CIC 2021

# 3rd Coatings and Interfaces Conference

24–26 NOVEMBER 2021 | ONLINE

**Abstract Booklet**

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# *3rd Coatings and Interfaces Conference*

VIRTUAL

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## Welcome from the Chairs

Dear colleagues,

It is our pleasure to invite you to the 3rd Coatings and Interfaces Conference (CIC2021). Following the two very successful electronic editions of this conference series, we are pleased to announce that CIC2021 will hold its 3rd edition virtually, allowing attendees to actively engage in discussions about the latest findings in the field. The event will take place on 24–26 November 2021.

The impact of coatings and interfaces in technology is growing at an unprecedented pace. Energy, sustainable mobility, pollution control, critical raw materials, preservation of cultural heritage, control of materials degradation, food safety, and health science are all challenges that critically depend on our capability to engineer surfaces. The aim of the CIC2021 is to give scientists and professionals a unique opportunity to keep up with this quickly evolving field, by providing a comprehensive overview of the latest findings regarding the fundamentals and application of coatings and interfaces.

CIC2021 will bring together scientists and technologists from academia and industry, encouraging the involvement of excellent early-stage investigators. Participation in and "attendance" to the CIC2021 are FREE of charge. Participants will have the opportunity to share their most recent findings with a focus on the following areas of Coatings and Interface Science and Technology:

- Coatings for mitigation of corrosion, wear, and erosion;
- Bioactive coatings, surfaces, and interfaces;
- Advances in coating deposition and surface functionalization;
- Coatings for food packaging and preservation;
- Coatings and interfaces in cultural heritage conservation and preservation.

A Coatings Special Issue dedicated to the conference will be open to the submission of selected outstanding contributions.

We look forward to your participation!

On Behalf of the Organizing Committee

The Conference Chair
Dr. Alessandro Lavacchi

**Certificate of Attendance**

Upon request, the participants of the event will receive an electronic Certificate of Attendance by email once the event is concluded.

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# General Information

*Coatings* (ISSN 2079-6412; CODEN: COATED) is an international, peer-reviewed and open access journal devoted to the science and engineering of coatings, thin and thick films, surfaces and interfaces. Coatings publishes original research papers and brief communications that report on the latest finding of research together with review papers that systematize the remarkable points on the state of the art. The Korean Tribology Society (KTS) is affiliated with Coatings and its members receive discounts on the article processing charges.

Journal Webpage: https://www.mdpi.com/journal/coatings
Impact factor: **2.881** (2020)
5-Year Impact Factor: 3.038 (2020)

Program

## Program at a Glance

| Wednesday<br>24 Nov. 2021 | Thursday<br>25 Nov. 2021 | Friday<br>26 Nov. 2021 |
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| **Break** | **Break** | **Break** |
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# Conference Program

## Day 1 - Wednesday, 24 November 2021

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|---|---|---|
| **12:00 - 12:05 (CET)** | **Welcome from the Organizers -** MDPI | |
| **12:05 - 12:15 (CET)** | **Welcome from the Chairs -** Dr. Alessandro Lavacchi, Prof. Dr. Massimo Innocenti | |
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| 13:00 - 13:30 | **Prof. Dr. Monica Santamaria**<br>University of Palermo, Italy | *Improvement of Corrosion Resistance of Light Alloys by Electrochemically Grown Coatings* |
| 13:30 - 14:00 | **Dr. Jesús Manuel Vega**<br>CIDETEC, Basque Research and Technology Alliance (BRTA), Donostia-San Sebastián, Spain | *Tribocorrosion Performance of Different Ni-Based Coatings: Ni/B by Electrodeposition and Multilayer Ni/P (Low Content) By Electroless* |
| **14:00 - 15:30 (CET)** | **Break** | |
| **15:30 - 16:30 (CET)** | **S4. Coatings for Food Packaging and Preservation**<br>**Session Chair: Prof. Dr. Stefano Farris** | |
| 15:30 - 16:00 | **Prof. Dr. Lluís Palou**<br>Valencian Institute of Agrarian Research (IVIA), Valencia, Spain | *Postharvest Disease Control and Quality Maintenance of Fresh Fruits and Vegetables by Antifungal Edible Coatings* |
| 16:00 - 16:30 | **Prof. Dr. Isabel Coelhoso**<br>Universidade Nova de Lisboa, Portugal | *Prickly Pears Bioactive Compounds Preservation by Edible Coatings* |

## Day 2 - Thursday, 25 November 2021

| | | |
|---|---|---|
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| 12:30 - 13:00 | **Prof. Dr. Yong Lei**<br>The Palace Museum, China | *The Identification of Green Pigments in Chinese Paintings* |
| 13:00 - 13:30 | **Dr. Francesca Gherardi**<br>Investigative Science Team, Historic England, Portsmouth, UK | *Nano Meets Heritage: Nanomaterials for the Conservation of Historical Buildings and Artworks* |
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| 15:05 - 15:10 | **Rubén del Olmo**<br>sciforum-052115 | *Wear Resistant Surface Treatments for Additively Manufactured Al10Si1Mg Alloy* |
| 15:10 - 15:15 | **Serdar Sonay Özbay**<br>sciforum-052272 | *Ion Release Measurements of Cu/Ag-TiN-Based Antibacterial Coatings on Textiles Deposited by Magnetron Sputtering* |
| 15:15 - 15:20 | **Lara Moreno**<br>sciforum-052065 | *Bioactive PEO Coatings for Al-free Mg Systems: Mg-Ca, Mg-Ca-Ag, Mg-Zn-Ca Alloys* |
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## Day 3 - Friday, 26 November 2021

| | | |
|---|---|---|
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| 13:00 - 13:30 | **Dr. Sara Ferraris**<br>INSTM and Politecnico di Torino, Italy | *Surface Modification of Bioactive Materials With Natural Molecules* |
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| 15:30 - 16:00 | **Dr. Kelsey Stoerzinger**<br>Oregon State University, USA | *Epitaxial Oxide Thin Films: New Insight Into Electrocatalysis and Corrosion* |
| **16:00 - 16:45 (CET)** | **Closing Plenary Talk**<br>**Prof. Dr. Giovanni Zangari**<br>University of Virginia, Charlottesvile, USA | *Materials, Coatings, and Energy in the time of COP26* |
| **16:45 - 17:00 (CET)** | **Chairs Closing Remarks -** Dr. Alessandro Lavacchi, Prof. Dr. Massimo Innocenti | |

## What is Sciforum?

Sciforum is an event planning platform that supports open science by offering the opportunity to host and participate in academic conferences. It provides an environment for scholarly exchange, discussion of topics of current interest, building of networks and establishing collaborations.

## The Benefits of Sciforum

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# Sessions

S1. Coatings for Corrosion Wear and Erosion Mitigation
S2. Bioactive Coatings, Surfaces and Interfaces
S3. Advances in Coatings Deposition and Surface Functionalization
S4. Coatings for Food Packaging and Preservation
S5. Coatings and Interfaces in Cultural Heritage Conservation and Preservation

# Abstracts

## Plenary Speakers

# Sciforum-055281: Materials, Coatings, and Energy in the time of COP26

Giovanni Zangari[1]

[1] Department of Materials Science and Engineering, University of Virginia, Charlottesvile, USA

Researchers working on materials and energy today have currently a tall order, no less than restoring the climate and reversing the land used during the industrial revolution. Currently, several technologies are available to abate the greenhouse gases, and emissions in the EU decreased by 20% in 2020. On the other hand, energy efficiency and decarbonization rates need to be strengthened. Raw materials, the energy required to processing and the greenhouse generated are correlated, making it is necessary to increase resource efficiency, recycling, and reuse.
In this context, I will try to discuss the most important technologies, their characteristics, and the relative importance of each. In particular, I will discuss electrochemical energy conversion, their relevance, including some emergent processes. Finally, I will discuss unconventional physical processes that could be used to generate electricity.

