth investigations of the inflammatory status of donors revealed that these specific effects are linked to a priming of neutrophils. Moreover, exposure to carbon nanoparticles led to the ROS-dependent activation of neutrophils determined by the loss of L-selectin and an increase in integrin CD11b. The described pro-inflammatory effects of carbon nanoparticles appear to be mediated by a ROS-dependent reorganization of membrane lipids.

Key messages:

1. Carbon nanoparticles act pro inflammatory via ROS-dependent reduction of apoptosis
2. Carbon nanoparticles activate neutrophils by intracellular ROS induction
3. Primed human neutrophils offer an experimental system for testing of pro-inflammatory effects of poorly soluble materials

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Innovative Binary Solvent Strategy to achieve a Highly Responsive NH_3 Gas Sensors Using Metal Halide Perovskite Films

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Key words: NH_3 gas, Binary solvent, Precursor preparation, DMF: DMSO mixture, Response

Ammonia (NH_3) gas is poisonous, requiring the deployment of sensitive gas sensors. This study introduces highly responsive NH_3 gas sensors using a binary solvent strategy. We used a mixture solvent strategy to optimize the preparation of Metal Halide Perovskite ($MAPbI_3$) film precursors. Previously, $MAPbI_3$ films for gas sensing were made in a single solvent. In contrast, we utilized a mixed solvent system comprised of dimethylformamide (DMF) and dimethyl sulfoxide (DMSO). When compared to DMF alone, this approach significantly improves NH_3 gas detection ability. Notably, perovskite precursor in a 4:1 (V/V) solvent combination of DMF and DMSO yields a high response of 190% in NH_3 gas sensing, and in DMF solvent achieved response of 31 %. Using mixed solvent to prepare the film precursor improves surface coverage and smoothness of the surface of the sensor, resulting in a better response [1]. In conclusion, this study offers a novel binary solvent technique to improve NH_3 gas detection utilizing $MAPbI_3$ film sensors and presenting its potential for future gas sensor technology.

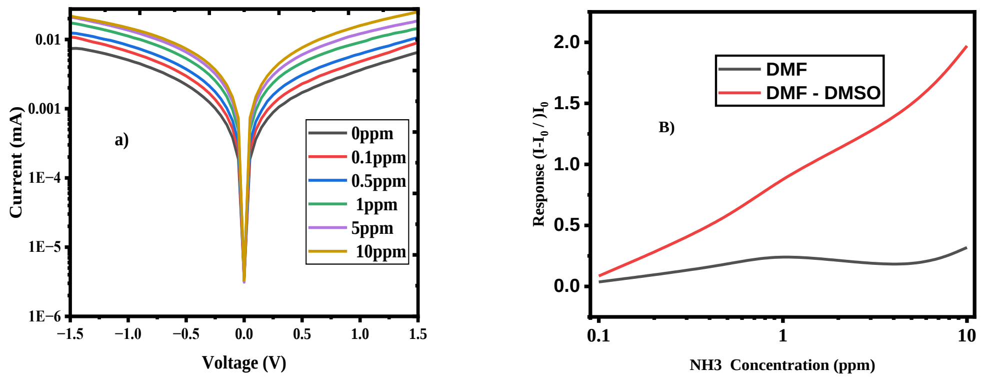

Figure 1. a) I – V characteristics of the sensor at various ammonia concentrations. B) Response of the sensor for different solvent

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The regulatory experience of SWNT named Tuball™

