Centre for advanced materials application v.v.i.

CEMEA

Questionnaire
Summary of the main activities of a research institute of the Slovak Academy of Sciences

In Bratislava 30.6.2022

Doc. Ing. Miroslav Hnatko, PhD.

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Period: January 1, 2016 - December 31, 2021

1. Basic information on the institute:

1.1. Legal name and address

Centre for advanced materials application v.v.i., (CEMEA),
Slovak Academy of Sciences,
Dúbravská cesta 5807/9,
845 11 Bratislava,
Slovakia

1.2. URL of the institute web site

http://www.cemea.sav.sk/

1.3. Executive body of the institute and its composition

Directoriat	Name	Age	Years in the position, from - to
Director	Doc. Ing. Miroslav Hnatko, PhD.	48	2022 -
Director	RNDr. Eva Majková, DrSc.	72	2017 - 2021
Deputy director	Ing. Karol Fröhlich, DrSc.	68	2017 -
Scientific secretary	Mgr. Peter Boháč, PhD.	34	2022 -

Add more rows for any changes during the evaluation period

1.4. Head of the Scientific Board

Dr. rer. nat. Peter Šiffalovič, DrSc. 2021-
Ing. Karol Fröhlich, DrSc. 2017 - 2021

1.4.1 Composition of the International Advisory Board

1.5. Basic information on the research personnel

1.5.1. Fulltime equivalent work capacity of all employees (FTE all), FTE of employees with university degrees engaged in research projects (FTE researchers)

2016		2017		2018		2019		2020		2021		2016-2021	
FTE all	FTE researchers	FTE all	FTE researchers	FTE all	FTE researchers	FTE all	FTE researchers	FTE all	FTE researchers	FTE all	FTE researchers	average FTE all per year	average FTE researchers per year
0,00	0,00	3,20	0,00	6,55	0,00	10,35	7,64	25,33	18,87	32,77	26,83	**13,03**	**8,89**

1.5.2. If applicable, add also a short information on the merger of the institute in the evaluation period. You can also add rows in the above table corresponding to the founding institutes

1.6. Basic information on the funding of the institute

1.6.1. Institutional salary budget, other salary budget[1], non-salary budget[2]

Salary budget	2016	2017	2018	2019	2020	2021	average
Institutional salary budget *[millions of EUR]*	x	0,02	0,14	0,05	0,08	0,17	**0,091**
Other salary budget *[millions of EUR]*	x	0,00	0,02	0,29	0,76	0,95	**0,404**
Total salary budget *[millions of EUR]*	0,000	0,020	0,158	0,340	0,841	1,115	**0,412**
Non-salary budget *[millions of EUR]*	x	0,01	0,03	0,08	0,21	0,47	**0,158**

1.7. Mission Statement of the Institute as presented in the Foundation Charter indicating the years when it was adopted and revised

The main activity of the organization is the implementation of research in the following disciplines of sciences and technology: Condensed Matter Physics and Acoustics (010304), Quantum Electronics and Optics (010309), Inorganic Chemistry (010402), Electrotechnology and materials (020205), Microelectronics (020211), Preparation and processing of metallic and non-metallic materials (020409), Physical engineering (020404), Nanomaterials (021101), Nanoprocesses (021102), Nanoelectronics (021103), Nanotechnologies and molecular electrical engineering (021104), other related fields nanotechnology (021199), Layers and films (020602), Composites (020603), Ceramics and Glass (020601), Macromolecular Chemistry (010409), Biochemistry (010403), Organic chemistry (010410), Materials chemistry (010407), Macromolecular technology substances (020506), Recycling technologies (020507), Biomaterials (021005), Bioplastics (021006), New biomaterials (021009), Molecular biology (010613), Cellular biology (010602), Oncology (010618), Genetics (010608), Virology (010621), and Microbiology (010612).

The activities of the organization are:

- Conducting research,
- provision and management of research and development infrastructure,

[1] Salary budget originating outside the regular budgetary resources of the organization, e.g. from the project funding.
[2] Includes Goods and Services and PhD fellowships

- obtaining, processing, and disseminating information in the field of science and technology and knowledge from our research and development,
- cooperation in the field of science and technology with universities, other legal entities conducting research and development, and entrepreneurs.

1.8. Summary of R&D activity pursued by the institute during the evaluation period in both national and international contexts. Describe the scientific importance and societal impact of each important result/discovery. Explain on general level – the information should be understandable for a non-specialist (recommended 5 pages, max. 10 pages for larger institutes with more than 50 FTE researchers as per Table 1.5.1.)

Establishment of the Centre for advanced materials application SAS (CEMEA) was initiated by the project Building-up Centre of Excellence for advanced materials application, CEMEA No. 664337 within the call of H2020 programme WIDESPREAD-1-2014-Teaming, which was awarded by the Seal of excellence and recommended for national funding. For these reasons, the Centre was established on the basis of a resolution of the SAS Presidium on 1.6.2017. Two years after the establishment of the Center (01.07.2019), an NFP contract was signed and the project began to be fully financed. The new project is complementary to the project of the call H2020 WIDESPREAD-1-2014-Teaming – Building-up Centre of Excellence for advanced materials application CEMEA. From this date, CEMEA SAS began operating as a standard institute of the Slovak Academy of Sciences.

The core activities of the project CEMEA are focused on the research in the field of materials science and new technologies aimed at modifying surfaces and interfaces in the domain of advanced nanomaterials, sustainable energy and biomedicine. In addition to the applicant SAS, seven research institutions (ElU SAS, FU SAS, UPo SAS, UMMS SAS, UACH SAS, BMC SAS and CEMEA SAS) support the project. The research subactivities include:

1. Thin films and surface properties
2. Functional polymer surfaces
3. Special light structural materials and composites
4. Advanced ceramic materials
5. Inorganic and organic nanostructures for electronics and sensorics
6. Advanced materials for biomedicine and biotechnologies

Thin films and surface properties

The CEMEA research and development plan was concentrated on surfaces and interface modifications of advanced materials. Activity 1.1 of the CEMEA research plan was focused on thin films and surface properties.

Part of our research is devoted to studying nanomagnetism, particularly the spin-wave dynamics at the nanoscale for information processing applications. Spin waves are elementary excitations in magnetically ordered systems, and magnon is their quasiparticle. Research in magnonics is focused on implementing spin waves into novel computing devices. The spin-wave is considered as a candidate for an information carrier in future ultrafast and energy-efficient devices due to its unique properties such as low heat dissipation, short wavelengths, possible manipulation at the nanoscale, reconfigurability, and operating frequency range from GHz to THz. An important example of promising nanoscale and reconfigurability properties of magnonic systems are noncolinear magnetic spin structures.

Another part of our investigations dealt with the application of thin-film structures in energetics. Thin-film structures were employed for water splitting under sun radiation and for battery application. Water splitting using sun radiation is a promising method for nature-friendly energy harvesting of sun radiation. Special attention was given to employing the atomic layer deposition (ALD) method to fabricate the studied structures.

Finally, nanotribological properties of 2D materials were pursued in this activity. Miniaturization of moving components in micro-electromechanical systems also requires reducing energy and material losses caused by friction and wear. The most promising solid lubricants for these applications are 2D materials such as graphene and transition metal dichalcogenides. These materials exhibit outstanding friction effects such as superlubricity, stick-slip, puckering, friction hysteresis, or directional anisotropy. We studied the friction properties of various 2D materials prepared by commonly used technologies, including chemical vapor deposition and thermally assisted conversion.

It is important to note that while spin-wave dynamics required deep theoretical knowledge of physics and magnetism, activities focused on water splitting and nanotribology of 2D materials requested an interdisciplinary approach based on cooperation between electrochemistry, material science, physics as well as mechanical engineering. Such synergy of the expertise has been made possible only thanks to the putting together CEMEA institute. Further, these new topics are complementary to those pursued by the founding institutions and extend the ability of SAS research teams to conduct inter- and multidisciplinary research.

Functional polymer surfaces

This subactivity research can be divided into two directions:

· surface modification of carbon or inorganic surfaces in order to introduce new surface properties for various applications

· preparation of polymeric materials with functional groups at the surface for biomedical applications.

Within the first direction, controlled radical polymerizations, such as atom transfer radical polymerization (ATRP) for surfaces modifications. Thus, graphene oxide (GO) was in situ reduced and at the same time the polymer was grafted from the surface during the ATRP of various monomers. Careful study of various influencing factors allowed control over the degree of GO reduction and thickness of the polymeric layer at the surface, while the dispersity in liquids as well as polymers was achieved. The prepared GO-based hybrids were successfully used in electro-rheological suspensions or polymer composites with photoactuating properties. Similarly, more ecological variation of ATRP using light for regeneration of ppm amount of catalyst was recently developed at the Polymer Institute of SAS and at CEMEA SAS, and its application on the wafer surface modification was investigated. Renewable monomer alpha-methylene-gamma-butyrolactone (MBL) was grafted from the wafer surface, while the conditions were optimized in order to control the polymer thickness over time. The grafted polymer contains pendant lactone rings which can be further post-functionalized. This approach can be applied to various inorganic (nano)particles with the aim of drug delivery or drug release targeting.

Within the second direction, the research is focused on the synthesis and application of poly(2-oxazoline)s, which are also called pseudopeptides due to their similar structure to peptides as well as their low nonspecific adhesion of proteins and cells. The activities were focused on the synthesis of gradient copolymers for the preparation of micelles as drug delivery systems. In addition, these polymers were used for modification of other polymeric surfaces in order to suppress the biofouling of the surfaces. Adhesion of fibroblasts was dramatically decreased by increasing the concentration of the poly(2-oxazoline) bonded at the surfaces.

Special light structural materials and composites

Our research has been oriented dominantly to novel structural bulk materials fabricated by the powder metallurgy (PM) approach, which form by the utilization of powders with a modified surface for various application fields. In the period of the last five years, the following main research activities have been pursued:

We described the stabilization mechanisms induced by nano in-situ Al_2O_3 dispersoids, which stem from amorphous films on atomized Al powder, into ultrafine-grained (UFG) Al matrix, the so-called HITEMAL® material family. We determined the limits of stabilization by Al_2O_3 in terms of imposed strain and thermal treatment. An effective stabilization by Zenner pinning mechanism by a small portion of nano Al_2O_3 dispersoids stabilized microstructure and hence the properties of UFG HITEMAL®, which can be then applied as an efficient heat and creep resistant, lightweight material with a high strength during a service at elevated temperatures not normally associated with the use of conventional Al alloys and metal matrix composites (MMC).

We applied a novel technique of small punch testing (SPT) to pursue the mechanical properties of HITEMAL® in a broad temperature range, including the creep characteristics. SPT technique allows, in a non-destructive way, a withdrawal of the samples from the metallic parts under service and testing of small samples in multiple directions, which is often a case of lab-scale fabricated materials. A mutual correlation of the properties derived from the tensile tests and SPT was established.

In-situ aluminum Al^+AlN MMC was manufactured by a PM cost-effective approach realized at a large industrial scale. In this approach, commercially available Al, Mg, and Sn powders were processed by readily available PM techniques of blending, CIP, gaseous nitridation, and direct extrusion to produce Al^+AlN MMC extruded bars. The stable and fine AlN dispersoids effectively stabilized the Al grain structure by Zener pinning action. In strict contrast to conventional Al alloys and MMC, this led to superior thermal stability, and no major changes to the tensile mechanical properties of the as-extruded Al^+AlN MMC were observed after severe annealing up to 500°C. At the same time, Al^+AlN MMC showed superior mechanical tensile properties at elevated temperatures, enhanced Young`s modulus, reduced thermal expansion, and reasonable thermal conductivity in addition to non-abrasive character. This predetermines the studied Al^+AlN fabricated at the upscaled level for lightweight structural parts, which operate at elevated temperatures not associated with the use of conventional Al alloys and MMC, and are subjected to intense mechanical loading.

We prepared, studied, and optimized the structure of porous Al anodes by the PM approach of partial sintering compaction of Al powders for the purpose of increasing the performance of the primary Al-air concept batteries. Metal-air batteries are considered candidates for a new generation of energy storage systems that have the potential to replace or replenish daily used lithium-ion batteries. Al-air battery seems to be a suitable candidate owing to their low cost, availability, and recyclability of Al.

We conducted fundamental research on the microstructure of an isothermal cut in the phase diagram of a unique Al-Pd-Co alloy with a scientific focus paid to the quasicrystal approximant and crystallization behavior description of the amorphous Al-Ni-Co-Gd alloys.

Advanced ceramic materials

In the field of "preparation of metallurgical materials from ALD-treated powders," we focus on the preparation and characterization of reference samples by using surface treatment of starting powders by ALD. Dense SiC-based composites with sintering additives in the form of Y_2O_3 and Sc_2O_3 and the addition of graphene nanoplates (GNP) or graphene oxide (GO) have been successfully prepared. The obtained results prove that the use of methods of freeze granulation, rapid hot press sintering, and annealing of samples in a nitrogen atmosphere makes it possible to obtain SiC-graphene composite materials with high electrical and thermal conductivity. In the second stage, the effort will be to apply sintering additives using ALD and compare the properties of the materials thus prepared with reference samples.