# Abstracts

## S1. Coatings for Corrosion Wear and Erosion Mitigation

## Invited Speakers

# Sciforum-054979: Improvement of Corrosion Resistance of Light Alloys by Electrochemically Grown Coatings

Monica Santamaria[1], Andrea Zaffora[1], Danilo Virtù[1], Davide Pupillo[1], Francesco Di Franco[1]

[1] Università degli Studi di Palermo, Dipartimento di Ingegneria, Viale delle Scienze, 90128 Palermo, Italy

Light metals and light alloys have low density and high strength-to-weight ratios. They are generally characterized by low toxicity in comparison to heavy metals, and include aluminium, magnesium, and titanium alloys. Light metals and alloys can form native oxide films on their surfaces that offer only limited protection to corrosion, thus it is often necessary to carry out surface treatments aimed to improve their resistance in aggressive environments.
Anodizing and hard anodizing are among the most used surface treatments to enhance the corrosion resistance of light metal alloys. They are both electrochemical processes that allow the growth of an oxide layer on the surface of metals, whose compositional and morphological features greatly depend on the process operating conditions, such as applied voltage/current density, electrolyte temperature and composition. Anodic oxide can be further functionalized for tailoring the physico-chemical properties of the material in view of the target application.
In this work, we discuss the effect on corrosion resistance of oxides layers grown by anodizing or hard anodizing of three selected light metal alloys, i.e., AA5083 aluminium alloy used for ship building, AZ31 magnesium alloy proposed for the fabrication of biodegradable implants, and Ti-6Al-4V alloys for orthopaedic implants.
Anodizing of AA5083 alloy was carried out in a tartaric and sulfuric acid solution at 37°C. Corrosion resistance was investigated by corrosion potential measurements and by electrochemical impedance spectroscopy (EIS) in 3.5% NaCl aqueous solution soon after anodizing, as well as after the electrodeposition of a superhydrophobic layer on top of the anodic oxide grown to reduce the contact time between the material and the aggressive environment.
Anodizing of AZ31 was carried out in a hot glycerol based electrolyte with the aim to influence the Pilling Bedworth ratio of the anodic layer and thus its adhesion to the alloy beneath. Corrosion resistance was investigated in simulated body fluid at 37°C by corrosion potential measurements and by EIS. Accurate evaluation of the hydrogen evolution was obtained by a method based on the measurement of the hydrostatic force resulting from the accumulation of hydrogen in a submerged container. In vitro studies were carried out to evaluate the cytocompatibility of the anodized AZ31 samples.
Cast and additive manufactured Ti-6Al-4V alloys were anodized in calcium acetate glycerophosphate aqueous solution to induce the growth of a porous oxide layer suitable to favor the formation of hydroxyapatite and thus to improve osteointegration. The anodizing process was optimized taking into account the different microstructure of alloy as a function of the production process. Corrosion resistance was investigated in simulated body fluid at 37°C by corrosion potential measurements and by EIS.

## Invited Speakers

# Sciforum-052259: Tribocorrosion performance of different Ni-based coatings: Ni/B by electrodeposition and multilayer Ni/P (low content) by electroless

Jesús Manuel Vega[1], Maria Lekka[1], Asier Salicio-Paz[1], Eva García-Lecina[1]

[1] Fundacion CIDETEC

Hard chromium coatings are characterized by their superior mechanical and tribological properties. Despite having cracks which worsen the corrosion resistance, it is used (with oil as a lubricant) in a wide range of industrial (e.g., hydraulic cylinders) and engineering applications (e.g., landing gears). However, such coatings are obtained from hexavalent-based baths which are known by their toxic and carcinogenic impact. Therefore, sustainable alternatives are needed to substitute them to fulfill the regulation given by the Registration, Evaluation, Authorisation, and Restriction of Chemicals (REACH). Under this scenario, several strategies can be used (plating, electroless, etc.) to develop innovative alternatives with optimum wear and corrosion resistance properties. In this research, different Ni-based coatings have been obtained to improve the tribocorrosion performance of hard chromium coatings on low carbon steel as substrate:
i) Ni/B electrodeposits with low B content (0.04 and 0.06% wt.);
ii) Ni/P coatings (three different architectures of coatings) by electroless. Their properties are manly governed by the phosphorous (P) content. A multilayer configuration was used in order to improve the corrosion resistance.
The following experimental methodology has been followed to evaluate the performance of the coatings. A pin-on-disk tribometer with an integrated three-electrode electrochemical cell was used. Samples were rubbed against an alumina ball under Open Circuit Potential (OCP), cathodic and anodic applied potentials in NaCl electrolyte. Worn surfaces were evaluated by confocal microscopy, SEM and metallographic analysis. The total wear volumes were quantified using a profilometer and the wear accelerated corrosion volumes were obtained using a mechanistic approach. Promising results were obtained with both Ni coatings, especially using the multilayer configuration for Ni/P ones.

## Flash Poster Presentations

# Sciforum-051991: How do lithium and cerium ions act as corrosion inhibitors in PMMA-silica coatings on AA7075? A mechanistic study

Andressa Trentin[1], Samarah V. Harb[1], Mayara C. Uvida[1], Peter Hammer[1]

[1] São Paulo State University

Protective organic-inorganic coatings based on polymethyl methacrylate (PMMA)-silica provide an excellent barrier against corrosion of aluminum alloys, thus representing an efficient and economical alternative for conventional polymeric systems. In addition to their effectiveness as a physical barrier, the addition of lithium and cerium ions can turn them into smart coatings showing self-healing activity in natural corrosion and mechanically induced defects. The key factor to develop smart high-performance coatings is an in-depth knowledge of the microstructure and phenomena occurring upon exposure to aggressive media, accessed by a set of surface and bulk characterization techniques. Transmission electron microscopy and small-angle X-ray scattering results showed that a balanced Ce(IV) loading promotes a dual effect: the formation of a homogenous hybrid structure and active protection of the AA7075 alloy. The addition of lithium carbonate yields coatings with increased connectivity of the silica domains, uniformly distributed in the PMMA matrix. Results of electrochemical impedance spectroscopy of coated AA7075, immersed in 3.5% NaCl, showed that the addition of Li or Ce restores the impedance modulus (up to two orders of magnitude) after corrosive damage, thus significantly improving the coating lifetime by the self-healing ability (up to 311 days). Time-of-flight secondary ion mass spectrometry and X-ray photoelectron spectroscopy have revealed that the regeneration occurs by leaching of Li or Ce ions from the surroundings of the corrosion spot, which is restored by a protective layer of precipitated species. An analog mechanism was found for artificially scratched coatings, showing after immersion a recovery of the impedance modulus, absent for Ce/Li free reference. These results evidence the dual role of lithium and cerium in improving the structure and extending the coating lifetime by the self-healing ability.

## Flash Poster Presentations

# Sciforum-052115: Wear resistant surface treatments for additively manufactured Al10Si1Mg alloy

Rubén del Olmo[1], Hugo Mora-Sanchez[2], Joaquín Rams[3], Belén Torres[3], Marta Mohedano[1], Endzhe Matykina[1], Raúl Arrabal[1]

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[2] Departamento de Ingeniería Química y de Materiales, Facultad de Ciencias Químicas, Universidad Complutense, 28040 Madrid, Spain.
[3] Dpto. Matemática Aplicada, Ciencia e Ingeniería de Materiales y Tecnología Electrónica, Universidad Rey Juan Carlos, C/Tulipán s/n, Móstoles 28933, Madrid, Spain.

Recent developments in additively manufactured Al alloys are focused on the Al-Si systems as they are the easiest to process due to their low melting point and fluidity.
However, a knowledge gap remains regarding their tribological performance and suitability for wear-resistance enhancing surface treatments. In this work, plasma electrolytic oxidation (PEO) and hard anodizing (HA) coatings are investigated on an additively manufactured (AM) Al10Si1Mg alloy obtained via direct metal laser sintering (DMLS). Results are compared to those obtained for a conventional A361 cast alloy in terms of surface modification process and coatings microstructure and properties.
Findings revealed that the microstructure of the AM alloy, consisting of $\alpha$-Al cells enclosed in a Si network, produced more uniform coatings—in terms of morphology, thickness, and roughness of the coating/substrate interface—than those obtained on the cast alloy.
Regarding the formation of HA and PEO coatings, enhanced oxidation of the fine Si network in the AM alloy led to an increased formation of crystalline SiO2, resulting in softer coatings. In both alloys, HA and PEO treatments demonstrated improved wear resistance in comparison to the bare substrates. PEO coatings revealed superior wear protection than HA due to the presence of crystalline mullite in the former. PEO coatings on the AM alloys presented slightly higher wear rates in comparison to the cast alloy.

# Sciforum-052273: The influence of CrAlN coating defects on die soldering in aluminum die casting

Dragan Kukuruzović1, Lazar Kovačević1, Pal Terek1, Vladimir Terek1, Branko Škorić1, Aleksandar Miletić2, Peter Panjan3, Miha Čekada3

[1] University of Novi Sad, Faculty of technical sciences, Novi Sad, Serbia,
[2] Polytechnique Montreal, Department of Engineering Physics, Quebec, Canada
[3] Jozef Stefan Institute, Ljubljana, Slovenia

Commonly used method for processing of aluminum alloys is the high-pressure die casting (HPDC) process. Due to high temperatures and high chemical affinity of aluminum towards iron, the molten metal has a tendency to stick to the tool surface. This type of sticking is called soldering and highly influences machine downtime and tool wear. The negative effects of soldering can be decreased by applying hard ceramic coatings on the tool surface. In this study, the performance and soldering resistance of CrAlN coating deposited by physical vapor deposition (PVD) was evaluated by using the detachment test. To simulate the effects of a large number of casting cycles, we employed a prolonged solidification method where cast alloy was heated and kept in a liquid state while in contact with the coating surface. After solidification, the castings and the samples were detached using a tensile testing machine. The contact surfaces were analyzed by a 3D profilometer and different microscopy techniques. Remains of solder (cast alloy) and coating delamination were found on the sample surface by using a scanning electron microscope (SEM). It was found that soldering mainly occurred through coating defects. At defect locations, molten metal and steel substrate were able to bypass inert ceramic coating and chemically interact, creating intermetallic compounds. After detachment, these compounds were found both on the surface of the coating and the substrate material. The amount of soldering and coating delamination increased with the solidification delay. The amount of soldered material was in direct correlation with the number of coating defects. Higher detachment forces were obtained for coatings with a higher number of defects. The results indicate that number and type of coating defects have a high influence on the soldering resistance of PVD ceramic coatings.