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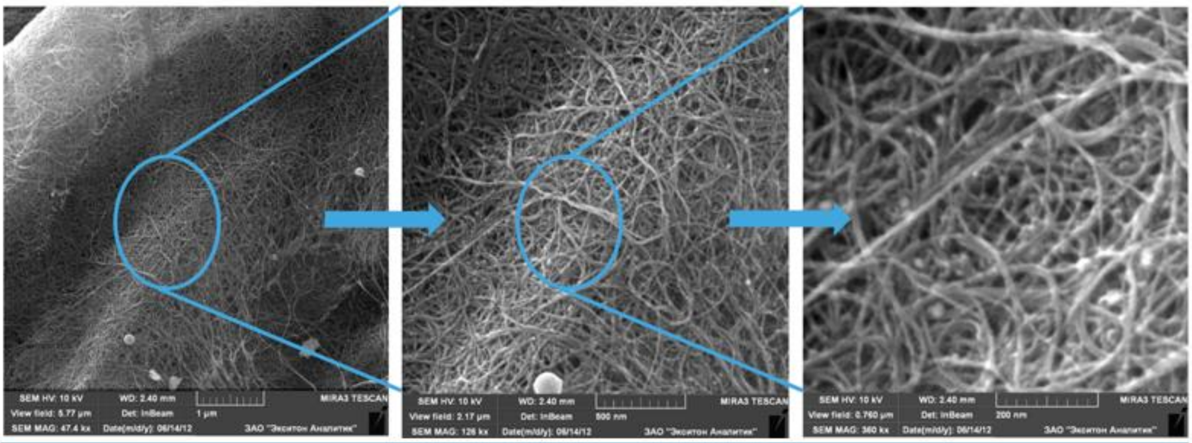
The company OCSiAl Europe Sarl is the first SWCNT manufacturer who has completed the EU-REACH registration and in the meantime allowed to commercialize up to 100 tons/y of his nanosubstance named Tuball™, being additionally compliant to the new REACH regulation for Nanoforms. Single wall carbon nanotubes (SWCNTs) are a highly innovative material that can be used as an additive to enhance the properties of most types of polymers and battery electrodes. OCSiAl plays the leading role in improving the accessibility of information on the nature of graphene nanotubes and forming the principles of their safe handling—as of today, the company has initiated almost 30 unique studies, including those required for EU-REACH and US-TSCA. We had some analytical - and other challenges during the different toxicity testing we had to perform for regulatory purposes. This poster explains our recent regulatory experiences of our TUBALL™.

1. This (SW)CNT differ significantly from other CNTs.
2. The devil is in the detail.
3. Substance properties can be a challenge.



TUBALL single wall carbon nanotubes are flexible due of its intrinsic morphology.

Investigation of ecotoxicological effects of fibrous and platelet-shaped advanced materials for deriving adapted testing strategies - the project FaPlaN

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Advanced materials are a very heterogeneous group of materials and used in many applications. Responsible use of these materials also includes the identification of potential threats to people and the environment as quickly and as precisely as possible. Hence it is unclear to date, whether OECD test methods in the field of ecotoxicology (already established and adapted for testing nanomaterials) may also be applicable for this class of materials.

Due to their special properties, fibrous and platelet-shaped materials represent advanced materials for which a reliable assessment of a potential environmental hazard based on the available test methods is challenging. The project presented here therefore aims to obtain information on the mechanisms of action (MoA) and thus a mechanistic understanding of potential toxic effects exerted by fibrous and platelet-shaped advanced materials. Based on this, methods will be adapted which will allow to identify related effects. By this, ecotoxicological assessment will be facilitated in the long term.

This poster will present initial results from a literature review on the effects of fibrous and platelet-shaped advanced materials in aquatic organisms, with a focus on identifying mechanisms of action. The aim of this poster is to exchange experiences with other toxicologists to learn more about possible mechanisms of action and to take these into account when adapting the testing strategies as the project progresses.

Key question 1	Which physical-chemical material properties must be taken into account?
Key question 2	Which mechanisms of action are relevant for fibrous and plate-shaped advanced materials?
Key question 3	Do testing strategies need to be adapted for fibrous and plate-shaped advanced materials?

Funding: The project FaPlaN is financed by the German Federal Ministry for the Environment, Nature Conversation, Nuclear Safety and Consumer Protection, Refo-Plan, FKZ: 3723 66 401 0.

Preparation of composite sorbents based on clay and magnetite

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The main part of research in the field of obtaining sorbents of organic pollutants and petroleum is devoted to the dispersion of natural sorbents and the determination of their sorption activity. The efficiency of using these sorbents to separate oil from water can be increased by giving them magnetic properties. Therefore, the aim of the study was to obtain magnetic composites of various clays.