A series of reference samples of SiC with a minimum content of sintering additives was prepared within the research activity entitled "Obtaining a systematic set of data on the corrosion properties of ceramic materials in fluoride melts." It is a promising ceramic material with expected high corrosion resistance in molten fluoride salts. In the past period, basic corrosion tests were performed, and subsequently, the corroded surfaces were characterized in terms of chemical and phase composition of corrosion products, the thickness of the corroded layer, and the like. Significant progress has also been made in researching the properties of new types of melt systems (based on Rb_3AlF_6, cryolite, and others).

Within the focus entitled "Process of preparation of inorganic-organic bioactive composite based on silicon nitride," we succeeded in mastering the preparation of trabecular bodies from silicon nitride. The aim was to develop a technology for preparing a porous, bioactive, antibacterial skeleton with sufficient strength, which could be used in the preparation of bone replacements of various shapes and sizes in a simple and fast way.

We consider it a new direction to investigate the possibility of using electrochemical polishing of Ti-based alloys using an environmentally friendly solvent - ethalin. It has been shown that electropolishing in ethanol has ensured the removal of surface defects, thus ensuring the smoothing of the surface and the reduction of its roughness. The analysis revealed that electrochemical polishing of the titanium alloy in ethanol provided the formation of specific patterns at the nanometer level with the shape of elongated hemispheres. Correlations between surface roughness coefficients and wettability parameters were determined and discussed. Adjusting the processing time and electrode potential of the electropolishing allows the surface roughness and wettability of the titanium-containing alloy to be controlled in a controllable and flexible manner.

Within bioactive materials, the process of compaction of bioactive material (Bioglass®45S5) in the form of powder (~98%) was successfully managed at room temperature. A mixture of Bioglass®45S5 with water or NaOH solution was tested. An isostatic pressure (400 MPa) was applied to such a mixture for 10 minutes. Due to hydrostatic conditions, a secondary phase formed around the undissolved bioglass particles. Chemical and phase analysis showed the formation of a C-S-H phase, with Raman and 29Si NMR spectroscopy showing that the sample treated in the water had higher silica connectivity compared to the sample where NaOH solution was used. The choice of solvent is crucial for dissolving the cations and anions of the bioglass.

Inorganic and organic nanostructures for electronics and sensorics

In the evaluated period, we focused our research on two types of materials for the fabrication of thin films for optoelectronic applications:

Organic semiconductors based on small molecules and conjugated polymers

Organic semiconductors may play an essential role in the next generation of optoelectronic devices such as flexible displays or sensors. In our research, we addressed a fundamental understanding of growth processes using a combination of different analytical techniques. The predominant method was in-situ time-resolved grazing-incidence wide- and small-angle X-ray scattering (GIWAXS/GISAXS), which allowed us to elucidate the fundamental growth modes of small semiconducting organic molecules. The most important result of our studies was the investigation of the role of low-dimensional substrates in the growth of organic molecules. As model systems, we studied the growth of pentacene (PEN) and diindenoperylene (DIP) molecules. The low-dimensional substrates used in our studies were graphene and MoS_2. By using GIWAXS in real-time, we have investigated the very early stages of growth and found that low-dimensional substrates tend to change the orientation of the crystallographic c-axis of PEN and DIP thin films from upright to lying in the substrate plane. In addition, we were able to track the subtle changes in the lattice parameters during the growth of the thin films, which were released after the formation of the thick films. This has important consequences for device fabrication, as the orientation of the c-axis affects optical absorption and electrical conductivity. In practice, this means that the growth of standing-up molecules is essential for in-plane electrical conductivity in thin-film transistors. In contrast, the lying configuration favors enhanced optical absorption in organic solar cells.

The second topic we studied in thin films of organic semiconductors was structural defects that affect the electronic structure and cause gap states that are detrimental to optoelectronic devices. We developed a new technique, energy-resolved electrochemical impedance spectroscopy (ER-EIS), which allows us to map the density of defect states in the bandgap of organic semiconductors. In our studies, we have been able to link the increased densities of gap states to structural properties. This has significant implications for the fabrication of thin organic films, as it allows us to determine the critical growth parameters responsible for generating defect states.

Another important class of our investigations was devoted to spatially-resolved studies of defect distribution in thin films of organic semiconductors. Using a powerful combination of s-SNOM with broadband illumination and FTIR-based detection, we analyzed the molecular orientation in thin films with a resolution of 20 nm. The main result was the local identification of structural defects related to the different molecular orientations, which may affect the functionality of organic thin film-based devices.

Hybrid organic-inorganic perovskite materials

Hybrid organic-inorganic perovskites attracted worldwide interest about ten years ago as a new cost-effective semiconductor material for the production of solar cells. Its main advantages include a tunable band gap and low activation energy compared to conventional semiconductors such as silicon. In our investigations, we concentrated on the formation kinetics with special emphasis on defect formation. It is well known that the defects are the main contributing factor responsible for the non-radiative recombination of excitons, which is detrimental to high-performance solar cell materials. To address this challenge, we designed and built a dedicated lab-scale device for simultaneous GIWAXS/GISAXS combined with photoluminescence. As a model system, we used methylammonium lead triiodide ($MAPbI_3$). Employing this approach, we were able to follow the nucleation and growth of perovskite crystals during the annealing of spin-coated films. The main result is a non-trivial dependence of the photoluminescence signal as a function of the total $MAPbI_3$ crystal volume. In particular, the photoluminescence signal was growing towards the coalescence phase as expected. However, at the beginning of the coalescence phase, the growth of perovskite grain boundaries led to a significant decrease in photoluminescence, which was attributed to the non-radiative recombination of defect states at the grain boundaries.

Moreover, a similar evolution was observed for the vacuum evaporated perovskite layers. This fact points to a more general conclusion that identifies grain boundaries as the main channel for non-radiative recombination in perovskite thin films. The direct consequence is that the developed monitoring technique allows to identify the right additives (molecules) to passivate the perovskite grain boundaries. In addition, our group has been active in the interfacial engineering of perovskite solar cells. We have incorporated a series of low-dimensional nanomaterials such as carbon nanodots and MXenes at the interfaces and bulk and observed positive effects on the energy conversion efficiency of perovskite solar cells.

Advanced materials for biomedicine and biotechnologies

We focused on two main areas:

- Novel materials for implantology – research and development of new progressive metal, ceramic, and polymer materials, health aids, and equipment for implantology.
- Nanomaterials in oncological diseases – research of mechanisms, innovative diagnostic and therapeutic procedures using advanced nanomaterials in biomedicine; study of nanocarriers for more effective treatment with conventional therapeutic agents whilst reducing adverse side effects; development of innovative targeted anti-tumor therapy combining a biological approach with advanced nanomaterials.

Novel materials for implantology

Among the R&D activities related to biomedical metallic materials, an emphasis was put on partially or fully biodegradable metals and MMC, while the main focus was oriented on the following studies:

Although dental implants (DI) from Ti and Ti alloys have been used with a high degree of success, their main shortcomings: i) so-called stress-shielding effect, i.e., a mechanical incompatibility with bone, and (ii) their insufficient surface bioactivity still remain insufficiently solved. Our innovative biomedical $Ti^{+}Mg$ MMC fabricated by PM is a partially biodegradable permanent material that minimizes the main disadvantages of conventional Ti materials for DI, while retaining sufficient mechanical properties and fatigue resistance. Two methods of DI surface stabilization by prewashing and mechanical surface treatment against a swift Mg corrosion, which is detrimental to cell adhesion and growth, acceptance of DI by patient and healing process, were proposed and studied with the help of corrosion studies and in-vitro biological response assays of the selected cell cultures. The achieved results are important from the point of view of promising production of $Ti^{+}Mg$ DI as well as fully biodegradable Mg implants.

Specific Mg-based alloys are promising materials for the application of fully biodegradable medical devices, namely orthopaedic internal fixators (screws, wires, plates). Though a high corrosion rate of Mg alloys, which is difficult to control, often results in toxic effects and necroses of surrounding tissue, which limits their applicability eventually. We have focused our attention towards the effect of the microstructural features of Mg materials fabricated by PM on their corrosion behavior.

In the last decade, current Zn-based materials have shown great potential as a suitable candidate for bioabsorbable implants, specifically endovascular stents, and internal orthopedic fixators. Zn materials have many advantageous properties over other bioabsorbable metallic (Mg and Fe) and polymeric (PGA / PLA) materials. Nevertheless, there are some unresolved problems of current Zn-based materials that limit their application potential. One of the most critical are: i) insufficient moss. Properties that do not meet the limits set for bioabsorbable implants; and (ii) post-deformation microstructural instability and subsequent moss instability. Properties at human body temperature. In our research, we focused on the development of a new group of Zn-based MMC with properties adapted for implantology, which address the shortcomings of contemporary Zn-based solutions. The excellent mechanical properties of Zn-based MMC, produced by the cold compaction PM approach, are due to the specific UFG structure of Zn stabilized by the low proportion of nanometric ZnO dispersoids. ZnO dispersoids stabilize the grain boundaries (GB) of UFG Zn structures by means of a Zener stabilization mechanism during plastic deformation and the post-deformation stage, which ensures an efficient and stable GB-mediated consolidation mechanism. In addition, dispersoids suppress the negative effect of GB slippage and rotation, key mechanisms of creep plastic deformation and fatigue in UFG metals. In addition, ZnO provides antibacterial properties, osteointegration potential and improves Zn-based MMC corrosion behavior. As part of the ongoing research, the PM production route has been optimized so far, a comprehensive microstructural characterization has been carried out, and we have performed detailed testing of mechanical properties, corrosion behavior, and in-vitro biological evaluation of $Zn^{+}ZnO$ MMC.

Nanomaterials in oncological diseases

Bioconjugated nanomaterials, especially low-dimensional nanomaterials, are promising agents for various bioapplications, such as drug delivery, therapy, and imaging. Selectivity of these processes is essential to avoid systemic toxicity and the survival of healthy cells. In our previous projects, we showed that 2D nanomaterials could be successfully linked with monoclonal antibodies to function as selective cancer-therapeutic nanoplatforms. We employed the biotin-avidin-biotin bridge, being the strongest known non-covalent interaction between a protein and ligand. Avidin is a quadrivalent molecule that can bridge up to four biotins. In our case, we use it to link two biotinylated compounds, a biotinylated antibody that clicks through avidin, to a biotinylated polyethylene glycol (PEG) linker attached to the nanoparticle. Antibodies M75 and antiCD33 were employed, serving as the nanoplatforms anchoring agents to cancer cells, expressing specific antigens to which the antibodies selectively bind. M75 is specific to the carbonic anhydrase IX (CA IX) antigen, which is expressed on tumor cells membrane during hypoxic conditions, a key feature of a tumor microenvironment. The protein antiCD33 is specific to CD33 receptors expressed by SKM-1 acute myeloid leukemia cells. We investigated the binding of graphene oxide (GO) conjugated with M75 antibody to Madin-Darby Canine Kidney (MDCK) cells. Higher intake was observed for GO-M75 towards MDCK cells ectopically expressing CA IX protein on their surface compared to control MDCK. The internalization rates of MoS_2 nanoflakes conjugated with M75 were observed in JIMT-1 breast carcinoma cell line and MRC5 fibroblasts. Employing the concept of antigen–antibody binding, we increased the probability of the endocytosis of MoS_2 nanosheets into CA IX expressing JIMT-1 cells by 30%. In our work on targeting acute myeloid leukemia cells by CD33 receptor-specific MoS_2-based nanoconjugates, we demonstrated that the (anti-CD33)-MoS_2 conjugates were present on the cell surface and within SKM-1 cells, presumably having been internalized via CD33-mediated endocytosis, while being highly specific to this receptor as showed a further comparison of cellular uptake with (anti-GPC3)-MoS_2 conjugates. These results regarding the selective targeting of cancer by nanoscale materials indicate the importance of appropriate functionalization of the nanomaterials by tumor-recognizing elements that significantly increase their specificity.

We apply original and modern strategies in the diagnostics of interactions between nanoparticles and biomolecules. These approaches allow in-situ monitoring of the nanoparticles biofunctionalization process and characterization of the biophysical properties of cells. In vitro label-free confocal Raman microscopy (CRM) of live cells enables the detection of bioconjugated nanoparticles in the intracellular space in real-time at a submicrometric resolution, as well as to differentiate individual cell compartments. The label-free character presents an advantage. Conventional fluorescent labels could be invasive and induce cell cytotoxicity, while photobleaching can cause the decomposition of fluorescent molecules, leading to a reduction in the fluorescent signal and the formation of free radicals and other highly reactive and toxic substances. We employed label-free CRM for the localization of nanoconjugates within cancer and healthy cells. MoS_2 and GO nanoflakes conjugated with monoclonal antibodies internalize preferentially within cancer cells in lysosome-rich cellular regions.

Moreover, we used the label-free live cell Raman imaging to assess the HaCaT human keratinocyte cell line morphological changes induced by essential oils encapsulated in poly(ε-caprolactone) nanocapsules. We showed the existence of lipoprotein aggregates inside the cells, in accord with concentration-dependent cytotoxicity studies. Lipid-rich protrusions are a response of cells to stress environment.

The method of single-molecule force spectroscopy (SMFS) is being implemented in our group, which can analyze a specific interaction between biomolecules and the cell membrane at a single-molecule level. In the frame of a pilot study, we investigated the physical properties of antifouling poly[N-(2-hydroxypropyl) methacrylamide] brushes. Polymer brushes are widely utilized in biomedical applications to prevent non-specific interactions with biological fluids.