# Sciforum-049576: Bio-based versus fossil-based UV-curable acrylate coatings in mechanical abrasion

Pieter Samyn[1], Joey Bosmans[1], Patrick Cosemans[1], Xavier Drujon[2]

[1] SIRRIS - Smart Coatings Lab
[2] Arkema, Centre de Recherche de l'Oise

The abrasion resistance for a series of UV-curable acrylates has been tested when applied as a protective coating on either hardwood (pine) or softwood (beech) substrates. In particular, the abrasive performance was systematically compared for acrylates originating from bio-based resources versus their traditional fossil-based equivalents. The acrylate systems are formulated by mixing a viscous oligomer with a monomer diluent in a given 50:50 ratio while incorporating monomers with different functionalities. Both the oligomer and monomers were synthesized from fossil-based (acrylic) or bio-based feedstock (wood, vegetable oil, lignocellulosic biomass), resulting in the same chemical composition. The effect of the bio-based content on coating performance was systematically investigated when either incorporated into the oligomer or the monomer fraction. Both the fossil-based and bio-based acrylates could be homogeneously applied through a bar-coating process and were characterized by comparable viscosities depending on the functionality rather than the resource origins. Interestingly, the abrasion under Taber testing conditions indicated systematically lower wear of the bio-based acrylate coatings, both when the bio-based content was augmented either in the oligomer or the monomer fraction. The ex situ evaluation of the wear track by profilometry indeed revealed that the bio-based acrylates were prone to a higher degree of ductility and recoverable elastic deformation, while the fossil-based acrylates showed more brittle cracks and permanent material loss. The different deformation behavior of the bio-based versus fossil-based grades was further confirmed by hardness and scratch resistance testing. The observations are in line with the development of a dual-phase microstructure inducing superior performance of bio-based grades

# Sciforum-042567: Cavitation erosion and cavitation slurry erosion of AlTiN films deposited on bronzes and stainless steel substrates

Mirosław Szala

[1] Department of Materials Engineering, Faculty of Mechanical Engineering, Lublin University of Technology, Nadbystrzycka St. 36D, 20-618 Lublin, Poland

The resistance to cavitation erosion in clean water and slurry of bronze and stainless steel can be improved by PVD coating deposition. This study aimed to investigate the cavitation erosion resistance of magnetron-sputtered AlTiN films deposited with different contents of chemical elements onto stainless steel and bronze substrates. The AlTiN films were deposited with different ranges of chemical elements. The surface morphology and structure of samples were examined by optical profilometry, light optical microscopy (LOM) and scanning electron microscopy (SEM-EDS). Mechanical properties (hardness, elastic modulus) were tested using a nanoindentation tester. The adhesion of the deposited coatings was determined by the scratch test. Cavitation erosion tests were performed according to ASTM G32 (vibratory apparatus), in compliance with the stationary specimen procedure. Two test mediums were used, i.e., distilled water and slurry composed of water and silica. The erosion curves indicate the higher wear resistance of bronze versus stainless steel. The results demonstrate that the cavitation erosion mechanism of the AlTiN coatings consists of the films' chemical composition and is strongly affected by the substrate properties. The slurry affects the wear mechanism and facilitates material degradation. Compared to the bare bronze and bare stainless steel reference samples, the deposition of PVD films exhibits superior resistance to cavitation erosion in pure water and slurry.

# Sciforum-051943: Characterization of surface-related and metallurgical phenomena for evaluation of CrN duplex coatings for HPDC tools

Pal Terek[1], Lazar Kovačević[2], Aleksandar Miletić[3], Branko Škorić[1], Dragan Kukuruzović[1], Aljaž Drnovšek[4], Peter Panjan[4]

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Application of physical vapor deposition (PVD) coatings for reduction of cast alloy soldering on surfaces of high pressure die casting (HPDC) tools provides many advantages in production. Quite a lot of research has already been done in this field, however understanding the aluminium alloy soldering mechanisms toward PVD coatings is still limited. Therefore, this was a motivation to perform to perform investigation in this field. In this work performance of CrN duplex coating with different roughness is evaluated by modified ejection test performed with delayed (DS) and conventional casting solidification (CS). After the ejection tests, morphological and chemical characteristics of sample surfaces and layers were analysed by various microscopy and spectroscopy techniques. In DS tests, considerably lower values of the ejection force were recorded than in CS tests. In CS tests, surface roughness played important role, while samples of different surface topography in DS tests performed in a similar way. Decrease in the ejection force, observed in DS tests, is attributed to formation of a thick Cr–O layer on CrN coating which reduced soldering and sliding friction against thick Al–O casting scale. The Cr–O layer formed in DS tests suffered from diffusion wear by cast alloy. Knowledge obtained in this investigation may be utilised in design of high performance non-sticking coatings for HPDC tools.

# Sciforum-052197: Comparison of two methods used for high temperature tribological testing of protective thin coatings

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This study aims to contribute to the better understanding of results obtained by different methods used for high temperature tribological evaluation of hard coatings. For these purposes tribological testing directly at high temperatures and testing of annealed coatings at room temperature were compared. In this study, high temperature tribological behavior of 3 μm thick TiAlN coating (3050 $HV_{0.05}$) was evaluated using high temperature pin-on-disk tribometer. Coating was prepared on EN X38CrMoV5 steel samples using cathodic arc deposition. Coated samples were tested against $Al_2O_3$ ball, in air atmosphere, at room temperature, 300 °C, 500 °C, 600 °C, and 700 °C, and after being previously annealed (PA) at these temperatures. Stylus profilometry, confocal microscopy, focused ion beam, and energy dispersive spectroscopy were employed for evaluation of the wear tracks. At room temperature (RT) the steady-state COF was 0.72. Tribo-tests at 300 °C and 500 °C resulted with steady COF which slightly increased to a maximum value of 0.7 and 1, respectively. COF for tests at 600 °C and 700 °C, after reaching a max value of 0.95 and 0.85, declined for both cases. Each of the tribo-tests on PA samples displayed COF values similar to RT tests, but with pronounced oscillations. Tribo-tests at RT and on PA samples produced similar wear tracks that displayed combination of both adhesive and abrasive wear mechanism, while abrasive and oxidative wear mechanism was observed at high temperatures. At 600 °C coating degradation due to oxidation of substrate initiated, and at 700 °C coating was completely damaged. It is suggested that declining COF at 600 °C and 700 °C is due to formation of Fe-O and Cr-O inside of wear tracks. Additionally, oscillations of COF on PA samples are suggested to be the consequence of adhesive wear of coatings. Finally, detailed analysis revealed that, apart from their COF, tribo-tests on PA samples are quite similar to RT tests, but significantly differ from high temperature tests.

# Sciforum-052245: Corrosion behavior of Fe-based metallic glass composite coating synthesized by high velocity oxy-fuel thermal spraying

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Recently, Fe-based metallic glass (MG) coating prepared by different thermal spraying methods is being investigated as a potential candidate for surface protection of various structures attributed to their remarkable combination of mechanical and chemical properties, including, superior strength, high hardness, and outstanding wear and corrosion resistance. Despite these appealing properties, the application of monolithic MG coatings are hindered gravely due to their inherent room temperature brittleness. Alternately, the preparation of MG composite coating has proven to be an effective approach to enhance its toughness owing to the hindrance to shear band propagation and promotion of multiple shear band formation caused by the crystalline phases. Accordingly, *an economical MG composite coating system based on a newly developed FeCrBPC alloy (Fe-10Cr-4B-4P-2C, wt %) was synthesized on the mild steel substrate via high velocity oxy-fuel thermal spraying* with different powder feed rates in this study. Microstructural characterization of the composite coatings revealed the correlation between level of amorphicity, as well as porosity content of the different coatings and the increased powder feed rate during the spraying process. The amorphicity of the coating increased, whereas the porosity content decreased gradually with the increment in feed rate. The electrochemical corrosion analysis of the various coatings displayed an improvement in the corrosion resistance of the composite coating deposited at elevated feed rate because of lower porosity content and higher amorphicity. This superior corrosion properties was attributed to presence of higher content of protective phases (chromium hydroxide and Cr substituted hematite) in the corrosion products. Additionally, all the MG composite coatings exhibited higher corrosion resistance than that of the substrate, as well as the SS316L coating prepared by optimized spray parameters. *The enhanced corrosion resistance of the economical Fe-based composite coating makes it a viable alternative to the conventional stainless steel coating.*

# Sciforum-051994: Effect of pre-anodizing and frequency on energy consumption, wear and corrosion properties of PEO coatings

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Plasma electrolytic oxidation (PEO) is a novel process capable of generating oxide ceramic coatings on Al, Mg, and Ti alloys with improved wear and corrosion properties. Nowadays, the major obstacle for a wider application of PEO technology is its high cost, which is associated with the high energy consumption (current densities and voltages are typically of the order of 20 A/dm2 and 400 Vrms) and low coating efficiency.
Among the different strategies for energy savings, the use of a conventional anodizing pre-treatment seems to be a very promising one. Precursor anodic films lead to a faster establishment of "soft sparking" under AC conditions, increasing the coating growth rate and reduced energy consumption.
The present work aims to investigate the effects of anodic film precursors on the wear and corrosion properties of PEO coatings produced on the AA6082 alloy at different frequencies. With that objective, different PEO coatings were produced at 50 Hz and 400 Hz with and without anodic layer. The coatings were evaluated in terms of thickness and morphology (Scanning Electron Microscopy), wear resistance (ball-on-disk test) and corrosion performance (Electrochemical Impedance Spectroscopy) in 3.5% NaCl.