By the Elmore method, magnetite particles were synthesized in the presence of bentonite, flask and vermiculite clays and clay–magnetite composites were obtained. By IR spectroscopy was shown that during the transition from clay minerals to clay-magnetite composites at an oscillation frequency of 1405 cm-1, a visual peak is formed related to deformation vibrations of the Fe–O bond. It shows that the FeO group has entered the clay structure. And the deceleration and displacement of deformation vibrations of Si-O–Si bonds in the range of 1039-1100 cm–1, small peaks of Si-O and Al-O bonds in 698 cm-1 and 630 cm–1, characteristic of silicates, indicate the interaction of silicate ions with magnetite.

The penetration of magnetite particles into the structure of bentonite, flask and vermiculite by X-ray phase analysis is proved by the appearance of its characteristic peaks on diffractograms of composites. In clays, the main peaks characteristic of silicates are observed at angle values of 2θ 19.8; 26.57 and 35.18 °, in magnetic composites, new peaks appear at angle values of 2θ 30.09; 35.47 and 74.22 °.

The dynamic scattering method revealed a decrease in the size of bentonite as a result of the formation of a clay-magnetite composite, as well as the growth of flask and vermiculite particles. These changes indicate that the processes of ion exchange, exfoliation of clay minerals and hetero coagulation of small particles of magnetite and dispersed clay layers occur during the formation of composites.

The adsorption capacity of magnetic composites was evaluated by the adsorption of methylene blue dye, and the adsorption data were processed within the framework of Langmuir and Freundlich models. Comparison of composites by A_∞ value showed that the sorption capacity of bentonite–magnetite composite is significantly higher than that of other composites.

This research is funded by the Science Committee of the Ministry of Science and Higher Education of the Republic of Kazakhstan (Grant AP19678156).

Neurotoxicity of metals and metal nanoparticles in cholinergic SH-SY5Y cells

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Metal nanoparticles (NP), such as silver based NP, aluminum oxide (Al_2O_3), titanium dioxide (TiO_2) or manganese oxide (MnO_2), have a wide range of applications and are used in everyday commodities like cosmetics or clothing. Different physical and chemical properties modify their biological effects [1]. Metal NP can easily pass the blood-brain-barrier or enter the brain via the olfactory route and cause neurotoxicity (reviewed by [2]). However, the mechanisms causing neurotoxicity as well as the role of their physicochemical properties are not fully unravelled, yet. To understand this mystery neuronal cell models are a good alternative to animal testing. Therefore, in a first, step we investigated the effects of TiO_2, $AlCl_3$ and $MnCl_2$ on the neuronal cell model of SH-SY5Y human neuroblastoma cells. These cells represent cholinergic neurons after differentiation with retinoic acid. $AlCl_3$ and $MnCl_2$ were chosen to first investigate the effect of the metal ions of the corresponding NPs. Both cell types were incubated with different concentrations of these compounds and the effects on cell viability and different neuron specific parameters like neurite area, neurite branching and the ability to respond to specific neurotransmitters were analysed over time. Whereas TiO_2 had no effect on either parameter, we found a significant increase of neurite area and neurite branching after 3 and 6h of $AlCl_3$ incubation with the highest concentrations of 5 and 10 mM but not after 24h. An acute exposure with 1 mM $AlCl_3$ led to a decreased response amplitude to acetylcholine (ACh) stimuli. A 24h incubation with $MnCl_2$ decreased cell viability at 0.5 mM and higher, concomitant with decreased neurite area and branching. The response amplitude to ACh was already decreased at 10 µM of $MnCl_2$.

1. The response behavior to neurotransmitter stimuli is a sensitive endpoint for metal neurotoxicity measures.
2. SH-SY5Y cells are a good cell model for human cholinergic neurons.
3. Different cell specific endpoints should be considered in risk assessment.