In recent years a new family of 2D nanomaterials has emerged that, in combination with selective tumor targeting elements, offers a very local cancer cell elimination strategy by cells ablation using photothermal therapy. Such nanomaterials are non-stoichiometric MoO_x (x between 2 and 3) that show localized surface plasmons in the NIR region (high penetration depth of radiation in tissue). We developed a method for their preparation by the facile liquid-phase exfoliation technique. We used two approaches: a) spontaneous oxidation of MoS_2 nanoflakes during exfoliation and b) exfoliation of crystalline MoO_2 powder. We have shown that two types of MoO_x nanoflakes with different morphology and optical properties coexist in the colloidal solution prepared by MoS_2 oxidation. The fraction containing smaller particles with diameters of 1–4 nm exhibited an increased absorbance peak in the NIR region and responded with a significant temperature increase to laser irradiation at the wavelength close to the maximal absorption. By gel filtration, we isolated the plasmonic MoO_x nanoparticles suitable for further bioconjugation and target photothermal treatment.

2. Partial indicators of main activities:

2.1. Research output

2.1.1. Principal types of research output of the institute: basic research/applied research, international/regional (in percentage)

At present, CEMEA's research activities are mainly focused on the area of basic research, which represents about 90% of the representation. Applied research represents about 10% of research activities. 100% of the research has an international character.

2.1.2 List of selected publications documenting the most important results of basic research. The total number of publications listed for the assessment period should not exceed the average number of employees with university degrees engaged in research projects. The principal research outputs (max. 5, including Digital Object Identifier – DOI if available) should be underlined. Authors from the evaluated organizations should be underlined.

KOVARICEK, Petr** - NÁDAŽDY, Peter - PLUHAROVA, Eva - BRUNOVÁ, Alica - SUBAIR, Riyas - VÉGSO, Karol - GUERRA, Valentino Libero Pio - VOLOCHANSKYI, Oleksandr - KALBAC, Martin - KRASNANSKY, Alexander - PANDIT, Pallavi - ROTH, Stephan Volker - HINDERHOFER, Alexander - MAJKOVÁ, Eva - JERGEL, Matej - TIAN, Jianjun - SCHREIBER, Frank - ŠIFFALOVIČ, Peter**. Crystallization of 2D Hybrid Organic-Inorganic Perovskites Templated by Conductive Substrates. In Advanced Functional Materials, 2021, vol. 31, no. 13, art. no. 2009007. (2020: 18.808 - IF, Q1 - JCR, 6.069 - SJR, Q1 - SJR). (2021 - Current Contents). ISSN 1616-301X. https://doi.org/10.1002/adfm.202009007

HASSAN IBRAHIM, Ahmed Mohamed - TAKÁČOVÁ, Martina - JELENSKÁ, Lenka - CSÁDEROVÁ, Lucia - BALOG, Martin** - KOPÁČEK, Juraj - ŠVASTOVÁ, Eliška - KRÍŽIK, Peter. The effect of surface modification of TiMg composite on the in-vitro degradation response, cell survival, adhesion, and proliferation. In *Materials Science and Engineering C*, 2021, vol. 127, no. 112259. (2020: 7.328 - IF, Q1 - JCR, 1.234 - SJR, Q1 - SJR). (2021 - Current Contents). ISSN 0928-4931. https://doi.org/10.1016/j.msec.2021.112259

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MRKÝVKOVÁ, Naďa, Tesařová** - HELD, Vladimír* - NÁDAŽDY, Peter - SUBAIR, Riyas - MAJKOVÁ, Eva - JERGEL, Matej - VLK, Aleš - LEDINSKÝ, Martin - KOTLÁR, Mário - TIAN, Jianjun - ŠIFFALOVIČ, Peter. Combined in situ photoluminescence and X-ray scattering reveals defect formation in Lead-Halide Perovskite films. In Journal of Physical Chemistry Letters, 2021, vol. 12, no. 41, p. 10156-10162. (2020: 6.475 - IF, Q1 - JCR, 2.563 - SJR, Q1 - SJR). (2021 - Current Contents). ISSN 1948-7185. https://doi.org/10.1021/acs.jpclett.1c02869

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2.1.3 List of monographs/books published abroad

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2.1.4. List of monographs/books published in Slovakia

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2.1.5. List of other scientific outputs specifically important for the institute, max. 10 items for institute with less than 50 FTE researchers, 20 for institutes with 50 – 100 FTE researchers and so on

2.1.6. List of patents, patent applications, and other intellectual property rights registered abroad, incl. revenues

-

2.1.7. List of patents, patent applications, and other intellectual property rights registered in Slovakia, incl. revenues

-

2.1.8. Table of research outputs

Papers from international collaborations in large-scale scientific projects (Dwarf team, ALICE Collaboration, ATLAS collaboration, CD Collaboration, H1 Collaboration, HADES Collaboration, and STAR Collaboration) have to be listed separately

Scientific publications	2016			2017			2018			2019			2020			2021			total			
	number	No. / FTE researches	No. / one million total salary budget	number	No. / FTE researches	No. / one million total salary budget	number	No. / FTE researches	No. / one million total salary budget	number	No. / FTE researches	No. / one million total salary budget	number	No. / FTE researches	No. / one million total salary budget	number	No. / FTE researches	No. /1 million total salary budget	number	averaged number per year	av. No. / FTE researches	av. No. / one million total salary budget
Scientific monographs and monographic studies in journals and proceedings published abroad *(AAA, ABA)*						0,000	0		0,000		0,000	0,000		0,000	0,000		0,000	0,000	**0**	**0,000**	**0,000**	**0,000**
Scientific monographs and monographic studies in journals and proceedings published in Slovakia *(AAB, ABB)*						0,000	0		0,000		0,000	0,000		0,000	0,000		0,000	0,000	**0**	**0,000**	**0,000**	**0,000**
Chapters in scientific monographs published abroad *(ABC)*						0,000	**0**		0,000	1	0,131	2,944		0,000	0,000	1	0,037	0,897	**2**	**0,667**	**0,075**	**1,617**
Chapters in scientific monographs published in Slovakia *(ABD)*						0,000	0		0,000		0,000	0,000		0,000	0,000		0,000	0,000	**0**	**0,000**	**0,000**	**0,000**
Scientific papers published in journals registered in Current Contents Connect *(ADCA, ADCB, ADDA, ADDB)*						0,000	5		31,678	12	1,571	35,331	38	2,014	45,166	58	2,162	52,027	**113**	**28,250**	**3,178**	**68,514**
Scientific papers published in journals registered in Web of Science Core Collection and SCOPUS not listed above *(ADMA, ADMB, ADNA, ADNB)*						0,000	1		6,336	1	0,131	2,944	4	0,212	4,754	5	0,186	4,485	**11**	**2,750**	**0,309**	**6,670**
Scientific papers published in other foreign journals (not listed above) *(ADEA, ADEB)*						0,000	0		0,000		0,000	0,000		0,000	0,000		0,000	0,000	**0**	**0,000**	**0,000**	**0,000**
Scientific papers published in other domestic journals (not listed above) *(ADFA, ADFB)*						0,000	0		0,000		0,000	0,000		0,000	0,000		0,000	0,000	**0**	**0,000**	**0,000**	**0,000**
Scientific papers published in foreign peer-reviewed proceedings *(AECA)*						0,000	0		0,000		0,000	0,000		0,000	0,000		0,000	0,000	**0**	**0,000**	**0,000**	**0,000**
Scientific papers published in domestic peer-reviewed proceedings *(AEDA)*						0,000	0		0,000		0,000	0,000		0,000	0,000		0,000	0,000	**0**	**0,000**	**0,000**	**0,000**
Published papers (full text) from foreign scientific conferences *(AFA, AFC)*						0,000	0		0,000	1	0,131	2,944		0,000	0,000	3	0,112	2,691	**4**	**1,333**	**0,150**	**3,234**
Published papers (full text) from domestic scientific conferences *(AFB, AFD)*						0,000	0		0,000	1	0,131	2,944		0,000	0,000	3	0	3	**4**	**1**	**0**	**3**

2.1.9. Narrative on the most important research outputs of the institute – especially focused on their importance for society (3-5 pages)

Thin films and surface properties

In the field of spin-wave dynamics at the nanoscale, we focused on developing novel ultrafast and energy-efficient computing elements based on spin waves. In work [1], we have reviewed the potential and challenges of noncolinear magnonic states and evaluated how they can contribute to the field of magnonics in the near future. Among the materials hosting the noncolinear states are the materials possessing antisymmetric exchange, also known as the Dzyaloshinskii–Moriya interaction. The Dzyaloshinskii–Moriya interaction induces not only the noncolinear magnetic states but, because of its chiral character, can also induce nonreciprocal dispersion of the spin wave. Our research contributes to developing next-generation computing devices that are predicted to go beyond the limitations of current CMOS technology.

In the field of thin-film structures in energetics, the aim of our work [2] was to evaluate the metal-insulator-semiconductor photoanodes for water splitting under solar radiation. As a top transparent catalytic layer, thin RuO_2 and RuO_2-IrO_2 films with a thickness of 5 µm were employed. The publication summarizes the potential of thin catalytic RuO_2 and RuO_2-IrO_2 films for water oxidation and shows that RuO_2 and RuO_2-IrO_2 thin films are promising as top catalytic layers for water splitting. Water splitting under sun radiation is an effective and nature-friendly technique for hydrogen production.

In the field of nanotribology of 2D materials, we highlight the study of frictional properties of few-layer and monolayer $MoSe_2$ grown by chemical vapor deposition (CVD). In the study [3], the anisotropic friction behavior between AFM tip and monolayer and few-layer $MoSe_2$ flakes grown by CVD was performed by nanofriction measurements at different crystallographic directions, applied loads, and tip scanning velocities. Our results reveal that the angular dependence of the friction forces is highly anisotropic for both types of $MoSe_2$ flakes, which can be explained by the coexistence of different friction mechanisms in ultra-thin $MoSe_2$ films. The work extends the understanding of the tribological properties of 2D materials and dry lubricants at the nanoscale.

[1] Mruczkiewicz, M. *et al*. The 2021 roadmap for noncollinear magnonics. *Solid State Physics : advances in Research and Applications*, 2021, vol. 72, p. 1-27. ISSN 0081-1947.

[2] Sahoo, P.P. *et al*. Si-based metal-insulator-semiconductor structures with RuO2-(IrO2) films for photoelectrochemical water oxidation. *ACS Applied Energy Materials*, 2021, vol. 4, p. 11162-11172.

[3] Kozak, A. *et al*. Angular dependence of nanofriction of mono- and few-layer MoSe2. *Applied Surface Science*, 2021, vol. 567, no. 150807.

Functional polymer surfaces

In our investigations, we focused on the synthesis of hybrid graphene oxide-based nanoparticles as active fillers for novel functional materials. As part of the cooperation with Tomas Bata University in Zlin and Technical University in Lodz, graphene oxide nanoparticles were modified by various polymers using surface-initiated atom transfer radical polymerization (ATRP). It was found that in addition to surface modification by polymer chains during the polymerization, a simultaneous reduction of graphene oxide surface by present tertiary amines, commonly used in ATRP as a ligand, was proceeded. At the same time, the conductivity of the prepared hybrids was increased up to 8 orders of magnitude. The degree of graphene oxide reduction and, thus, the conductivity of the hybrid nanoparticles could be controlled by polymerization conditions. The effect of prepared graphene oxide hybrids as fillers in elastomers and polymer blends on their properties was investigated. Various composite elastomers filled with graphene oxide hybrids showed excellent photo-actuation properties [1,2]. The graphene oxide hybrids with finely adjusted electrical conductivity provided excellent materials for electro-rheological systems. In addition, the graphene oxide hybrids increased the stability of emulsions and miscible PMMA/SAN blends against the phase separation at high temperatures [3]. The developed one-pot synthesis of electrically conductive hybrids and composites provides a simple approach for novel functional materials applicable in various sensors, brake systems, and electro-rheological fluids applicable in biomedicine.

[1] Osicka, J. *et al*. Controllably coated graphene oxide particles with enhanced compatibility with poly(ethylene-co-propylene) thermoplastic elastomer for excellent photo-mechanical actuation capability. *Reactive & Functional Polymers*, 2020, vol. 148, art. no. 104487,

[2] Zygo, M. *et al*. Effect of structure of polymers grafted from graphene oxide on the compatibility of particles with silicone-based environment and the stimuli-responsive capabilities of their composites. *Nanomaterials-Basel*, 2020, vol. 10, no. 3, art.no. 591,

[3] Ilčíková, M. *et al*. The effect of short polystyrene brushes grafted from graphene oxide on the behavior of miscible PMMA/SAN blends. *Polymer : the International Journal for the Science and Technology of Polymers*, 2020, vol. 211, art. no. 123088,

Special light structural materials and composites

Our study [1] introduces aluminium (Al) – aluminium nitride (AlN) metal matrix composites (MMCs) manufactured by a powder metallurgy cost-effective approach realized at a large industrial scale. Commercially available, atomized Al, magnesium (Mg), and tin (Sn) powders were processed by readily available blending techniques, cold isostatic pressing, solid-state nitridation in static gaseous nitrogen, and direct extrusion. Two Al samples 8.8 and 14.7 vol.% AlN MMCs were fabricated in the form of extruded bars with a cross-section of 80x15 mm. The microstructure of the nitrided Al-AlN and extruded MMCs were presented in detail. The stability of tensile mechanical properties of the as-extruded Al-AlN MMCs was pursued after the MMCs were annealed between 300 and 600°C for 24 h. No major changes to their mechanical properties occurred by annealing up to 500°C owing to an effective stabilization by stable and fine nanoscale AlN dispersoids by Zener pinning action. The results predetermine Al-AlN MMCs to be targeted for structural load-bearing applications at elevated temperatures not normally associated with the use of conventional Al alloys and MMCs.