# Sciforum-049815: Functionalized polysiloxanes as hybrid precursors for coating materials with anti-corrosion properties

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Metals, such as iron, aluminium, copper, and magnesium, and their alloys are used in a myriad of structural, marine, aircraft applications, and cultural heritage, etc. Although these metals are useful because of their physical characteristics, such as stiffness and high strength to weight ratios, they are highly susceptible to corrosion in aggressive environments. Corrosion is always the major reason of energy and material loss. Recently 70% of the world's manufactured coating materials contains two main active corrosion protective agents, such as lead oxide and chromium compounds, mainly zinc-potassium chromate. Additionally commonly used, e.g., in automobile industry, are phosphate coatings that unfortunately has harmful impact on natural environment through eutrophication. Use of these traditional highly effective agents was drastically reduced, due to their high toxicity and for this reason a new, environmentally safe corrosion inhibitors are being searched for.
Polysiloxanes enjoys great interest for many years due to their unique physicochemical and dielectric properties. In recent years, special attention has been paid to functionalized polysiloxanes, which have the properties provided by the flexible siloxane chain and the organic moieties that modify this chain. Functionalised polysilcosans can be used to produce protective coatings that protect materials against the harmful effects of the environment.

# Sciforum-044241: Hydrophobic Surface Modification of Sintered UHMWPE Ski Base Materials

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Ultra-high-molecular-weight polyethylene (UHMWPE) is the material of choice for many tough applications, including high-strength fibers, biomaterials for hip and knee replacements, as a manufacturing material for other thermoplastics, and as the base material of choice for nearly all skis and snowboards in production. However, UHMWPE is highly susceptible to abrasion. In ski bases, abrasion produces UHMWPE "micro-hairs", which drastically increase friction and have been partially responsible for producing the need for topical waxes, which are subsequently abraded from ski bases into the snow pack and watershed during use. Ski waxes contain many additives in an effort to enhance their performance in many environmental conditions, including air temperature, humidity, snow temperature, snow crystal structures, and many others. The best-performing waxes are fluorocarbon-based waxes, which are known sources of PFOA and have been linked to many health hazards due to the tendency of PFOA to bioaccumulate in both the human body during application and in the environment. This has resulted in a full ban of fluorocarbon-based waxes by all major ski bodies starting with the 2020–2021 competitive season, which has resulted in the need for new non-toxic, high-performance products in the snowsport industry. This project focuses on the development of a permanent surface modification of UHMWPE using non-toxic polymers that can improve the baseline toughness and wear resistance, thereby preventing the occurrence of micro-hairs that reduce long-term glide performance. We have determined both the porosity and diffusion kinetics of small monomers into sintered UHMWPE and how they affect the wear rate of the base polymer. We report on the scientific principles surrounding surface modification, on-snow friction, and the functional groups of polymers and organic molecules that result in broad-range, high-performance ski base treatments.

# Sciforum-052179: Plasma Electrolytic Oxidation of Electron Beam surface structures in Ti6Al4V alloy

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The development of surface modification strategies to enhance the osteoconductivity of metallic implants is a research field of major interest. It has been proved that multiscale surface roughening and surface functionalization are two effective strategies to promote the generation of new bone on the implant surface.
The aim of this work is to combine Electron Beam (EB) surface structuring and Plasma Electrolytic Oxidation (PEO) to tailor the surface topography and chemistry of Ti6Al4V alloy: i) topographical features with lateral and vertical dimensions between thousands and tens of micrometres were produced via EB structuring; ii) PEO was used to fabricate Ca- and P-containing thin ( 10 μm) coatings on the EB surfaces.
EB surface structures were designed to maximize the structured area while providing multiscale topographies. Specific EB structures were produced to study the effect of the as-processed microstructure and the topography scale on the PEO treatment. Uniform PEO coatings were successfully produced on the EB structures maintaining similar morphology and chemistry in comparison to PEO coatings on the non-structured Ti6Al4V alloy. Moreover, the EB topographies were retained after PEO treatment. PEO coatings provided with additional micrometre porosity (1–6 μm in diameter) and sub-micrometre scale surface roughness (Sa 0.9–0.1 μm) and enhanced the corrosion resistance of the surface in physiological media.
These results are presented in detail in the present contribution together with the discussion on the effect of the EB structuring on the PEO process.

# Sciforum-052255: Reactive molecular dynamic study of aluminum–magnesium surface during dry corrosion

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Aluminum–magnesium alloy is an important category of materials due to their high technological value and a wide range of industrial applications, including automotive, aerospace, defense, and manufacturing industries. The corrosion resistance of Al–Mg alloys is good at ambient conditions, but becomes reduced at elevated temperatures. Therefore, there is a need to investigate the mechanisms of Al–Mg alloy corrosion in dry environments by considering different factors, such as oxygen gas concentration, temperature, and composition of Al–Mg alloy. The corrosion mechanism is a complex one, and its studies require deep understanding of the early stages of Al–Mg surface oxidation, as very little is known to date about the structure and properties of oxide films formed during this process.
In this contribution, we discuss the results of atomistic simulations and compare them with available experimental data on thermal oxidation of an Al–Mg alloy [1, 2]. Molecular dynamics simulations based on the reactive force field, ReaxFF, were performed at selected temperatures according to the phase diagram [3], including 300 K, 500 K, and 773 K. The structure and chemistry of oxide thin films grown on the Al–Mg alloy surface during corrosion in dry oxidizing environment was investigated by computing chemical composition, bond lengths, and respective structural properties of the thin films. The topography of Al–Mg alloy surface before and after corrosion was analyzed in terms of surface roughness, determined from a 3D map (height profile) of the Al–Mg surfaces. To inspect in detail the structure of both thin oxide film and Al-Mg substrate, Voronoi analyses were performed. The kinetics of thin film growth upon dry corrosion was also investigated by computing the thickness and effective diffusion coefficient to assess the corrosion rate.
The simulations show that the thickness of the formed oxide layer increases with the increase in oxidation temperature. The obtained results give an atomic-level insight into the mechanism of oxide formation on the surface of Al–Mg alloys, and also provide detailed information about the kinetics of the structure and property evolution of the alloy surface upon corrosion. Future research will consider the oxidation processes of the Al–Mg alloy in contact with harsh environment, including halide ions [4]. The planned studies will allow for modelling of protective coatings against the corrosive agents.

Acknowledgments:
The presented results presented results were obtained using computational resources provided through PLGrid Infrastructure at Academic Computer Centre Cyfronet AGH.
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# Sciforum-049405: SELF-HEALING PROTECTIVE COATINGS BASED ON EPOXY-LOADED POLYMERIC MICROCAPSULES

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Protective coating failure can lead to excessive substrate wear, thus increasing the need for maintenance. Self-healing systems can offer autonomous crack repair and increase a coating's service lifetime. Polymeric microcapsules (MCs) containing healing agents can be used in that perspective and exhibit significant potential. In the case of micro-cracks, microcapsules are ruptured and the healing agent flows into the crack. The released agent comes into contact with the catalyst that is also embedded in the matrix and is polymerized, bonding the crack faces, increasing the coating service lifetime and protecting the substrate from corrosion with significant benefits for industrial applications, such as marine. Epoxy-loaded microcapsules with a poly(urea-formaldehyde) shell were successfully prepared within the current study using one-step in situ polymerization based on the work of Tzavidi et al. (Journal of Applied Polymer Science, 2020). Microcapsules were obtained as a colorless free-flowing powder with a diameter of 37 μm and 78 % encapsulation efficiency (ratio of encapsulated substance to microcapsule mass). In order to study the self-healing properties of the microcapsules, they were dispersed in a commercially available alkyd-based paint at a content of 5, 10, or 15 % wt. along with the catalyst. Steel specimens were coated using a paintbrush with either an MC-loaded paint or pure paint as reference. A scratch was manually made on the coating with a blade, and electrochemical impedance spectroscopy (EIS) was used to evaluate the self-healing properties of the coating before and after the scratch. Based on the EIS tests, the MC-containing coating was found to offer corrosion protection even in the case of the low 5 % wt. microcapsule content.