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Reliable risk communication on advanced materials safety - The DaNa4.0 *Knowledge Base Materials*

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Worldwide, research on the safety and risks of advanced materials such as nanomaterials has been ongoing for more than 20 years. In times of social transformations, science has a special responsibility to provide evidence-based answers and solutions to the pressing issues of our time, such as climate change or digitalization. Today, the responsibilities of science also include communication, dialog with society, objectification of current debates, and education about the challenges and opportunities of new scientific developments.

In 2009, the online knowledge base on nanomaterials www.nanoobjects.info was initiated within the framework of the BMBF-funded project DaNa. Thus, scientific results on the safety of nanomaterials were communicated to the public in a value-neutral way at an early stage. In 2020, this information platform was expanded as part of the DaNa4.0 project to include advanced materials in order to make an understanding and awareness of safety-related data on these materials available to the public as early as possible. This so-called *Knowledge Base Materials* is providing safety-relevant information on 30 advanced materials, including nanomaterials. The project focuses on the effects on human health and the environment and, since 2023, on the sustainability of innovative materials. A continuously updated list of standard operating procedures (SOPs) and laboratory protocols of different categories is available for download. A template for creating SOPs has been developed and can be downloaded too. A monthly spotlight research article on a recent scientific publication as well as numerous cross-cutting articles on topics such as advanced materials for environmental remediation or materials for 3D printing complement this knowledge base. In addition, social media channels (*X*, LinkedIn) are used in order to achieve the widest possible reach for the dissemination of information.

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Redox-Responsive Porous Materials: Their Preparation, Switchability and Sustainable Recycling

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Metallopolymers are an exciting class of functional polymers based on their stimuli-responsive properties. Especially ferrocene-based polymers are outstanding candidates because of their fast and fully reversible switching capabilities between hydrophobic ferrocene and hydrophilic ferrocenium by redox chemistry or the application of an electrical current. This enables a manifold of new applications e.g., in batteries, catalysis, or ion sorbents. [1-3] The covalent attachment of these polymers on surfaces offers high stability and precise adjustment of the resulting properties. [4] Because of this, we establish the surface-initiated living anionic polymerization as a catalyzed free immobilization strategy for methacrylate-based polymers on highly porous organic microparticles. [5]

Poly(ferrocenylmethyl methacrylate) functionalized particles were investigated in terms of their switching behavior wet-chemically and electrochemically. The accessibility of all ferrocene units in the porous system in combination with the high stability of 1000 cycles of oxidation and reduction with no loss in capacities paves the way for long-term applications. Moreover, a second life-cycle of the particles can be achieved by ceramization due to their iron-based functionalization. The morphology and size of the ceramic particles are well adjustable depending e.g. on the polymer degree of the precursors. In addition, the composition can be set regarding the iron oxide species, the iron, and carbon content leading to the possibility of a broad range of applications in batteries or catalyzes of the recycling materials. Throughout the particles' life cycles, a remarkable sustainability of the particles was pursued, while simultaneously the iron-based materials at the end are harmless to the environment.

1. Immobilization strategies of redox-responsive polymers
2. Switchability of ferrocene-polymer functionalization
3. Ceramization as sustainable recycling strategy

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Impact of mucus modulation by N-acetylcysteine on nanoparticle toxicity

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Respiratory mucus is a biological hydrogel that covers the underlying epithelium, offering considerable protection not only against environmental particles, but also drug delivery systems [1]. Modulation of the mucus layer has been applied as a strategy to enhance transmucosal drug carrier transport. However, a successful modulation protocol should not permanently impair mucus barrier properties, in particular in situations with an increased exposure to particles [2].

We investigated the impact of mucus modulation on its protective role. We used pulmonary mucus produced by Calu-3 cells, cultivated at the air-liquid interface for 21 days. Confocal imaging revealed that Calu-3 cells secrete a mucus layer with a thickness of 24 ± 6 µm after differentiating for 21 days. Mucus confined the penetration of 500 nm carboxyl-modified polystyrene particles only to the upper layers (5-10 µm). Moreover, we established a mucus modulation protocol using aerosolized N-acetylcysteine (NAC), which enhanced the penetration of these particles to deeper mucus layers (20-25 µm). These findings were supported by cytotoxicity data, indicating that intact mucus protects the underlying epithelium from particle-induced effects on membrane integrity. Using 50 and 100 nm amine-modified and 50 nm carboxyl-modified polystyrene nanoparticles, we could probe the impact of mucus modulation by NAC on the protective properties of mucus. Cytotoxicity was only induced by the amine-modified nanoparticles, implying the reduced protective function of modulated mucus.