[1] Balog, M. *et al*. Industrially fabricated in-situ Al-AlN metal matrix composites (part A): processing, thermal stability, and microstructure, *J. Alloys Compd*. 883 (2021) 160858.

Advanced inorganic materials

The intensive development of such industries as medicine, mechanical engineering, rocket science, shipbuilding, and electronics requires the improvement of the characteristics of the manufactured metals and alloys, which can be achieved by their surface modification. In this connection, as part of the sub-activities of CEMEA, we focused our attention on highly efficient, resource-saving, and environmentally-friendly electrochemical surface modification of metals and alloys in new generation ionic liquids (deep eutectic solvents). Deep eutectic solvents (DESs) as natural non-water bio-degradable solvents have proven to be a promising alternative to the classical most-common acidic electrolytes for the electrochemical processing of metals and alloys. The room-temperature technology of electrochemical surface treatment of metals and alloys in DESs, proposed by the researchers of CEMEA, allows not only cleaning the surface, giving it an attractive appearance and increased corrosion resistance, but also flexibly modeling surface properties, obtaining surfaces with previously known and desired characteristics (specific morphology, topography, certain chemical composition, wettability, etc.). It was demonstrated that electrochemical processing of stainless steels in DESs could be used for renovation of stainless-steel constructions and tools, corrosion protection, and antibacterial protection (reduction of bacterial and viral activity is very important for stainless steel medical instruments, especially during epidemic times). Also, it was shown that galvanostatic and potentiostatic electrochemical surface treatment of Ti and Ti-based alloys in DESs provide dissolution of the surface defects and contaminations, noticeable improvement in corrosion resistance, and possibilities with different treatment conditions influence the chemical composition of the protective oxide layer, surface roughness, and wettability. It revealed the possibility of the formation of micro and nano-rough structures on surfaces of Ti and Ti-alloy samples for bio-inspiration of Ti-products for medical applications. The formation of chemically pure nano-structured protective oxide layers opens up wide opportunities for improving the quality of titanium implants and prostheses. Moreover, electrochemically modified in DESs Ti and Ti-based alloys can be successfully applied as efficient photocatalysts. Besides, it should be noted a promising application of DESs for electrochemical surface treatment of WCu composites for microelectronics proposal. Short-time room-temperature electropolishing of WCu composite in DESs causes significant leveling of the surfaces accompanied by advantageous changes in the elemental surface composition, which meet the high standards of materials for microelectronics [1-3].

[1] Kityk, A. *et al*. Electropolishing of WCu composite in a deep eutectic solvent. *Chemical Papers*, 2021, vol. 75, no. 4, p. 1767-1771.

[2] Kityk, A. *et al*. Enhancement of the surface characteristics of Ti-based biomedical alloy by electropolishing in environmentally friendly deep eutectic solvent (Ethaline). *Colloids and Surfaces A: Physicochemical and Engineering Aspects*, 2021, vol. 613, p. 126125-1-126125-14.

[3] Kityk, A. *et al*. Electrochemical surface treatment of manganese stainless steel using several types of deep eutectic solvents. *Materials Research Bulletin*, 2021, vol. 141, p. 111348-1-111348-11.

Inorganic and organic nanostructures for electronics and sensorics

Recently discovered two-dimensional (2D) nanomaterials have shown many outstanding chemical and physical properties. In our research, we concentrated on the preparation and application of 2D materials as templates for the growth of organic semiconductors and perovskites for optoelectronic applications. We investigated the preparation of 2D materials by liquid-phase exfoliation and their self-assembly in thin films. In particular, we investigated the exfoliation of 2D MoS_2 flakes as a function of the initial concentration of MoS_2 powder and found a non-trivial dependence of the final MoS_2 flake concentration on the initial concentration. In addition, we demonstrated the use of exfoliated MoS_2 flakes to fabricate self-assembled thin films employing modified Langmuir-Schaefer deposition [1]. In addition, we have generalized the Langmuir-Schaefer deposition technique to a large family of different low-dimensional materials. 2D nanomaterials are known to influence the growth of organic semiconductor films. Using in-situ and time-resolved X-ray scattering (GIWAXS), we have studied the growth of diindenoperylene thin films on MoS_2 substrates with different c-axis crystallographic orientations. Our published studies provide a deeper understanding of the growth processes of organic semiconductor thin films in terms of their crystallographic orientations and stresses and confirm the tuning capability of 2D substrates to fabricate specialized films for optoelectronic applications. Perovskite solar cells are one of the most rapidly developing research topics of the last decade. By combining time-resolved photoluminescence and X-ray scattering (GIWAXS), we tracked the nucleation and growth of perovskite layers during annealing. Our studies allowed us to determine the best fabrication parameters leading to perovskite layers with the lowest defect density. We also followed the crystal lattice changes during the directional growth of 2D perovskite on graphene [2]. A significant result was the association of emerging grain boundaries during the coalescence phase with the formation of non-radiative recombination of excitons in ultrathin perovskite layers [3]. Our recent findings in the field of templated growth of organic semiconductors and perovskites are likely to have an impact on the improved performance of next-generation optoelectronic devices and thus on the rapidly growing market for electronic consumables in telecommunications and solar power generation.

[1] Kálosi, A. *et al*. Tailored Langmuir-Schaefer Deposition of Few-Layer MoS2 Nanosheet Films for Electronic Applications. *Langmuir*, 2019, vol. 35, no. 30, p. 9802-9808.

[2] Kovaricek, P. *et al*. Crystallization of 2D Hybrid Organic-Inorganic Perovskites Templated by Conductive Substrates. *Advanced Functional Materials*, 2021, vol. 31, no. 13, art. no. 2009007.

[3] Mrkývková, N. *et al*. Combined in situ photoluminescence and X-ray scattering reveals defect formation in Lead-Halide Perovskite films. *Journal of Physical Chemistry Letters*, 2021, vol. 12, no. 41, p. 10156-10162.

Advanced materials for biomedicine and biotechnologies

Titanium (Ti) and Ti alloys belong among the materials most frequently used for the production of dental implants (DI). Although DI from Ti and Ti alloys are used with a high success rate, their major shortcomings still remain unsolved. Innovative biomedical Ti-Magnesium composite is a partially biodegradable permanent material that minimizes the main disadvantages of conventional materials for DI. Biologically degradable Mg component provides an ideal solution to a number of problems associated with Ti DI, however, TiMg is more prone to corrosion in physiological environment. This can strongly restrain the initial cell adhesion and proliferation on the implant surface. The rate of Mg corrosion is usually moderated chemically by surface modification but despite of its effectivity it results in the formation of pores on the surface, where undesirable bacterial infections can arise. In our article, we propose a new way of TiMg surface stabilization by optimizing the conditions of mechanical surface treatment, which can be easily and effectively applied in the production of DI [1]. The results confirmed that a smooth and less deformed surface of TiMg samples efficiently reduced the corrosion rate and improved in-vitro cell response to an acceptable level, comparable with chemically stabilized TiMg samples. The results we have achieved are important from the point of view of prospective production of TiMg DI and fully biodegradable Mg implants.

Despite the obvious benefits of nanotherapeutics in healthcare strategies, biocompatibility, and the clearance of imaging agents and nanocarriers from the body following their application generates concerns about their safety for health. Considering the nanoparticles-induced nephrotoxicity as a frequent adverse event developing during NPs application, the impact of magnetic nanoparticles (MNPs) on renal cells forming the filtration apparatus of the kidney was studied [2]. We have revealed that the type of cell and the type of the MNPs coating might be the strongest determinants of cellular response e.g. immune response, cell injury, proteinuric kidney diseases, toward nanoparticle exposure. These results are essential in the field of nanomaterial testing for medical purposes and underline the importance of in vitro tests aimed at nephrotoxic side effects of such materials.

One of the main aims of the theranostic is to increase the delivery efficiency and specificity of the nanoparticles in line with the reduction of unspecific accumulation in different organs. The most promising approach is a functionalization with antibodies that selectively recognize the antigens exclusively expressed in tumors but not in healthy tissues. We developed a new bioconjugation approach to target the cancer cells by linking monoclonal antibodies specific to a dual hypoxia/acidosis marker of aggressive tumors, carbonic anhydrase IX (CAIX), to MoS_2 2D nanomaterials [3]. Flow cytometry measurements and label-free molecular imaging studies revealed cell type-dependent internalization rates, with high specificity towards CAIX-expressing cells. Thus, we showed that appropriately functionalized nanoplatforms can potentially serve as platforms for the diagnosis or therapy of different types of cancer. Moreover, the label-free molecular imaging of cells and tissues is an emerging modern technique that we employ in our workspace using a confocal Raman Microscope (CRM). Tumor targeting for diagnostic and therapeutic purposes via nanomaterials-based approach combined with anti-CAIX antibody ensures highly selective application with potential benefits in the clinical environment.

[1] Ibrahim A.M.H., *et al*. The effect of surface modification of TiMg composite on the in-vitro degradation response, cell survival, adhesion, and proliferation, *Mater. Sci. Eng*., C 127 (2021) 112259.

[2] Šelc, M. *et al*. Surface coating determines the inflammatory potential of magnetite nanoparticles in murine renal podocytes and mesangial cells. *RSC Advances*, 2020, vol. 10, no. 40, p. 23916-23929.

[3] Kálosi, A. *et al*. A bioconjugated MoS2 based nanoplatform with increased binding efficiency to cancer cells. *Biomaterials Science*, 2020, vol. 8, no. 7, p. 1973-1980.

2.2. Measures of research outputs (citations, etc.)

2.2.1. Table with citations per annum (without self-citations)

Citations of papers from international collaborations in large-scale scientific projects (Dwarf team, ALICE Collaboration, ATLAS collaboration, CD Collaboration, H1 Collaboration, HADES Collaboration, and STAR Collaboration) are listed separately

Citations, reviews	2016		2017		2018		2019		2020		2021		total		
	number	No. / FTE researchers	number	No. / FTE researchers	number	No. / FTE researchers	number	No. / FTE researchers	number	No. / FTE researchers	number	No. / FTE researchers	number	averaged number per year	av. No. / FTE researchers
Citations in Web of Science Core Collection (1.1, 2.1)					1		12	1,57	42	2,23	13	0,48	**68**	**17,00**	**1,91**
Citations in SCOPUS (1.2, 2.2) if not listed above								0,00	1	0,05	1	0,04	**2**	**1,00**	**0,11**
Citations in other citation indexes and databases (not listed above) (3.2,4.2)								0,00		0,00		0,00	**0**		
Other citations (not listed above) (3.1, 4.1)								0,00		0,00		0,00	**0**		
Reviews (5,6)								0,00		0,00		0,00	**0**		

2.2.2. List of 10 most-cited publications published any time with the address of the institute, with number of citations in the assessment period (2015 – 2020)

ELIÁŠOVÁ SOHOVÁ, Marianna - BODIK, Michal - ŠIFFALOVIČ, Peter - BUGÁROVÁ, Nikola - LABUDOVÁ, Martina - ZAŤOVIČOVÁ, Miriam - HIANIK, Tibor - OMASTOVÁ, Mária - MAJKOVÁ, Eva - JERGEL, Matej - PASTOREKOVÁ, Silvia. Label-free tracking of nanosized graphene oxide cellular uptake by confocal Raman microscopy. In Analyst, 2018, vol. 143, no. 15, p. 3686-3692. (7. Cit)

BALOG, Martin - KRÍŽIK, Peter - BAJANA, Otto - HU, Tao - YANG, Hanry - SCHOENUNG, Julie M. - LAVERNIA, Enrique J. Influence of grain boundaries with dispersed nanoscale Al2O3 particles on the strength of Al for a wide range of homologous temperatures. In Journal of Alloys and Compounds, 2019, vol. 772, p. 472-481. (7. Cit)

KÁLOSI, Anna - DEMYDENKO, Maksym - BODIK, Michal - HAGARA, Jakub - KOTLÁR, Mário - KOSTIUK, Dmytro - HALAHOVETS, Yuriy - VÉGSO, Karol - ROLDAN, Alicia Marin - MAURYA, Gulab Singh - ANGUS, Michal - VEIS, Pavel - JERGEL, Matej - MAJKOVÁ, Eva - ŠIFFALOVIČ, Peter. Tailored Langmuir-Schaefer Deposition of Few-Layer MoS2 Nanosheet Films for Electronic Applications. In Langmuir, 2019, vol. 35, no. 30, p. 9802-9808. (5. Cit)

SUBAIR, Riyas - DI GIROLAMO, Diego - BODIK, Michal - NÁDAŽDY, Vojtech - LI, Bo - NÁDAŽDY, Peter - MARKOVIC, Zoran - HOFBAUEROVÁ, Monika, Benkovičová - CHLPIK, Juraj - KOTLAR, Mario - HALAHOVETS, Yuriy - ŠIFFALOVIČ, Peter - JERGEL, Matej - TIAN, Jianjun - BRUNETTI, Francesca - MAJKOVÁ, Eva. Effect of the doping of PC61BM electron transport layer with carbon nanodots on the performance of inverted planar MAPbI(3) perovskite solar cells. In Solar Energy, 2019, vol. 189, p. 426-434. (5 cit)