# Sciforum-052262: Synthesis of pH-sensitive poly(melamine-formaldehyde) microcapsules containing 8-hydroxyquinoline as a corrosion inhibitor

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PH-sensitive Polymelamine formaldehyde microcapsules containing 8-hydroxyquinoline inhibitors were prepared as an in vitro corrosion inhibitor. The Polymelamine formaldehyde microcapsule was detected by Fourier transform spectroscopy (FTIR) and its particle size was determined by scanning electron microscopy (SEM). A thermal resistance test (TGA) was performed to ensure the encapsulation of the inhibitor inside the microcapsules and to determine the contents of the core, the results of which confirmed the presence of the inhibitor in the core and its amount. To investigate the anti-corrosion properties of microcapsules containing corrosion inhibitors, these microcapsules were dispersed in epoxy resin with different weight percentages, and electrochemical impedance test (EIS) in 3.5 wt.% sodium chloride solution were performed. The results showed that coatings containing inhibitory microcapsules performed well to prevent corrosion reactions.

# sciforum-052212: Wear properties of Iron Based Alloy Coatings produced by Plasma cladding

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Plasma cladding has been widely applied in surface modification, repairing, and remanufacturing. In this work, the multiple cladded thick coatings were deposited on the compacted graphite cast iron with iron based powders through plasma cladding technology at different cladding currents to enhance the wear resistance. The phase and microstructure of the coatings were characterized by XRD, SEM, and EDS. The microhardness and wear resistance of the coatings were characterized. Results showed that iron based alloy coatings composed of pearlite, graphite, austenite, and secondary carbides. Due to the heat influence during multiple cladding, a spheroidal graphite transition zone appears between the coating and the substrate. The microhardness of the claddings varied from 363HV to 402HV according to the varied plasma cladding current from 45A to 60A. With the increase of plasma cladding current, the cladding's microhardness increased. The minimum friction coefficient and wear mass loss of coating was about 0.45 and 5.4mg, respectively, when the current was 50A, which were lower than that of the compacted graphite iron substrate with the friction coefficient and wear mass loss of 0.55 and 8.2mg. Compared with the substrate, the iron-based alloy cladding layer achieved the effect of reducing friction and wear resistance simultaneously, which resulted from the self-lubricating effect of graphite and high wear-resistance of carbides in the claddings

# Abstracts

## S2. Bioactive Coatings, Surfaces and Interfaces

## Invited Speakers

# Sciforum-054967: Tuning Surfaces to Improve Bacterial Attachment in Bioelectrochemical Systems

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In the majority of the systems, bacterial attachment on surfaces and biofilm growth is usually not a desired process. For example, bacterial growth on cooling systems can generally lead to issues, such as biocorrosion, causing enormous damages and it can increase significantly the operational cost and the maintenance. In parallel, in bioelectrochemical systems, bacterial attachment and biofilm formation is a desired process on the anode but undesired on the cathode. On the anode in fact, bacterial are actually the biocatalyst for the oxidation reaction of organics. Therefore, the colonization of the anode electrode has to be improved and optimized. Surface chemistry and surface morphology affect the bacterial attachment. Few examples will be presented related to: 1) the presence/absence of polytetrafluoroethylene on the surface of carbon paper; 2) Hydrophilic (-$N(CH_3)_3^+$, -OH, -COOH) and hydrophobic (-$CH_3$) functional groups on self-assembled monolayers. It will be shown how the surface chemistry affect importantly the startup time of a bioelectrochemical system and its electrochemical performance. Biofouling and inorganic fouling at the cathode electrode instead are unwanted due to the fact that this layer cover the catalytic layer and enhance the proton mass transfer resistance, in turn reducing the cathode catalytic performance. This might occur due to the alkalization of the cathode that in turn enhance the precipitation of salts on the cathode electrode. Examples of biofouled cathodes will be presented through studies conducted using X-ray micro tomography.

## Invited Speakers

# Sciforum-055337: Surface Modifications of Titanium Alloys for Antibacterial Implants

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Surface modifications and coatings are commonly applied to medical implants in order to improve biocompatibility and/or bioactivity. In this context, various types of surface coatings have been researched as biocompatible and anti-bacterial coatings. Antibacterial coatings can be synthesised on medical grade titanium alloys using various methods including electroplating of silver, titania nanotubes by anodising, silver nanoparticles or ZnO nanowires by sol-gel process which have their own advantages and disadvantages. Bioactive nano hydroxyapatite can also be deposited on top of the antibacterial coatings. Antibacterial and biocompatibility performance was evaluated and reported with some speculations about the related mechanisms. The results showed that both silver and ZnO exhibit excellent biocidal performance against S. aureus. The overlay of hydroxyapaptite nanoparticles improves biocompatibility without significant effect on the biocidal performance.

## Invited Speakers

# Sciforum-054972: Surface Modification of Bioactive Materials With Natural Molecules

Ferraris Sara[1], Riccucci Giacomo[1], Cazzola Martina[1], Reggio Camilla[1], Gobbo Virginia Alessandra[1], Miola Marta [1], Bosso Antonella [2], Guaita Massimo [2], Örlygsson Gissur[3], Chuen How Ng[4], Verné Enrica[1], Spriano Silvia [1]

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The surface of biomaterials is their visiting card for the biological environment. Proper surface modifications of bioactive materials are powerful tools for the modulation of their biological response in challenging practical situations.
The use of natural molecules (e.g. polyphenols) obtained from food and wine byproducts, with a sustainable and circular approach, is a promising strategy for the development of smart multifunctional biomaterials.
The talk will give an overview of recent research on the surface functionalization of bioactive materials (nanotextured bioactive titanium alloy, bioactive glasses, and hydroxyapatite) with natural polyphenols obtained from grape pomaces.
Polyphenols from Barbera and Moscato pomaces were successfully grafted to the selected biomaterials maintaining their redox and radical scavenging activities. Surface reactivity and the composition of the solution used for the functionalization are crucial factors for an effective grafting. A set of techniques were implemented and optimized for the characterization of functionalized biomaterials. XPS analyses suggest the formation of polyphenols-metal ions complexes in some cases. Polyphenols can be gradually released in aqueous solutions.
In conclusion, active polyphenols can be extracted from grape pomaces and coupled with biomaterials in order to combine their properties. The proposed technique can transform abundant local byproducts in high added value molecules for biomedical applications.

## Flash Poster Presentations

# Sciforum-052272: Ion release measurements of Cu/Ag-TiN-based antibacterial coatings on textiles deposited by magnetron sputtering

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The use of antibacterial textile surfaces that functionalise Ag and Cu nanoparticles as antibacterial agents has become a common practice to counter healthcare-acquired infections (HAI) by reducing the horizontal transmission of pathogens between patients and healthcare workers. Although the exact mechanisms of nanoparticle toxicity are still being investigated, one popular option is the release of metal ions from nanoparticle surfaces. As ion release measurement is easier and quicker than analysing antibacterial properties, it can be used as a predictor tool to estimate the antibacterial performance of the coatings. Controlling the ion release can provide an opportunity for long-term antibacterial activity without causing any unwanted side effects on humans. However, the parameters that affect the release are still not fully understood. Our study focuses on investigating the controlling parameters on ion release as well as tuning it to achieve a steady ion release profile. The deposition of antibacterial coatings on PET textiles, consisting of Ag and Cu metals as antibacterial agents and TiN as ceramic phase, was prepared using magnetron sputtering. We conducted a comprehensive study to understand the effects of deposition parameters (cathode current, deposition time), Ag/Cu composition (75/25, 50/50, 25/75), and multilayer/nanocomposite structures on coatings' ion release characteristics, surface morphology, and adhesion strength. Sputtered samples were characterised using various techniques, e.g., Scanning Electron Microscopy (SEM), conductivity measurements, adhesion tests. Ion release tests were performed by immersing coated textiles in deionised water over a 7-day period, and the released metal ion concentrations were measured by ICP-OES. We show that for each coating composition and design, deposition parameters can be altered to yield an optimised ion release rate and profile, which can be tuned to provide long-term antibacterial efficacy.