Overall, our results suggest that evaluation of the impact of mucus modulation on the protective role of the mucus barrier is imperative for developing therapeutical protocols to improve the penetration of drug delivery systems through mucus.

1. Human respiratory mucus is a viscous hydrogel that forms a protective barrier for the underlying epithelium.
2. Modulation of the mucus layer can potentially reduce the protective barrier properties and increase environmental/occupational exposure of respiratory epithelium.
3. Assessing the protective function of mucus upon modulation is essential for the development of therapy approaches that aim to enhance the penetration of drug delivery systems.

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Inhibition of monamino oxidase by benzofurane Derivatives

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Parkinson's disease is a condition where a part of your brain deteriorates, causing more severe symptoms over time. While this condition is best known for how it affects muscle control, balance and movement, it can also cause a wide range of other effects on your senses, thinking ability, mental health and more [1]. Monoamine oxidase B (MAO B) is an enzyme in the body that breaks down several chemicals in the brain, including dopamine. An MAO B inhibitor makes more dopamine available to the brain. This can modestly improve many PD movement symptoms [2 ,3]. A series of benzofuran derivatives were synthesised and evaluated as inhibitors of MAO B, In general, the derivatives were found to be selective MAO B inhibitors with IC50 values [4] In our work, the interaction between bioactive structures will be studied by molecular modeling methods (MM, Docking (Molecul ar Operating Environment (MOE)[5]). We conclude that these benzofuran derivatives are promising reversible MAO B inhibitors with a possible role in the treatment of neurodegenerative diseases such as Parkinson's disease (PD).

Keywords:

Parkinson's disease (PD), Monoamine oxidase (MAO), benzofurane derivatives, molecular modeling

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Preparation of physiologically active bionanocomposites based on Kazakhstan montmorillonite

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Currently, the creation of bionanocomposites, i.e. new generation hydrogel carriers for prolonged release of biologically active substances immobilised in them, remains an urgent task for research in chemistry, medicine and pharmacology worldwide.

New promising areas of bentonites use include the synthesis of bionanocomposites used in the production of composite materials of new technology, polymeric forms of prolonged-acting drugs, long-lasting bactericidal agents, various cosmetics, biodegradable and edible forms of food packaging, liquid gloves, etc. [1-3]. Silver and other drug compounds are proposed to create bactericidal forms of bionanocomposites based on natural polymers and montmorillonite [4].

Existing silver-based preparations such as collargol, protargol, lapis, etc. have long been known and successfully used in medicine for decades. Unfortunately, there is a belief that silver-based preparations are quite expensive. In fact, the price of one therapeutic or prophylactic dose of silver in these preparations does not exceed or is even less than the cost of a similar dose of modern antibiotics. Therefore, now instead of using antibiotics the advantage of antiseptic preparations is increasing. The proposed bionanocomposites can be used for application to damaged and intact skin, mucous membranes, cavities and wounds in order to treat and prevent the development of local infectious lesions and sepsis [5]. The aim of this study is to synthesise bionanocomposites based on Kazakhstan montmorillonite, silver ions, sodium salt of alginic acid and to study their physicochemical properties.

The results of these studies allowed us to establish the optimal mode of formation of bionanocomposites and to determine the kinetics of hydrogel swelling and the kinetics of release of colloidal silver ions from hydrogels into saline solution. From the results of the analysis, it was found that as the pH of the saline solution and the colloidal silver content in the hydrogel increased, the silver yield increased. The release kinetics was analysed for 20 days, which proves the prolonged release of silver ions. Due to the prolonged release of active substances, hydrogels can be used as antibacterial and healing dressings and patches. The content of montmorillonite with silver in the hydrogel allows to absorb secreted blood and heal wounds at the same time.

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