OSIČKA, Josef - MRLIK, Miroslav - ILČÍKOVÁ, Markéta - HANULÍKOVÁ, Barbora - SEDLAČIK, Michal** - MOSNÁČEK, Jaroslav. Reversible actuation ability upon light stimulation of the smart systems with controllably grafted graphene oxide with poly (glycidyl methacrylate) and PDMS elastomer: Effect of compatibility and graphene oxide reduction on the photo-actuation performance. In Polymers : Open Access Polymer Science Journal, 2018, vol. 10, art. no. 832. (3. Cit)

SOJKOVÁ, Michaela - VÉGSO, Karol - MRKÝVKOVÁ, Naďa, Tesařová - HAGARA, Jakub - HUTÁR, Peter - ROSOVÁ, Alica - ČAPLOVIČOVÁ, M. - LUDACKA, U. - SKÁKALOVÁ, V. - MAJKOVÁ, Eva - ŠIFFALOVIČ, Peter - HULMAN, Martin. Tuning the orientation of few-layer MoS2 films using one-zone sulfurization. In RSC Advances, 2019, vol. 9, no. 51, p. 29645-29651. (3. Cit)

KARKI, Akchheta - VOLLBRECHT, Joachim - GILLETT, Alexander J. - SELTER, Philipp - LEE, Jaewon - PENG, Zhengxing - SCHOPP, Nora - DIXON, Alana L. - SCHROCK, Max - NÁDAŽDY, Vojtech - SCHAUER, Franz - ADE, Harald - CHMELKA, Bradley F. - BAZAN, Guillermo C. - FRIEND, Richard H. - NGUYEN, Thuc-Quyen. Unifying Charge Generation, Recombination, and Extraction in Low-Offset Non-Fullerene Acceptor Organic Solar Cells. In Advanced Energy Materials, 2020, vol. 10, no. 29, 2001203. (3. Cit)

BALOG, Martin - ROSOVÁ, Alica - SZUNDIOVÁ, Bronislava - OROVČÍK, Ľubomír - KRÍŽIK, Peter - ŠVEC, Peter Jr. - KULICH, Miloslav - KOPERA, Ľubomír - KOVÁČ, Pavol - HUŠEK, Imrich - IBRAHIM, Ahmed Mohamed Hassan. HITEMAL-an outer sheath material for MgB2 superconductor wires: The effect of annealing at 595-655 degrees C on the microstructure and properties. In Materials and Design, 2018, vol. 157, p. 12-23. (2. Cit)

HOFBAUEROVÁ, Monika, Benkovičová - HOLOŠ, Ana - NÁDAŽDY, Peter - HALAHOVETS, Yuriy - KOTLÁR, Mário - KOLLÁR, Jozef - ŠIFFALOVIČ, Peter - JERGEL, Matej - MAJKOVÁ, Eva - MOSNÁČEK, Jaroslav - IVANČO, Ján. Tailoring the interparticle distance in Langmuir nanoparticle films. In Physical Chemistry Chemical Physics, 2019, vol. 21, no. 18, p. 9553-9563. (2. Cit)

BODIK, Michal - ANNUŠOVÁ, Adriana - HAGARA, Jakub - MIČUŠÍK, Matej - OMASTOVÁ, Mária - KOTLÁR, Mário - CHLPÍK, Juraj - CIRÁK, Július - ŠVAJDLENKOVÁ, Helena - ANGUŠ, Michal - ROLDÁN, Alicia Marín - VEIS, Pavel - JERGEL, Matej - MAJKOVÁ, Eva - ŠIFFALOVIČ, Peter. An elevated concentration of MoS2 lowers the efficacy of liquid-phase exfoliation and triggers the production of MoOx nanoparticles. In Physical Chemistry Chemical Physics, 2019, vol. 21, no. 23, p. 12396-12405. (2. Cit)

2.2.3. List of 10 most-cited publications published any time with the address of the institute, with number of citations obtained until 2020

Beginning of research at the institute CEMEA SAS v.v.i. started in 2019; therefore, the outputs are identical to chapter 2.2.2

2.2.4. List of 10 most-cited publications published during the evaluation period (2016-2021) with the address of the Institute, with number of citations obtained until 2021

ELIÁŠOVÁ SOHOVÁ, Marianna - BODIK, Michal - ŠIFFALOVIČ, Peter - BUGÁROVÁ, Nikola - LABUDOVÁ, Martina - ZAŤOVIČOVÁ, Miriam - HIANIK, Tibor - OMASTOVÁ, Mária - MAJKOVÁ, Eva - JERGEL, Matej - PASTOREKOVÁ, Silvia. Label-free tracking of nanosized graphene oxide cellular uptake by confocal Raman microscopy. In Analyst, 2018, vol. 143, no. 15, p. 3686-3692. (9. Cit)

BALOG, Martin - KRÍŽIK, Peter - BAJANA, Otto - HU, Tao - YANG, Hanry - SCHOENUNG, Julie M. - LAVERNIA, Enrique J. Influence of grain boundaries with dispersed nanoscale Al2O3 particles on the strength of Al for a wide range of homologous temperatures. In Journal of Alloys and Compounds, 2019, vol. 772, p. 472-481. (7. Cit)

OSIČKA, Josef - MRLIK, Miroslav - ILČÍKOVÁ, Markéta - HANULÍKOVÁ, Barbora - SEDLAČIK, Michal** - MOSNÁČEK, Jaroslav. Reversible actuation ability upon light stimulation of the smart systems with controllably grafted graphene oxide with poly (glycidyl methacrylate) and PDMS elastomer: Effect of compatibility and graphene oxide reduction on the photo-actuation performance. In Polymers : Open Access Polymer Science Journal, 2018, vol. 10, art. no. 832. (5. Cit)

KÁLOSI, Anna - DEMYDENKO, Maksym - BODIK, Michal - HAGARA, Jakub - KOTLÁR, Mário - KOSTIUK, Dmytro - HALAHOVETS, Yuriy - VÉGSO, Karol - ROLDAN, Alicia Marin - MAURYA, Gulab Singh - ANGUS, Michal - VEIS, Pavel - JERGEL, Matej - MAJKOVÁ, Eva - ŠIFFALOVIČ, Peter. Tailored Langmuir-Schaefer Deposition of Few-Layer MoS2 Nanosheet Films for Electronic Applications. In Langmuir, 2019, vol. 35, no. 30, p. 9802-9808. (5. Cit)

SUBAIR, Riyas - DI GIROLAMO, Diego - BODIK, Michal - NÁDAŽDY, Vojtech - LI, Bo - NÁDAŽDY, Peter - MARKOVIC, Zoran - HOFBAUEROVÁ, Monika, Benkovičová - CHLPIK, Juraj - KOTLAR, Mario - HALAHOVETS, Yuriy - ŠIFFALOVIČ, Peter - JERGEL, Matej - TIAN, Jianjun - BRUNETTI, Francesca - MAJKOVÁ, Eva. Effect of the doping of PC61BM electron transport layer with carbon nanodots on the performance of inverted planar MAPbI(3) perovskite solar cells. In Solar Energy, 2019, vol. 189, p. 426-434. (5. cit)

BODIK, Michal - ANNUŠOVÁ, Adriana - HAGARA, Jakub - MIČUŠÍK, Matej - OMASTOVÁ, Mária - KOTLÁR, Mário - CHLPÍK, Juraj - CIRÁK, Július - ŠVAJDLENKOVÁ, Helena - ANGUŠ, Michal - ROLDÁN, Alicia Marín - VEIS, Pavel - JERGEL, Matej - MAJKOVÁ, Eva - ŠIFFALOVIČ, Peter. An elevated concentration of MoS2 lowers the efficacy of liquid-phase exfoliation and triggers the production of MoOx nanoparticles. In Physical Chemistry Chemical Physics, 2019, vol. 21, no. 23, p. 12396-12405. (4. Cit)

PUCHÝ, Viktor - HVIZDOŠ, Pavol - IVOR, Michal - MEDVEĎ, Dávid - HNATKO, Miroslav - KOVALČÍKOVÁ, Alexandra - SEDLÁK, Richard - DUSZA, Ján. Preparation, friction, wear, and fracture of the Si3N4-Ag-GNPs composites prepared by SPS. In Journal of the European Ceramic Society, 2020, vol. 40, no. 14, p. 4853-4859. (3. cit)

CSANÁDI, Tamás - GALL, Marián - VOJTKO, Marek - KOVALČÍKOVÁ, Alexandra - HNATKO, Miroslav - DUSZA, Ján - ŠAJGALÍK, Pavol. Micro scale fracture strength of grains and grain boundaries in polycrystalline La-doped beta-Si3N4 ceramics. In Journal of the European Ceramic Society, 2020, vol. 40, no. 14, p. 4783-4791. (3. cit)

SOJKOVÁ, Michaela - VÉGSO, Karol - MRKÝVKOVÁ, Naďa, Tesařová - HAGARA, Jakub - HUTÁR, Peter - ROSOVÁ, Alica - ČAPLOVIČOVÁ, M. - LUDACKA, U. - SKÁKALOVÁ, V. - MAJKOVÁ, Eva - ŠIFFALOVIČ, Peter - HULMAN, Martin. Tuning the orientation of few-layer MoS2 films using one-zone sulfurization. In RSC Advances, 2019, vol. 9, no. 51, p. 29645-29651. (3. Cit)

KARKI, Akchheta - VOLLBRECHT, Joachim - GILLETT, Alexander J. - SELTER, Philipp - LEE, Jaewon - PENG, Zhengxing - SCHOPP, Nora - DIXON, Alana L. - SCHROCK, Max - NÁDAŽDY, Vojtech - SCHAUER, Franz - ADE, Harald - CHMELKA, Bradley F. - BAZAN, Guillermo C. - FRIEND, Richard H. - NGUYEN, Thuc-Quyen. Unifying Charge Generation, Recombination, and Extraction in Low-Offset Non-Fullerene Acceptor Organic Solar Cells. In Advanced Energy Materials, 2020, vol. 10, no. 29, 2001203. (3. Cit)

2.2.5. List of most-cited authors from the Institute (at most 10 % of the research employees with university degree engaged in research projects) and their number of citations in the assessment period (2015– 2020). The cited papers must bear the address of the institute

Šiffalovič Peter	32
Majková Eva	32
Balog Martin	10
Mosnáček Jaroslav	7
Mrkývková - Tesařová Naďa	7

2.2.6. List of most-cited authors from the Institute (at most 10 % of the research employees with university degree engaged in research projects) and their number of citations obtained until 2020. The cited papers must bear the address of the Institute

Beginning of research at the institute CEMEA SAS v.v.i. started in 2019; therefore, the outputs are identical to chapter 2.2.5

2.2.7. List of most-cited authors from the Institute (at most 10 % of the research employees with university degree engaged in research projects) and their number of citations obtained until 2021 of their papers published during the evaluation period (2016– 2021). The cited papers must bear the address of the Institute

Šiffalovič Peter	36
Majková Eva	36
Balog Martin	11
Mosnáček Jaroslav	10
Mrkývková - Tesařová Naďa	7

2.3. Research status of the institute in international and national context

- **International/European position of the institute**

2.3.1. List of the most important research activities demonstrating the international relevance of the research performed by the institute, incl. major projects (details of projects should be supplied under Indicator 2.4). Max. 10 items for institute with less than 50 FTE researchers, max. 20 for institutes with 50 – 100 FTE researchers and so on

The Center for Advanced Materials Application (CEMEA) was founded in 2017 by the Slovak Academy of Sciences (SAS). CEMEA started to operate in 2019 after receiving project support from the Research Agency. Within just a few years of its existence, CEMEA has become the leading institution in the field of battery technology research in Slovakia. CEMEA has the ambition to coordinate not only national but also international projects within HORIZON EUROPE Programme.

CEMEA was successful in the M-ERA.NET Call 2021 with the project:

Title: Enhancing the mechanical stability of interfaces in solid-state Li batteries for energy-intensive applications, SOLIMEC
Coordinator: Univ. Autonoma Madrid, Spain
Partners: CEMEA, Univ. Leoben, Austria, Univ. Trondheim, Norway, CSIC, Madrid, Spain, AVL List, graz, Austria
The project starts in 2022 and lasts until 2024.

CEMEA was also active in the HORIZON EUROPE program. In 2021 we submitted two projects in the field of battery technology. In both projects, CEMEA was the coordinator of the proposal:

Identification number, call: HORIZON-CL5-2021-D2-01-02
Title: High performance and safe Li-ion battery cell with electrodes protected by atomic layer deposition, LiBALD
Coordinator: CEMEA
Partners: WUT Poland, Univ. Helsinki, Finland, Technion, Israel, Beneq OY, Finland, InoBat, Slovakia, Heyrovsky Inst. CAS, Czech Republic, Fraunhofer IKTS, Germany, Univ. Surrey, United Kingdom.
For this proposal, we received 11 out of 15 points. Although this was above the threshold (10 points), the project was not funded.

Another proposal from the HORIZON EUROPE programme was submitted in the frame of Widening participation and strengthening the European Research Area, call Teaming for Excellence:

Identification number, call: HORIZON-WIDERA-2022-ACCESS-01-01-two-stage
Title: Battery Technology Research in the Centre of Excellence for Advanced Materials Application, BATTERCEMEA
Coordinator: CEMEA
Partners: Fraunhofer IKTS, Germany, Univ. Helsinki, Finland.
Unfortunately, the proposal received a score of 8 out of 10 and was not selected for the second stage.