## Flash Poster Presentations

# sciforum-052065: Bioactive PEO coatings for Al-free Mg systems: Mg-Ca, Mg-Ca-Ag, Mg-Zn-Ca alloys

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AC bioactive plasma electrolytic oxidation (PEO) coatings enriched in Ca, P, Si, and F were developed on Mg0.6Ca, Mg0.6Ca2Ag and $Mg_xZn_yCa$ alloys (two cast alloys and one extruded; x=1, 3 or 0.5; y=1, 0.4 or 0.2) in order to improve the corrosion resistance, bioactivity, and cytocompatibility of the alloys. Surface characteristics, morphology, and chemical composition of studied materials were evaluated using optical profilometry, electron-optic microscopy, energy dispersive X-ray spectroscopy, and X-ray diffraction. The coating thickness on all alloys ranged within 40 to 50 μm and phases, such as hydroxyapatite and fluorapatite, were formed. Corrosion investigations were performed for uncoated and coated materials using hydrogen evolution measurements at 37ºC in physiological media. For Mg0.6Ca and Mg0.6Ca2Ag alloys, $H_2$ evolution was measured during 60 days of immersion in simulated body fluid. In case of Mg-Zn-Ca alloys, $H_2$ was collected in inorganic part of $\alpha$-MEM during 5 days. The results showed that the PEO coatings improved the corrosion resistance of cast Mg0.6Ca and extruded Mg0.5Zn0.2Ca alloys. Strong microgalvanic coupling effect in the rest of the alloys had a detrimental effect on protective properties of the PEO coatings.

# Sciforum-052054: Biofunctionalization of Ti nanostructured surfaces with hydroxyapatite-based coatings intended for medical applications

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The current research aim is to biofunctionalize pure titanium (cp-Ti) substrate with titania nanotubes and Zn doped hydroxyapatite-based coatings, by applying a duplex electrochemical treatment and to evaluate the influence of Zn content on the physico-chemical properties of HAp. Thus, initially the cp-Ti substrate was anodized for 30 min. at a constant potential of 20 V in a 0.5 % wt. HF solution. The obtained nanostructured surfaces were covered with hydroxyapatite-based coatings doped with Zn in different concentration by electrochemical deposition in pulsed galvanostatic mode. The obtained surfaces were characterized in terms of morphology, elemental and phasic composition, and roughness. The nanostructured surface consisted in titania nanotubes (NT), aligned, vertically oriented, and hollow, with an inner diameter of ~ 70 nm. XRD analysis showed that the nanostructured surface mainly consists in anatase phase, and some rutile peaks as secondary phase. The morphology of all coatings consisted in ribbon-like crystals and by increasing the Zn content the dimension of the crystals was reduced. The elemental and phasic composition evidenced that HAp was successfully doped with Zn through pulsed galvanostatic method on the cp-Ti nanostructured surfaces. Based on the obtained results it can be said that by addition of Zn, the properties of hydroxyapatite can be controlled and thus, leading to materials with tuneable features.
This research has been funded by a grant of the Romanian Ministry of Education and Research, CNCS - UEFISCDI, project number PN-III-P1-1.1-TE-2019-1331, within PNCDI III (project no. TE 172/2020; 3B-CoatED).

# Sciforum-052252 Active biofilms of mango (*Mangifera indica*) kernel starch containing hydroethanolic extract of mango peel

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In recent years, the plastic packaging industry has been investigating how to replace non-biodegradable petroleum-based polymers with environmentally friendly alternatives. In this sense, starch-based edible biofilms and coatings are becoming interesting options for food packaging because they are renewable, biodegradable, nontoxic, and economically cost-effective. Different research shows unconventional starch sources have the potential to provide new characteristics and are viable alternatives for the production of bioplastics. Furthermore, the addition of extracts or essential oils from plant material to starch films can improve their antioxidant, antibacterial, and barrier properties, such as permeability to oxygen, UV rays, and water vapor, can reduce the reproduction of microorganisms and prolong the shelf life of packaged foods; therefore, the objective of this work was to evaluate the physical, mechanical, and rheological properties of biofilms elaborated with mango kernel starch and hydroethanolic extract of mango peel.
Mango kernel starch presented extraction yields of 44.05 ± 2.58 % with amylose values of 34.35 ± 0.46. Hydroethanolic extract of mango peel obtained by ultrasound-assisted extraction presents yields of 33.24 ± 2.48 %, total phenolic compounds with values 305.04 ± 10.70 mg GAE/g and antioxidant activity analyzed by ABTS assay with TEAC values of 1470.41 ± 59.75. Different biofilms were developed evaluating the percentage of extract (0.5%–2%). Their properties depend mainly on the starch properties, that is, the source, the ratio of amylose to amylopectin, the size of the granule will influence the physical, mechanical, and rheological properties of the films. In addition, mango peel extract imparts bioactive properties to films, such as improved antioxidant properties. This research provides the possibility of using mango by-products to develop bioactive films that can be successfully used in the food packaging industry.

# Sciforum-052427: Corrosion control of magnesium alloys using Mg doped hydroxyapatite based coatings

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In the medical field, using a material to replace a body part has been made since the late nineteenth century. Over time, several types of biomaterials have been used, and one of the most widely used categories is represented by metallic biomaterials. Among these, the biodegradable metallic materials represent a hot topic in the medical field, especially in orthopedics, with a new direction to follow with multiple advantages, mainly for the patient and medical staff but also in terms of materials science, by combining aspects of bone regeneration and biocompatibility related to structural analysis, mechanical and corrosion properties. According to the studies conducted in recent decades, Mg alloys are biocompatible and biodegradable and can be used as implantable medical devices, such as bone implants, vascular stents, etc. Even though they have good mechanical properties, with values close to those of the human bone, it is desired to improve their corrosion resistance. Thus, this can be achieved through addition of bioactive coatings, and especially those based on doped or undoped hydroxyapatite (HAp). The aim of the present study is to evaluate the electrochemical behavior of Mg alloys coated with Mg doped HAp. The deposition was carried out using RF magnetron sputtering method. The samples were characterized in terms of elemental composition, morphology, roughness, and electrochemical behavior. In order not to affect the integrity of the MgCa alloy substrate, which undergoes structural transformations at temperatures higher than 300 °C, the depositions were achieved at a temperature of 100 °C. Acknowledgement: We acknowledge the support of the Romanian Ministry of Education and Research, CNCS - UEFISCDI, project ERANET-M-ISIDE-1, no. 171/2020 (INOE partner) and 172/2020 (UPB partner), within PNCDI III.

# Sciforum-052265: Development of an antimicrobial formulation of polyurethane-based lacquer

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Humans spend almost 90% of their lives in indoor environments, which are characterized as confined and multi-shared spaces[1,2]. In such environments, the surfaces are envisioned as a reservoir for potential harmful microorganisms, offering important opportunities to exposure to pathogens[2]. In this context, we propose to develop different bioactive coatings for polymeric substrates to inhibit the surface colonization and avoid transmission and spreading of pathogenic microorganisms among humans.
In this work, transparent coating formulations were produced based on a commercial polyurethane resin supplemented with a range of antimicrobial compounds: phenolic-based; ionic-based and a copper-based. It was evaluated the effect of those compounds on the optical and surface properties of the coating.
The incorporation of the antimicrobial compounds slightly impacted the color, the gloss, and the transmittance of the produced films, while FTIR analysis did not reveal any differences among control and test samples. Despite these minor changes in the optical properties of the coating films, the final product revealed a uniform and homogeneous surface.
The lacquers were tested for their antimicrobial activity against *Staphylococcus aureus* and *Escherichia coli*, as well as their cytocompatibility against the fibroblast cell line L929. Copper-based materials exhibited a significant antimicrobial activity against both bacteria, with a 100% reduction of the bacterial load. Ionic-based materials also revealed a similar antimicrobial activity against *S. aureus*, but only an 84% reduction for *E. coli*. In contrast, neither of the phenolic-based materials shown relevant antimicrobial activity against the tested bacterial strains. Regarding biocompatibility, a cytotoxic effect was only observed for the highest concentration of ionic-based materials.
Our findings reveal that copper-based compounds exhibited the most effective antimicrobial activity and a good biocompatibility, being a promising candidate to be incorporated in polyurethane formulations for finish coatings of polymeric substrates.

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# Sciforum-050963: Investigation of Biofouling at CoaST Maritime Test Centre

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Biofouling is unwanted organisms that accumulate on immersed surfaces. A common method to prevent biofouling on, e.g., ships is by using fouling control coatings. There are different techniques to prove the effectiveness of a new fouling control coating either by static or dynamic exposure in the ocean. The new CoaST Maritime Test Centre (located in the northern part of Zealand in Denmark) established by the Technical University of Denmark is an ideal place for the testing of different fouling control coatings. The test centre has a capacity for more than 4500 panels of standard size 20x10 cm and the possibility for both full immersed or splash zone exposure. In addition, there are three pools designed for special test equipment such as dynamic tests or live underwater monitoring, etc. The biofouling is seasonal, ranging from March to October with temperatures from 10°C to 25°C and salinity around 15–22 ppm.
Initial experiments to investigate the propensity for biofouling were performed at the test centre. For this purpose, 56 panels were coated with a commercial polyurethane topcoat without any fouling control properties. These were placed on eight frames, two in each corner, with different graphical directions. All panels were fully covered after six weeks of exposure, indicating high biofouling intensity. The panels facing South and East showed more algae fouling compared to North and West, which is explained by the access to sunlight. The biofouling has been categorised as light and dense slime, macroalgae (green, red, and brown algae), and animals (barnacles, mussels, and tunicates). The biofouling coverage was evaluated both manually and documented through images for the development of an image library, which is to be used in developing a pixel classification model for biofouling recognition and classification.

# Sciforum-043065 Investigation of sputtered CaP coatings doped with Mg

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The purpose of the current paper is to show the effect of Mg addition on the CaP sputtered coatings as possible resorbable material used for biomedical applications. The coatings were produced by RF magnetron sputtering method on silicon and Mg alloy substrates. Comparatively examinations were performed in terms of their elemental and phase composition, mechanical characteristics, and degradation rate in two acellular media (SBF and DMEM) at 37°C for a period ranged from 1 to 21 days. CaP coating without Mg addition was used as reference coating. The results showed that the Mg addition into CaP decreased the degradation rate of CaP coatings, being an advantage for the biomedical degradable products.
We acknowledge the support of the Romanian Ministry of Education and Research, CNCS - UEFISCDI, project ERANET-M-ISIDE-1, no. 171/2020 (INOE2000 partner) or 172/2020 (UPB partner), within PNCDI III, and no. 19PFE/2018 (PROINSTITUTIO) – institutional project.

# Sciforum-052302: Loading fibrous electrospun mats with antiviral essential oils for COVID-19 protection

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In December 2019, a novel strain of coronavirus, SARS-CoV-2, was identified. Hoping to prevent transmission, many countries adopted mandatory mask usage in closed public spaces. However, most mask options display a passive-like action against COVID-19. To overcome such restrictions, this work proposes the incorporation of antiviral essential oils (EOs) loaded onto a fibrous layer that can be adapted to both community and commercial masks. Twenty EOs selected based on their antimicrobial nature were examined for the first time against the *Escherichia* virus MS2. The most effective were the lemongrass (LGO), Niaouli (NO), and eucalyptus (ELO) with a virucidal concentration (VC) of 356.0 mg/mL, 365.2 mg/mL, and 586.0 mg/mL, respectively. Polycaprolactone (PCL) was prepared at 14 wt.% in chloroform/dimethylformamide (9/1 v/v) and processed via electrospinning, with processing parameters being optimized to 23 kV, 0.7 mL/h, and 26 cm. Uniform, beadless nanofibers were obtained. Mats were characterized as mechanically resilient, to endure movements arising from mask positioning, and hydrophobic in nature, to repel droplets coming from the exterior. Loading of the nanofibrous mats was accomplished via two ways: (1) physisorption and (2) by combining the EOs with the polymer solution (electrospinning parameters adjusted to 26 kV). In both cases, EOs were loaded at 10% of VC concentration (saturation) for 24 h. Presence of the EOs was confirmed along the mats (ATR-FTIR and UV-visible). Presence of EOs increased the mats water repellence and water vapor transition rate. Antimicrobial testing revealed the mats' ability to retain the virus (preventing infiltration) and to eliminate it (log reduction > 1). The most effective mats were those modified via strategy 2 (blending) using LGO as the bioactive molecule. Data demonstrated the potential of these EOs-loaded PCL fibrous mats to work as COVID-19 active barriers for individual protection masks.

# Sciforum-051859: Molecular dynamics simulation of surface interaction between the Magnetic spinel ferrite nanoparticles with chitosan and polyethylene glycol coatings.

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Molecular dynamics (DM) is a powerful method for gaining a better understanding of complex atomic and molecular interactions. In this paper, the aim is to investigate the surface interaction behavior of with $FeO$-$Fe_2O_3$ ferrite spinel nanoparticles with chitosan and polyethylene glycol polymer coatings. According to the energy obtained from the interaction between the (100) $Fe_3O_4$ plane and the polymers, it was observed that the interaction between chitosan and the (100) $Fe_3O_4$ plane is stronger than polyethylene glycol. The weak interaction between polyethylene glycol and (100) $Fe_3O_4$ plane is due to the intermolecular force between the oxygen and nitrogen atoms in this polymer and the iron atoms at the (100) plane of the $Fe_3O_4$. Structure. In contrast, the presence of hydrogen bonds between the chitosan functional groups and the (100) $Fe_3O_4$ plane was due to the strong interaction between the polymer and the surface.

# Sciforum-051858: The coated magnetic $Fe_3O_4$ nanoparticles as carriers in targeted drug delivery

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Magnetic nanoparticles are of interest to a broad range of scientific fields of researchers such as magnetic fluids, catalysts, biotechnology, medicine, information storage, and environmental issues. One of these applications is the use of nanotechnology in the field of treatment and drug delivery. Ferrite magnetic nanoparticles with spinel crystal structure are one of the most interesting and at the same time the most complex ceramic crystal structures. In this research, Fe3O4 is synthesized, using co-precipitation method under nitrogen gas atmosphere. Then, chitosan and polyethylene glycol were used as biopolymer coatings on the synthesized nanoparticles. To determine the morphology of the magnetic nanoparticles, field emission electron microscopy has been used. The results indicate the formation of a uniform coating by both of chitosan and polyethylene glycol. Totally, these coated nanoparticles have spherical morphology are suitable candidates for use in the field of treatment and drug delivery.

# Sciforum-049792: Using of hydrogels as biocompatible coatings for medical device biofabrication: innovations and patentability

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There are a variety of hydrogels commonly used as coatings for medical device applications. Hydrogels are synthetic matrices made up of a network of hydrophilic polymers that absorb water and/or biological fluids. They can be created from a large number of water-soluble materials including synthetic polymers (e.g., polyglycolic acid), proteins (e.g., collagen), and polysaccharides (e.g., alginate). The 3D structure of these hydrogels is due to crosslinking which forms a structure which is insoluble in environmental fluid. The resemblance to different biological tissues, due to the elasticity and the presence of a large amount of water, allows the use of hydrogels in the regeneration of several types of damaged tissues (e.g., fibrin hydrogel is seeded with neural cells to regenerate brain tissue, keratinocytes are seeded in collagen hydrogel to regenerate skin tissue)
This work in the form of patent analysis englobes information which could be used as a reference by researchers in the fields of coatings and interfaces, biofabrication, biomaterials, tissue engineering and biomedical engineering, as well as those interested especially in formulation of hydrogel coatings. The state of the art has been reviewed by introducing what has been patented in relation to hydrogel coatings. Furthermore, a detailed analysis of the patentability of hydrogel applications such as in the coating of medical devices to enhance its clinical performance, have been provided by determining publication years, classifications, inventors, applicants, owners, and jurisdictions. Finally, this work which gives an analysis of the past, present, and future trends lead to various recommendations that could help one to plan and innovate research strategy.

# Abstracts

## S3. Advances in Coatings Deposition and Surface Functionalization

## Invited Speakers

# Sciforum-051464: Multifunctional Plasma Electrolytic Oxidation (PEO) Coatings on Mg alloys

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The demand of modern technological society for light structural materials (in particular Mg alloys) emphasizes a combination of good corrosion resistance with wear properties and functionalized surfaces. Mg based materials field of applications ranges from mechanical aspects and transport components to bioengineering. Regardless of the final application, improved tailored surfaces are required to prolong service life and reduce long-term costs.
Plasma electrolytic oxidation (PEO) is an exceptional candidate to achieve that goal: it enables a considerable improvement of the mechanical properties and corrosion resistance of Mg alloys together with other characteristics, such as improved biocompatibility. PEO is an advanced electrochemical technique based on anodizing at high voltages in an appropriate electrolyte with the generation of a large number of short-lived microdischarges caused by dielectric breakdown. These shortlived plasma microdischarges facilitate a rapid growth of the coating by formation of new phases derived from complex reactions between the electrolyte and substrate species.
The present talk compiles recent studies of PEO-coated Mg alloys for structural and biomedical applications focused on corrosion protection and surface functionalization.
In the case of structural Mg alloys, it was explored the design and multidimensional screening of Flash-PEO Coatings in comparison to commercial chromium(VI) conversion coating.
In the field of biomedical application, bioactive PEO coatings on Al-free Mg alloy (with incorporated of bioactive agents) were investigated to control de degradation rate and hydrogen evolution during the process.

## Invited Speakers

# Sciforum-055398: Epitaxial oxide thin films: new insight into electrocatalysis and corrosion

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The intermittent nature of renewable energy sources requires a clean, scalable means of converting and storing energy. One Earth-abundant storage option is water electrolysis: storing energy in the bonds of $O_2$ and $H_2$, and later extracting electricity by the electrochemical reaction of gasses in a fuel cell. Perovskite oxides ($AMO_3$) can be highly active for the oxygen evolution reaction (OER). I will present studies of model oxide electrodes grown by pulsed laser deposition (PLD) and molecular beam epitaxy (MBE) on single crystal substrates that display a known crystallographic orientation, strain, surface area, and path for charge transport. Electrochemical measurements on these heterostructures can establish the intrinsic activity of oxide catalysts in a way that cannot be realized with polydisperse nanoparticle systems, and we use these findings to rationally design the composition and structure to maximize activity while maintaining stability. This fundamental understanding aids in the design of active, earth-abundant electrocatalysts for efficient conversion of renewable energy into chemical fuels.