2.3.2. List of international conferences (co)organised by the institute

-

2.3.3. List of edited proceedings from international scientific conferences

-

2.3.4. List of journals edited/published by the institute and information on their indexing in WOS, SCOPUS, other database or no database, incl. impact factor and other metrics of journals in each year of the assessment period

-

- **National position of the institute**

2.3.5. List of selected activities of national importance

In 2020, CEMEA initiated and organized the first seminar on batteries in Slovakia, SEMBAT2020. More than 50 participants from Slovak universities (STU, TUKE, UPJŠ, Univ. Žilina) and private companies took part in the event. The event was organized in the Congress Centrum SAS Smolenice on January 20-21. 2020. The symposium focused on the following topics:

Raw materials for batteries available in Slovakia.

Technology of battery cells.

Battery management systems.

Recycling of used batteries.

Education.

Cooperation with industry.

In 2020, CEMEA stimulated the formation of the National Battery Center (NBC). A consortium of several SAS institutes led by the Centre for Advanced Material Application (CEMEA), several research universities, and private companies associated in the NBC intends to develop a strategic national research initiative to develop new battery technologies and support their commercialization. The project aims to develop and commercialize battery technologies and systems at EU Technology Readiness Level 1 to 6 (basic/application research - prototype - validation in the real environment). The project is divided into three work packages and two cross-sectional activities:

WP1 Raw materials, active materials, and cells

WP2 Battery system and its management

WP3 Recycling and re-use of batteries

Cross-sectional activity – Talent and education

Cross-sectional activity – Knowledge transfer and commercialization

The NBC project covers the most important and, in Slovakia, also the most promising components of the battery value chain. In addition, NBC is preparing its activities for the Slovakia's Economic Recovery and Resilience Plan approved by the EU Commission.

In 2019, CEMEA became a founding member of the **Slovak Battery Alliance, SBaA**. The Slovak Battery Alliance is an independent advocacy group composed of legal entities and operating as an industry cluster. The only cluster in Slovakia, SBaA operates in the fields of strategy, legislation, and communication to build a comprehensive battery chain in Slovakia. It is an executive platform for cooperation among the public and private sectors, innovators, the academic community, and financial institutions. Its aim is to participate in the battery value chain in Europe. The main goal of SBaA is to promote long-term competitiveness, merger, and mobilization of its members' resources in order to establish an innovative and competitive battery eco-system in Slovakia. Furthermore, it wants to carry out activities aimed at increasing the awareness of this eco-system's importance for the industry. By membership in SBaA CEMEA obtained access to activities in the field of battery as well as the opportunity to establish contacts with the most important players in this field in Slovakia.

2.3.6. List of journals (published only in the Slovak language) edited/published by the institute and information on their indexing in WOS, SCOPUS, other database or no database, incl. impact factor and other metrics of journals in each year of the assessment period

-

- ### Position of individual researchers in the international context

2.3.7. List of invited/keynote presentations at international conferences, as documented by programme or invitation letter

2021:

MOSNÁČEK, Jaroslav - KOLLÁR, Jozef - BONDAREV, Dmitrij - HOLOŠ, Ana - ZAIN, Gamal - KARIM, Rubina - ECKSTEIN ANDICSOVÁ, Anita - BORSKÁ, Katarína - MORAVČÍKOVÁ, Daniela. Oxygen tolerant copper mediated photo-ATRP under specific polymerization conditions. In VESPS 2021: Virtual European Symposium of Photopolymer Science dedicated to Ewa Andrzejewska: book of abstracts. - Gumpoldskirchen, Austria: ChemIT e.U. - Book-ofabstracts.com, 2021, p. 63. ISBN 978-3-9504809-3-1.

BALOG, Martin** - IBRAHIM, Ahmed Mohamed Hassan - KRÍŽIK, Peter - CATIC, Amir -SCHAUPERL, Zdravko - CETIN, Yuksel - BESIROVIC, Hajrudin. From the powder to implantation - the development of novel biomedical TiMg Composite (Biacom©). In Book of Abstracts: 21th International Conference on Materials, Tribology & Recycling MATRIB 2021. Danko Ćorić, Sanja Šolić, Franjo Ivušić. - Zagreb, Croatia: HDMT - Hrvatsko Društvo za Materijale i Tribologiju, 2021, p. 9-31. ISSN 2459-5608. MATRIB 2021: International Conference on Materials, Tribology & Recycling.

HASSAN IBRAHIM, Ahmed Mohamed** - TAKÁČOVÁ, Martina - BALOG, Martin - ŠVASTOVÁ, Eliška. Ti+Mg composite with a mechanically modified surface: the in-vitro degradation response and cytocompatibility. In Book of Abstracts: 21th International Conference on Materials, Tribology & Recycling MATRIB 2021. Danko Ćorić, Sanja Šolić, Franjo Ivušić. - Zagreb, Croatia: HDMT - Hrvatsko Društvo za Materijale i Tribologiju, 2021, p. 210-220. ISSN 2459-5608. MATRIB 2021: International Conference on Materials, Tribology & Recycling.

ŠVEC, Peter Jr. - MIHALKOVIČ, Marek - RUSANOV, B. - JANIČKOVIČ, Dušan - SIDOROV, V. - ŠVEC, Peter. Phase evolution clarification in Al-Ni-Co-RE amorphous alloys with varying. In MC 2021 Microscopic conference: Proceedings. - Vienna, Austria, 2021, p. 113.

CAGALINEC, Michal. Mitochondrial dynamics and calcium homeostasis in experimental models of Wolfram syndrome. Physiopathological Consequences of MAM Alterations in Diseases. 24. 9. 2021. UM, Montpellier, France.

2020:

K. FRÖHLICH, - M. MIKOLÁŠEK, - P.P. SAHOO, - K. HUŠEKOVÁ, - P. ONDREJKA, - V. ŘEHÁČEK, - L. HARMATHA. Preparation and performance of photoanode with thin RuO2- and IrO2-RuO2-based oxide electrocatalysts for water splitting Int. Conf. Functional Materials and Nanotechnologies, 23-26.11. 2020 Vilnius, Lithuania, on-line

2018:

E. MAJKOVÁ et al. Uniform assemblies of 2D nanosheets: formation, properties and applications.3rd Int. Conference on Nanomaterials: Synthesis, Characterization and Applications (ICN 2018), 11-13. 5. 2018 Kottayam, Kerala, India

2.3.8. List of researchers who served as members of the organising and/or programme committees

-

2.3.9. List of researchers who received an international scientific award

-

- **Position of individual researchers in the national context**

2.3.10. List of invited/keynote presentations at national conferences, as documented by programme or invitation letter

2019:

E. MAJKOVÁ.: Nanolayers prepared by physical vapor deposition. 21. School of vacuum technology. Strbske Pleso 2019.

2.3.11. List of researchers who served as members of organising and programme committees of national conferences

-

2.3.12. List of researchers who received a national scientific award

-

2.4. Research grants and other funding resources

(List type of project, title, grant number, duration, total funding and funding for the institute, responsible person in the institute and his/her status in the project, e.g. coordinator “C”, work package leader “W”, investigator “I”. Add information on the projects which are interdisciplinary, and also on the joint projects with several participating SAS institutes)

- **International projects and funding**

2.4.1 List of major projects of Framework Programmes of the EU (which pilar), NATO, COST, etc.

-

Add information on your activities in international networks

- **National projects and their funding, incl. international projects with only national funding**

2.4.2. List of ERA-NET projects funded from SAS budget

-

2.4.3. List of projects of the Slovak Research and Development Agency (APVV)

1. Nanotechnology preparation of a MIS photoelectrode with metallic oxides for systems for production of solar fuels, APVV-17-0169, 1.7.2018 / 30.6.2021, 250 000 Eur / 70 000 Eur for CEMEA, Karol Fröhlich.

2. Development of the bioactive silicon nitride by surface modification, APVV-18-0542, 1.7.2019 / 31.12.2022, 167 425 € / 34 000 € for CEMEA, Miroslav Hnatko.

3. Advanced Oxygen Tolerant Photochemically Induced Atom Transfer Radical Polymerization, APVV-19-0338, 1.7.2020 / 30.6.2024,250 000 Eur / 7552 Eur for CEMEA, Jaroslav Mosnáček.

4. Carbon-silicon based composite anodes for Li-ion batteries, APVV-19-0461, 1.7.2020 / 30.6.2024, 250 000 Eur / 150 000 Eur for CEMEA, Jaroslav Sedláček.

5. Towards lithium based batteries with improved lifetime, APVV-20-011, 1.7.2021 / 30.6.2025, 250 000 Eur / 72 254 Eur for CEMEA, Peter Šiffalovič

6. Nanomedical approach to fight pancreatic cancer via targeting tumorassociated carbonic anhydrase IX, APVV-20-0485, 1.7.2021 / 30.6.2025, 249 668 Eur / 69 742 Eur for CEMEA, Peter Šiffalovič

7. Development of unique TiMg composite dental implant, APVV-20-0417, 1.7.2021 / 30.6.2025, 249 908 Eur / 65 154 Eur for CEMEA, Eliška Švastová

8. Tribological properties of 2D materials and related nanocomposites, APVV-17-0560, 1.8.2018 / 30.6.2022, 249 599 Eur / 80 000 Eur for CEMEA, Milan Ťapajna

2.4.4. List of projects of the Scientific Grant Agency of the Slovak Academy of Sciences and the Ministry of Education (VEGA)

1. Use of photochemically induced radical polymerization with atom transfer in targeted surface modification, VEGA 2/0129/19, 1.1.2019 / 31.12.2022, 20582 €, Jaroslav Mosnáček.

2. Low energy synthesis of high performance NaSICON-like structured cathodes for rechargeable Sodium-Ion Batteries (SIBs) (Low energy synthesis of high performance NaSICONlike structured cathodes for rechargeable Sodium-Ion Batteries (SIBs). VEGA 2/0110/21, 1.1.2021 / 31.12.2024, 78 000 €, Gianmarco Taveri.

2.4.5. List of projects supported by EU Structural Funds

1. Building a centre for advanced material application SAS, 313021T081, 1.7.2019 / 30.6.2023, 1148851 €, Eva Majková

2.4.6. List of other projects funded from national resources

1. Reaction bonding of advanced SiC-based ceramics, Mobility SAV-AV ČR-21-04, 1.1.2021 / 31.12.2022, 351 €, Gianmarco Taveri

2.4.7. List of projects funded from private funds

-

2.4.8. List of projects funded from other competitive funds

-

2.5. PhD studies and educational activities

At the moment, CEMEA SAS v.v.i is not authorized to educate PhD students. We are working to become an external educational institution with the right to educate doctoral students.

2.5.1. List of accredited programmes of doctoral studies, period of validity, source of funding

-

2.5.2. Summary table on doctoral studies (number of internal/external PhD students at the end of the year; number of foreign PhD students, number of students who successfully completed their theses during the year, number of PhD students who quit the programme during the year*)*

PhD study	2016			2017			2018			2019			2020			2021		
Number of potential PhD supervisors																		
PhD students	number, end of year	defended thesis	students quitted	number, end of year	defended thesis	students quitted	unumber, end of yea	defended thesis	students quitted	number, end of year	defended thesis	students quitted	number, end of year	defended thesis	students quitted	number, end of year	defended thesis	students quitted
Internal total																		
from which foreign citizens																		
External																		
Other supervised by the research employees of the institute																		

2.5.3. PhD carrier path – Information on the next career steps of the PhD graduates who received their degree from the institute

-

2.5.4. Summary table on educational activities

Teaching	2016	2017	2018	2019	2020	2021
Lectures (hours/year)*	0	0	0	0	0	0
Practicum courses (hours/year)*	0	0	0	0	0	0
Supervised diploma and bachelor thesis (in total)	0	0	0	0	0	0
Members in PhD committees (in total)	0	0	0	0	0	0
Members in DrSc. committees (in total)	0	0	1	0	0	1
Members in university/faculty councils (in total)	0	0	0	0	0	1
Members in habilitation/inauguration committees (in total)	0	0	0	0	1	0

2.5.5. List of published university textbooks

-

2.5.6. Number of published academic course books

-

2.5.7. List of joint research laboratories/facilities with universities

-

2.5.8. Supplementary information and/or comments on doctoral studies and educational activities – focused on what changes have occurred since the last evaluation in 2016

CEMEA intends to become an external educational institution with the opportunity to train PhD students from the school year 2023/24.

2.6. Societal impact

2.6.1. The most important case studies of the research with direct societal impact, max. 4 for institute with up to 50 FTE researchers, 8 for institutes with 50 – 100 FTE researchers and so on. Structure: Summary of the impact; Underpinning research; References to the research; Details of the impact; Sources to corroborate the impact. One page per one case study

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2.6.2. List of the most important studies and/or other activities commissioned for the decision-making authorities, the government and NGOs, international and foreign institutes (title, name of institution, contract value, purpose (max 20 words))

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2.6.3. List of contracts and research projects with industrial and other commercial partners, incl. revenues (study title, name of institution, contract value, country of partner, purpose (max 20 words))

-

2.6.4.1 List of intangible fixed assets (internally registered IP (confidential know-how), patent applications, patents granted, trademarks registered) denoting background IPR

-

2.6.4.2 List of licences sold abroad and in Slovakia, incl. revenues (background IPR identification, name of institution, contract value, country of partner, purpose (max 20 words))

-

2.6.5. Summary of relevant activities, max. 300 words (describe the pipeline of valorization in terms of Number of disclosure, Number of registered IP internally, number of CCR/LIC contracts and their respective summary values, the support you are receiving in specific points internally at the institute, at SAS, externally – also the limitations and drawbacks.

CEMEA is a member of the **Slovak Battery Alliance** (SBaA) since its establishment in 2019. CEMEA has a representative in the Alliance presidium. The goal of the SBaA is to promote Slovak battery production and to assist in the development of a comprehensive battery chain in Slovakia, from the mining of raw materials to battery regeneration and recycling. Research activities of CEMEA are concentrated mostly on the application of new materials for the next generation of batteries. By membership in the SBaA, CEMEA has direct contact to all important players in the battery business in Slovakia.

CEMEA has signed **Memorandum of Understanding** with Automotive Industry Association of the Slovak Republic (ZAP), Slovak Electrical Vehicle Association (SEVA) and company Innobat. Memorandum of understanding determines the main directions for future collaboration between CEMEA, associations and company Innobat.

2.7. Popularisation of Science (outreach activities)

2.7.1. List of the most important popularisation activities, max. 20 items

Appearance in television:

- Martin Balog - The experiment program on TV channel Dvojka “Materials and medicine – the implants”
- Karol Frohlich: 15.07. 2021 13:30: Future of batteries for electrical vehicles. Discussion on future of batteries for electrical vehicles, TV TA3.

Podcast:

- Podcast “Na plný prúd”: https://podcasts.google.com/feed/aHR0cHM6Ly9hbmNob3IuZm0vcy9lMjJjZTc0L3BvZGNhc3QvcnNz/episode/YWI1N2JmZjAtZTg5OC00NzA2LWFmOTMtZDRhN2YzZTA0YzE5?sa=X&ved=0CAUQkfYCahcKEwjQ9_Knt4XuAhUAAAAAHQAAAAAQAQ
- Scientific Podcast of Slovak Academy of Sciences: https://www.sav.sk/?lang=sk&doc=services-news&source_no=71&news_no=10233

Web:

- In 2020 in collaboration with Media Planet company we have prepared leaflets for advertising research program of CEMEA. The title of the leaflets was:

  1. Surface modification for advanced batteries. (https://www.info-lifestyle.sk/technologie-a-inovacie/efektivne-uchovanie-vyrobenej-energie-povrchova-uprava-materialov-pre-pokrocile-baterie/)

  2. Development of advanced biomaterials. (https://www.info-lifestyle.sk/technologie-a-inovacie/vyskum-progresivnych-biomaterialov-inovacie-pre-biomedicinu-a-biotechnologie/)

The leaflets were distributed using internet media (Facebook) or as printed documents.

Public popularisation lectures:

2.7.2. Table of outreach activities according to institute annual reports

Outreach activities	2016	2017	2018	2019	2020	2021	total
Articles in press media/internet popularising results of science, in particular those achieved by the Organization	x	0	0	0	0	0	0
Appearances in telecommunication media popularising results of science, in particular those achieved by the Organization	x	0	0	0	0	0	0
Public popularisation lectures	x	0	0	0	0	0	0

2.8. Background and management. Infrastructure and human resources, incl. support and incentives for young researchers

2.8.1. Summary table of personnel

2.8.1.1. Professional qualification structure (as of 31 December 2021)

	Degree/rank				Research position		
	DrSc./DSc	CSc./PhD.	professor	docent/ assoc. prof.	I.	II.a.	II.b.
Male	7	28	0	1	8	10	17
Female	2	14	0	2	3	4	10

I. – director of research with a degree of doctor of science/DrSc.

II.a – Senior researcher

II.b – PhD holder/Postdoc

2.8.1.2. Age and gender structure of researchers (as of 31 December 2021)

Age structure of researchers	< 31		31-35		36-40		41-45		46-50		51-55		56-60		61-65		> 65	
	A	B	A	B	A	B	A	B	A	B	A	B	A	B	A	B	A	B
Male	2,0	0,8	9,0	8,2	4,0	3,1	7,0	4,2	8,0	3,9	0,0	0,0	4,0	1,6	1,0	0,1	2,0	1,1
Female	0,0	0,0	5,0	4,3	5,0	3,6	2,0	1,0	1,0	0,5	0,0	0,0	0,0	0,0	2,0	0,6	2,0	1,5

A – number

B – FTE

2.8.2. Postdoctoral fellowships (list of positions with holder name, starting date, duration. Add brief information about each fellow's career path before and after receiving PhD degree, etc.)

2.8.2.1. MoRePro and SASPRO fellowships

-

2.8.2.2. Stefan Schwarz fellowships

-

2.8.2.3. Postdoctoral positions from other resources (specify)

-

2.8.3. Important research infrastructure introduced during the evaluation period with the information about the sources of funding *(max. 2 pages)*

The aim of the CEMEA project is to stimulate multidisciplinary research and motivate deeper cooperation of project partners, to create a model "open access" approach to the consortium's research infrastructure and to create a platform for formulating coherent research plans. A Memorandum of Understanding was signed between the partners, which defined the basic framework of cooperation and CEMEA SAS as an institutional platform within which the partners want to operate and cooperate according to the agreed competencies and rules.

As part of CEMEA project, infrastructure modernization was planned, while CEMEA SAS has signed a contract for the supply of several major equipment and a number of small devices that will certainly contribute to increasing the quality of scientific results at CEMEA SAS and partners' SAS institutes. The total number of purchased devices is more than 100 with a total value of over 16 million euros.

The important devices we consider:

- **Mass cytometer with imaging system** - device used to monitor the influence / effect of specific inorganic nanomaterials on biological mechanisms / signaling pathways in tumor cells and their interactions with immune cells of the tumor microenvironment in 3D models (using tested advanced materials, e.g. bone substitutes, trabecular structures and other porous / adhesive biomaterials) in humanized mouse models in in vivo studies. It will also be used to reveal the effect of nanomaterials on individual types of tumors. (~1.891.000, -eur)

- **X-ray photoelectron spectrometer with UPS and cluster cannon** - compact device for X-ray photoelectron (XPS) and ultraviolet (UPS) photoelectron spectroscopy with sources of monochromatic X-rays as well as Ar ions and clusters with high-resolution spectrometer for precise surface point (line) mapping and in-depth qualitative and quantitative analysis of the chemical composition of solid electrically conductive and non-conductive solid materials and thin films, including complete control, analytical and evaluation software. (~1.061.000, -eur)

- **Hybrid hot press combined with electric field sintering technology -** the device is designed for sintering ceramic and composite materials using years of proven hot pressing technology in combination with the latest and most modern electric field sintering technology. (~1.058.000, -eur)

- **Scanning FTIR microscope operating in near-field mode -** the device allows co-localization of surface morphology with their infrared absorption spectra with a spatial resolution better than 10-20 nm. (~860.000, -eur)

- **Ultra-fast scanning power microscope combined with an inverted confocal microscope -** ultra-fast scanning power microscope combined with an inverted confocal microscope. The scanning force microscope allows fast in-situ measurements in a liquid directly in an inverted confocal microscope. (~756.000, -eur)

- **High-temperature non-graphite vacuum furnace with resistance heating** - the device is designed for free (pressureless) sintering of ceramic and composite materials at temperatures of at least 1800 ° C. (~681.000, -eur)

- **Device for the application of thin layers on particles -** the device uses the technology of application on atomic layers and will be used for the application of thin layers of oxides on metal and ceramic particles of micrometer dimensions. Thanks to the use of Fluidized bed reactor technology (particles are buoyed by the gas stream) and mechanical vibration, the device enables the preparation of homogeneous thin films on submicrometer particles. The coated particles will be used for the preparation of skeleton composites with a metal matrix (Al, Mg, Ti) with unique properties as well as for the preparation of new types of ceramic materials. This is a unique device that is not yet available in Slovakia (~623 000, -eur).

- **Vacuumable FTIR spectrometer -** a device for optical analysis of samples from a wide range of wavelengths. (~511 000, -eur)

- **Vacuumable tribometer -** a device for measuring tribological properties (friction, wear, lubrication) using the "pin-on-disk" or "ball-on-disk" method, while the measurement itself takes place in a vacuum chamber, which also allows controlled filling of the working gas. (~419 000, -eur)

- **Equipment for 3D printing of ceramic components** - equipment for the preparation of 3D structures from materials based on ceramics and metals using lithographic technology. (~377 000, -eur)

- **Optical profilometer -** the device enables hte mapping of morphology and thickness of organic and inorganic thin films by an optical method. The specificity of the device is the mapping of roughness in the area below 0.1 nm on large areas up to 10 cm. (~376 000, -eur)

- **Vapor deposition system -** a device for the deposition of thin metal layers (units up to tens of nanometers) by the method of vacuum vapor deposition using the evaporation of material with an electron beam. The device will be used for the application of functional and contact metal multilayers of various metals, including refractory metals. (~372 000, -eur)

- **Scanning probe microscope** - device for measuring resp. 2-dimensional mapping of the sample surface in the lateral range of nanometers to micrometers with vertical resolution at the sub-nanometer level. (~352 000, -eur)

- **System for simulation and modeling of physical processes** - a system based on the finite element method will be used for simulation and modeling of physical processes in the preparation and interpretation of the properties of thin films and thin-film structures. The use of software based on the finite element method will make it possible to predict the properties of the prepared structures and compare them with experimental data. The basic equipment is supplemented by modules for calculations of structural mechanical quantities, heat transfer, design module, module for simulation and modeling of fatigue of materials and components, multiparticle module, acoustic module, etc. (~256 000, -eur)

- **Ellipsometer for measuring the thickness of layers on the device for application on atomic layers** - the device is designed for measuring the thickness of thin layers prepared by the method of application on atomic layers. Thin-film structures are designed for the decomposition of water by the action of solar radiation. The device will be located on the inlet chamber of the Beneq TSF 200 and is able to measure thickness without interrupting the working vacuum. The device is able to measure layer thicknesses up to 1000 nm (~149 000, -eur).

- **Potentiostat** - the device will be used to measure basic electrical properties such as. impedance spectroscopy of Li-based thin-film structures for electrodes of new types of batteries (~76,000).

Reconstruction of 2 buildings

We also consider the fact that two ground-floor buildings, which are in an extremely poor technical condition, will be reconstructed as part of the CEMEA project. According to the call, the buildings will be primarily used as laboratories for new infrastructure, the necessary rooms for service staff and evaluation rooms for researchers using specific equipment. The total investment for the reconstruction of buildings and other workspaces is a total of approximately five million euros.

2.9 Supplementary information and/or comments on all items 2.1 – 2.8 (max. 2 pages in total for the whole section)

The Center for Advanced Materials Application (CEMEA) was founded by the Slovak Academy of Sciences (SAS) in 2017. CEMEA started to operate in 2019 after receiving project support from the Research Agency. Thanks to a close partnership with six founding institutes of SAS (Inst. Phys, Inst. Electrical Eng., Inst. Mater. Machine Mechanics, Inst. Inorg. Chem., Polymer Inst. and Biomed Res. Center), the research conducted in CEMEA is multidisciplinary. From the very beginning, the collaboration with the SAS institutes leads to publications in high-ranking international journals.

Since 2019, when the project was approved by the research agency, CEMEA has hired new employees. Some of the employees have been employed jointly with the SAS founding institutes on a part-time basis to maintain contacts and develop a joint research strategy. More than 50% of the employees were hired from abroad, mainly from third-world countries such as India, Pakistan, and Iran. Unfortunately, the recruitment of new employees from abroad was hampered by the COVID pandemic. However, in 2021 and 2022, we have attained an almost complete number of employees. Some of these new employees have achieved good research results, and we would like them to stay for the next period.

An important mission of CEMEA in the period since the beginning of Structural Funds support has been the procurement of research infrastructure worth as much as 15 million euros. Unfortunately, public procurement in Slovakia is a very complicated process and requires a lot of effort. Nevertheless, after almost three years of the administrative process, the delivery of the research infrastructure has already started in 2022.

Even more complex still appears to be the reconstruction of two buildings planned as part of the Structural Funds project. The total cost of reconstructing the buildings is about 7 million euros. Similar to the research equipment also, the planned reconstruction of two buildings requires a high personnel effort.

Within just a few years of its existence, CEMEA has become the leading institution in the field of battery research in Slovakia. CEMEA has the ambition to coordinate not only national but also international projects within the HORIZON EUROPE program. In 2021, CEMEA participated in 8 national projects (APVV) and received support for 5 projects from VEGA.

CEMEA was particularly active in the field of battery technology. This topic is relatively new and was not covered by any SAS institute. In this field, CEMEA has stimulated the establishment of the National Battery Center. Therefore, we believe that the National Battery Center can apply for support under the Slovakia's Recovery and Resilience Plan.

The unique research focus of the materials-research oriented community within CEMEA and the biomedical oriented groups of the Biomedical Center SAS on advanced biomaterials research is very promising. We believe that this direction will lead to several new discoveries and offers good prospects for future research.

3. ***Implementation of the recommendations from the previous evaluation period***

CEMEA was not evaluated in the previous evaluation period

4. ***Research strategy and future development of the institute for the nextfive years*** (Recommended 3 pages, max. 5 pages)

Research strategy of the institute in the national and international contexts, objectives, and methods (including the information on when the strategy was adopted)

The research strategy and future development of the Institute in the next five years are aimed at future developments in the areas of battery technology, materials for biomedicine and advanced materials/nanomaterials. In the following text, we will describe basic ideas of how the research will be developed in the next five years.

1. Future developments in the field of battery technology.

Future developments in battery technology will focus on improving the performance of Li-ion batteries, developing new generations of Li-ion batteries such as Li-S and solid electrolyte Li-ion batteries, and developing batteries beyond Li-ion.

Improvement of performance of Li-ion batteries covers the following topics:

- Development of a silicon/graphite anode for Li-ion batteries. The incorporation of silicon particles into the graphite anode increases its capacity, however volumetric changes of the silicon particles during lithiation/delithiation of the anode lead to mechanical instability. We intend to solve this problem by using self-healing binders.
- Modification of the electrode surface by atomic layer deposition (ALD). The application of ultrathin oxide layers (Al_2O_3, ZnO and TiO_2) increases the cycling stability and C-rate capability of lithium-ion batteries. We aim to determine what type of oxide films and what parameters are required to improve the performance of lithium-ion batteries.

Development of new generations of Li-ion batteries comprises:

- Improvement of the performance of Li-S battery. Li-S battery suffers from dissolution of sulfur cathode, which leads to capacity degradation and poor cycle life. We aim to stabilize the capacity and lifetime of Li-S batteries by employing an ultra-thin interfacial layer prepared by means of ALD. The goal of this activity is to determine appropriate film composition and thickness.
- Development of all-solid-state Li-ion batteries (SSBs). Li-ion batteries with solid-state electrolytes can achieve high energy density and safety. We intend to direct our activities towards improved mechanical stability of electrode/solid-electrolyte composites. Interfacial modification by ALD can potentially stabilize ionic conductivity at solid-electrolyte/cathode interfaces.

Development of batteries beyond Na-ion system.

- Na-ion battery is one of the promising candidates. Sodium-based batteries offer a combination of attractive properties, i.e. low cost, sustainable chemistry and secure raw material supply. We aim to develop a Na-ion battery using NASICON (sodium super ionic conductor) type material, which serves as a cathode but also as a solid-state electrolyte.

Development of advanced characterization techniques for SSBs:

Unlike conventional batteries with liquid electrolytes, SSBs are subjected to significant stresses during battery cycling due to the substantial change in volume of the redox-active materials used in cathode and anode materials. Consequently, mechanical stresses can lead to premature aging due to loss of physical contact between the redox-active and solid-electrolyte or electron-conducting materials. To mitigate these problems, developing specific analytical techniques to track the stress fields during lithiation/delithiation is essential. We have already agreed to collaborate on this topic at the EU level (M-ERA.NET project), focusing on the characterization of stress fields with synchrotron radiation. In addition, we have also been awarded a smaller project with the Massachusetts Institute of Technology, USA (MIT) that also addresses this heavily studied topic.

In the upcoming period, we will concentrate on the following two experimental techniques that can be used to study the mechanical stresses in SSBs.

- Development of special Raman cells for SSBs. This cell will allow stresses to be imaged using a standard confocal Raman microscope with a spatial resolution down to 1 mm. However, this technique will only monitor phase/stress changes in the volume just below the surface.
- Development of a synchrotron-grade cell for wide- and small-angle X-ray scattering (WAXS/SAXS). This cell will use a highly focused X-ray beam that allows spatial resolution below 100 nm. This will be done in collaboration with the University of

Leoben, Austria (group of Prof. J. Keckes). In contrast to the Raman cell, the stress information provided by this type of cell will also be sensitive to changes in bulk.

Developing novel rechargeable batteries with high energy storage capacity and recycling technology remains a major scientific and technological challenge. CEMEA-SAV has made complementary efforts to achieve a better fundamental understanding of the chemical and electrochemical properties of hybrid inorganic-organic materials for batteries. As a logical extension of these efforts, CEMEA proposes a new class of high-energy battery electrodes comprising functional nanostructured polymers with ultra-high-capacity inorganic particles for next-generation high-performance metal-ion/air batteries, along with a new approach to battery materials reuse. In view of this extension, we will focus in the coming period on the synthesis and fabrication of novel battery electrode systems from high-performance polymers that synergistically integrate nanostructured conductive media and electrochemical catalysts to address the fundamental challenges faced by metal-air batteries using ionic liquids.

CEMEA proposes a new concept of solid-state metal-ion batteries by fabricating a single phase for the anode, electrolyte, and cathode, and thus, eliminating the highly resistive interfaces between the battery components found in conventional SSBs. In this part, efforts will be focused on developing ionic conductive separators based on innovative functionalized polymeric substrates with tunable surface area and very low surface tension. Although metal-air batteries offer high energy capacities, expensive platinum-based catalysts are required for oxygen reduction and oxidation reactions. The use of metals, metal oxides, and/or metal-free bifunctional electrochemical catalysts for metal-air batteries is another approach of CEMEA to develop rechargeable metal-air batteries. In this part, CEMEA focuses on two primary research approaches (1) using hydrothermal technology as green chemistry to produce metal oxides and (2) synthesizing heteroatom-doped anthraquinone-based bifunctional electrochemical catalysts.

Replacing lithium and cobalt in Li-ion batteries would result in a more environmentally and socially responsible technology. Battery recycling has been challenging because materials with similar properties had to be isolated and extracted. Instead of separating and sorting the individual elements, CEMEA proposes a new approach to battery materials reuse to synthesize new composite materials with high potential.

Metal-air batteries are considered candidates for a new generation of energy storage systems that have the potential to replace or complement the Li-ion batteries used every day. Aluminum (Al)-air batteries seem to be a suitable candidate due to the low cost, availability, and recyclability of aluminum. We propose two solutions to suppress the corrosion and passivation of the porous Al anode: i) replacement of pure Al powder with Al alloys containing Sn, Zn and Mg as starting materials for the porous anode production, ii) use of anhydrous electrolytes. Currently, corrosion and electrochemical studies are being conducted on ethaline (a eutectic mixture of choline chloride and ethylene glycol) as a potential electrolyte for an Al-air battery. Pilot tests show higher corrosion resistance of Al compared to ethaline, but the primary battery exhibits lower initial voltage as well as low discharge currents. By optimizing the composition of ethaline, we aim to achieve the above parameters while maintaining the high corrosion resistance of Al.

Another important area is the recycling of used batteries. Pyrometallurgy or hydrometallurgy are typical recycling methods for recovering active materials from Li-ion batteries. We intend to develop bioleaching to recover metals from used batteries using bacteria.

Battery technology offers plenty of scope for research developments. We have indicated several research activities that could contribute to development in this field. Depending on funding opportunities, we will be involved in some of the activities described and thus contribute to future scientific development and its impact on society.

2. Future developments in materials for biomedicine and advanced materials/nanomaterials.

Targeted drug application is among the main areas where nanotechnology can contribute, in a revolutionary way, to more effective treatment of various diseases, including cancer. Inorganic nanomaterials represent promising diagnostic and therapeutic systems of modern medicine. Their use implies more precise diagnostics as well as a possibility of targeted therapy (nanovectors) which would mean a significant improvement, especially in the treatment of oncological diseases. Progress in identifying specific oncomarkers allows the development of a new generation of nanodrugs. Attachment of specific molecules such as aptamers, proteins, peptides, and small molecules to nanoparticles facilitates their selective recognition and interaction with tumor cells. The development of multifunctional nanomaterials carrying a therapeutic substance, the accumulation of which can be concurrently and easily monitored in a tumor, thus enabling the identification of a disease stage, represents the basis of so-called theranostics.

To prepare selective, tissue-specific nanoparticles for theranostics, it is necessary to elucidate laws that determine the increased affinity of nanomaterials to separate organs/tissues. Despite a considerable progress achieved in this area, the questions of the nanomaterials safety for human health have not been sufficiently answered and explored yet, which hampers their clinical application. Thanks to their features, gold nanoparticles appear as an ideal candidate for theranostics as they do not show acute toxicity and their unique optical properties allow excellent monitoring of their presence in the body. Intensive research concentrates especially on the acute toxicity of gold nanomaterials; however, not enough attention is paid to the long-term effects connected with their accumulation in the organism. Although gold nanoparticles are currently considered the safest metal nanoparticles, their toxicity was shown several times. Therefore, our research will aim at chronic tissue exposure to gold nanoparticles, which results from the accumulation of therapeutic nanoparticles. Besides the long-term biological effects of gold nanoparticles accumulated within tissues, our study will generate novel data about the transport, distribution and accumulation of gold nanoparticles in the organism and data about their elimination from the body. The acquired knowledge will contribute to a more efficient development of a new generation of nanotherapeutic agents and their smoother introduction into clinical practice.

The majority of nanomaterials need to be conjugated with organic molecules or/and biomolecules before their possible use in biomedicine, imaging or theranostics. Attachment of organic ligands to the nanoparticle surface can influence the stability and biocompatibility of a nanoparticle complex. Moreover, it also enables the binding of therapeutic substances. In the treatment of liver disease, conventional therapy fails due to the inability to deliver adequate drug concentrations to the organ. Au nanoparticles with an average of 20 nm have the ability of a long-term accumulation in the liver. We aim to investigate in vivo anti-fibrotic effect of silibinin bound to gold nanoparticles via polyethylene glycol. This is an example of passive targeting when drug carriers accumulate in target tissues based on their physical and chemical properties. Conjugation with functional biomolecules (enzymes, peptides, antibodies) represents a way how to empower nanocomplexes with advanced functions and unique features. Active targeting relies on a biological interaction between a targeting agent located on the surface of functionalized nanoparticles and a specific receptor/protein existing on the surface of tumor cells. In our national projects and in the framework of the international collaboration with LVTS - SMBH - INSERM U1148 (Université Sorbonne Paris Nord), we will focus on the interaction between antibody and antigen and on the functionalization with tumor-targeting peptides (RGD - sequence Arg-Gly-Asp), while the subjects of the modification are newly discovered low-dimensional nanomaterials - MXenes and MoO_x. Thanks to the very efficient conversion of light energy to heat, they are considered promising candidates for drug delivery, diagnostics, imaging, and photothermal nanotherapeutics. Photothermal therapy leads to efficient conversion of light to heat and consequently to ablation of tumor cells (localized hyperthermia) while healthy cells remain undamaged. The key to an effective anti-tumor treatment seems to lie in synergic use of active targeting via a specific tumor marker together with therapeutic approaches that are strictly spatially localized and minimally invasive. Our research will focus on using these innovative nanomaterials in theranostics for targeted therapy of hypoxic tumors. We will concentrate mainly on plasmon nanoparticles functionalized by antibody recognizing CAIX protein which is strongly associated with aggressive hypoxic tumors and is almost exclusively present on the surface of tumor cells. Functionalizing plasmon NPs with an anti-CAIX antibody increases the specificity of a drug being developed and its accumulation within tumors, which should also reduce adverse effects in healthy organs. Our selected nanomaterials based on MoO_x and MXenes display photothermal properties and thus can be used for photothermal therapy. In addition, these innovative nanomaterials represent nanoplatforms that can be functionalized by various substances. Hence they may become a diagnostic tool, detectable by standard imaging methods (MRI, CT), and a therapeutic tool. Moreover, we want to expand the use of targeted therapy via tumor-specific CAIX recognition to the preparation of oxazoline micelles that can carry commonly used chemotherapeutic drugs inside them. This targeted delivery at the tumor site can reduce a used therapeutic dose and their adverse side effects, which is a significant benefit for a patient in case of treatment with chemotherapeutics. Furthermore, oxazoline micelles can be used as a packaging for other potential therapeutics and their combinations, such as a specific inhibitor of the enzymatic activity of CAIX, which can decrease extracellular acidosis – as an important factor of aggressive tumor microenvironment. In our approaches, we will test the combined antitumor therapy based on the targeting of aggressive TME through CAIX antibody conjugated with oxazoline spheres enveloping other therapeutic drugs like i, cytokine / chemokine network inhibitors; ii, conventional systemically administered chemotherapeutics, iii, immune-checkpoint inhibitors (anti-PD1 antibodies, anti-CTLA4 antibodies, etc.). In addition, we want to focus on the use of antigen-specific delivery of nanomaterials (Fe_2O_3, gadolinium, etc.) applicable in the early detection of cancer using common screening imaging methods e.g. MRI. Finally, we are working on innovative approaches to track proteins in dense media similar to intracellular space. Together with German, Swedish, and French teams, we submitted a proposal to the European XFEL addressing dynamics, interactions and aggregation phenomena in protein solutions.

In the area of novel metallic materials for biomedical applications, we intend to focus our R&D activities in the near future primarily on Zn-based+ZnO MMC:

- The positive effect of ZnO dispersoids on creep and fatigue performance of $Zn^{+}ZnO$ MMC.
- Indirect in-vitro biological evaluation assay in DMEM medium of selected cultured cells.
- Microstructure and chemistry optimization of Zn matrix by selecting suitable fine alloyed Zn powders in order to meet the requested characteristics for biodegradable endovascular stents and internal orthopedic fixators while maintaining stability, as confirmed in a case study for pure $Zn^{+}ZnO$ MMC.

Furthermore, we aim to explore the possibility of TiMg MMC fabrication with an extremely low Young`s modulus, which significantly minimizes the stress-shielding effect by using so-called “gum-metal” TNTZ alloys, specifically TiTa alloy matrix.