## Flash Poster Presentations

# Sciforum-052240: Deposition of stoichiometric $VO_2$ on ultra-thin glass in roll-to-roll process.

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Vanadium dioxide ($VO_2$) exhibits different polymorphic structures, among them $VO_2$(B) and $VO_2$(M1), which are widely studied in science in technology development for their application potential: $VO_2$(B) can be used as, e.g., electrode materials for batteries and $VO_2$(M1) as thermochromic layer for Intelligent Glass Units (IGU).
Through reversible, temperature-dependent semiconductor-to-metal transition of low-temperature monoclinic $VO_2$(M1) to high-temperature tetragonal $VO_2$ (R); electrical and optical properties are changed. Especially the transmission in infrared (IR) wavelength range can be significantly reduced. Such thermochromic behaviour can lead to a reduction of the energy consumption of buildings, particularly for cooling.
We present the deposition of crystalline stoichiometric $VO_2$(B) and thermochromic $ZrO_2/V_{1-x}W_xO_2$(M1)/$ZrO_2$ thin films on ultra-thin glass (300 mm width and 100 μm thickness) in a roll-to-roll process with High Power Impuls Magnetron Sputtering (HiPIMS) with a pulsed $O_2$ flow control. The bottom and top $ZrO_2$ antireflection layers optimize the optical properties of the film, the top $ZrO_2$ layer increases the mechanical and chemical stability and the crystalline bottom $ZrO_2$ layer improves the $VO_2$ crystallinity and the process reproducibility. The doping of W leads to reduction in the switching temperature of $VO_2$ from 57 °C for thin films to even 30 °C. The deposition process is run without substrate bias at a low deposition temperature of 400 °C.

## Flash Poster Presentations

# Sciforum-048210: Deposition of synthetic and bio-based polycations onto negatively charged solid surfaces: Effect of the polymer cationicity, ionic strength, and the addition of an anionic surfactant

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The deposition of layers of different polycations (synthetic or derived from natural, renewable resources) onto oppositely charged surfaces has been studied using ellipsometry and quartz crystal microbalance with dissipation monitoring (QCM-D). Information about the thickness of the deposited layers and their water content was ascertained. The adsorption of the different polycations onto negatively charged surfaces was found to be a complex process, which is influenced by the chemical nature of the polymer chains, ionic strength, polymer concentration, and the addition of additives, such as surfactants. The experimental picture shows a good agreement with theoretical calculations performed using the self-consistent mean field (SCF) approach. The results show that the electrostatically-driven deposition can be tuned by modifying the physico-chemical properties of the solutions and the chemical nature of the adsorbed polymer. This versatile approach is a big step forward in aiding the design of new polymers for many industrial applications and, in particular, the design of sustainable washing formulations for cosmetic applications

## Flash Poster Presentations

# Sciforum-050603: Compositionally Graded Sodium Tantalate Thin Films Deposited by Chemical Beam Vapour Deposition

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Among $ABO_3$ perovskite oxides, sodium tantalate has attracted much attention as an efficient photocatalyst for overall water splitting and photodegradation of organic pollutants under ultraviolet radiation. The remarkable photocatalytic properties of this semiconductor have been mainly ascribed to the favourable band-edges position and efficient carrier delocalization due to the distortion of the $TaO_6$ octahedra [1]. A significant research effort has been dedicated to improve the visible-light activity of sodium tantalate, as well as to tune its crystallinity, particle size, and morphology, equally important for developing effective photocatalysts [2].
Chemical beam vapour deposition (CBVD) with combinatorial approach is a technique developed in the early 2000s for the growth of multi-element and multi-functional thin films. This deposition method makes use of molecular beams of chemical precursors emitted from several punctual sources with Knudsen-like effusion into a deposition chamber under high vacuum conditions. As gas phase collisions are negligible, the precursor molecules reach the heated substrate with ballistic trajectories and decompose thermally [3]. Ballistic regime and configuration of active sources allow stoichiometric gradients, leading to combinatorial investigation of material properties: we control the amount of each precursor reaching a given position on the substrate used for deposition, thus enabling stoichiometry tuning.
In this work, we focus on the deposition of sodium tantalate thin films by CBVD and on the characterisation of their composition, structural, and morphological properties. The used CBVD reactor relied on up to six effusive sources for each precursor distributed in a circular geometry [3]. Two different source configurations were tested: 1) one active source for Ta opposite to one active source for Na precursor (1_1); 2) one active source for Ta and six active sources for Na precursor (1_6). The 1_1 configuration ensured the widest range of the Na/Ta element ratio (2.5-0.6) in the deposited materials at the expense of the growth rates, which were up to ten times lower compared to those achieved in 1_6 configuration. The effects of varying the substrate temperature and the Na flow were investigated in this second configuration. The crystallinity of the deposited thin films was significantly impacted by the precursors flow ratio with the growth of orthorhombic structure at Na/Ta > 1, leading to gradual loss of crystallinity at Na/Ta 1 and eventually to the growth of amorphous material at Na/Ta=0.6-0.7. Amorphous phase was also deposited at substrate temperature below 500°C and converted to orthorhombic structure upon post-annealing at 750°C in argon atmosphere. Scanning electron microscopy (SEM) revealed the formation of well-defined crystalline grains. Our results show how CBVD is a powerful combinatorial technique for the fabrication of graded sodium tantalate thin films with wide compositional and crystallinity spreads.

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# Sciforum-053264: Pulsed Laser Deposition of $TiO_2$ thin film and their functionalization with folic acid

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$TiO_2$ thin films and nanostructures functionalized with specific biomolecules have been used in the manufacture of highly sensitive and selective electrochemical biosensors.[1] In particular, nanomaterials functionalized with folic acid for detection of folate receptors are highly interesting, because these receptors are over-expressed in most cancer cells and, therefore, their identification can allow the detection and even the photothermal treatment of cancer. [2-3] In this work, a methodology for the manufacture of $TiO_2$ thin films and their functionalization with folic acid is presented. $TiO_2$ thin films were obtained by pulsed laser deposition at different fluence values of the laser light between 1.3 and 2.5 J/cm$^2$ at a constant deposition time of 5 min. The deposition chamber had a base pressure of 7.4x10-3 Pa and the deposition of the film was carried out on a Si substrate at room temperature, under a pressure of 4.6 Pa of oxygen. Thin films with and without functionalization were characterized by X-ray photoelectron spectroscopy (XPS), atomic force microscopy (AFM), and Raman spectroscopy. AFM images of the obtained films show that as the fluence of laser light increases, the thickness and RMS roughness of thin film increases. The AFM analysis of the functionalized films evidenced a decrease in roughness, with respect to the non-functionalized film, indicating that the folic acid molecules were mainly anchored in the valleys of the film. The Raman analysis as by XPS showed evidence of the interaction of folic acid with the surface of $TiO_2$ through the pteridine ring. In this way, the reported methodology allows for obtaining $TiO_2$ thin films functionalized with folic acid that can be tested in future research in the detection of cancer cells.

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# Sciforum-052109: Additive effect of Cu doped $CH_3NH_3PbI_3$ perovskite solar cells

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Perovskite solar cells have high potential to use the photovoltaic application because of high conversion efficiency, low cost, and easy fabrication process. Additive effects of copper (Cu), guanidinium (GA) and potassium (K) compounds to lead-based perovskite solar cells on the photovoltaic properties and microstructures were investigated in the present work. The stability of the conversion efficiencies was achieved for a device containing +CuCl 2% +KI 2%. Electronic structures and stabilities were also investigated by first principles calculation. Effects of co-addition of Cu and alkali metals were discussed.

# Sciforum-052106: Additive effects of methyl ammonium bromide or formamidinium bromide in methylammonium lead iodide perovskite solar cells using decaphenylcyclopentasilane

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The mixed cation lead halide perovskite compounds having chemical elements and crystal structure have the advantage for developing the photovoltaic devices with improving stabilities of conversion efficiency. Controlling composition ratio of organic cation in the mixed perovskite crystal optimized the photovoltaic performance related with the surface uniformity and smoothing. The methylammonium bromide (MABr) or formamidinium bromide (FABr) added perovskite solar cells with decaphenylcyclopentasilane (DPPS) were fabricated and characterized for improving the photovoltaic performances and the surface morphologies. Additive effects of MABr or FABr into the perovskite crystal with DPPS were investigated by the photovoltaic characteristics. The addition of 5% MABr or FABr into the perovskite layer with DPPS formed the uniform morphologies with monodispersed grains in the perovskite layer, improving the photovoltaic parameters, such as conversion efficiency related with short circuit current density, shunt resistance, open-circuit voltages, and external quantum efficiency. Addition of FABr into the perovskite layer with DPPS promoted the uniform surface morphologies while reducing the appearance of pinholes in the perovskite layer. The photovoltaic performances depended on the morphologies condition, uniform dispersion of the crystalline grains, the crystal growth and orientation for promoting the carrier-diffusion with suppression of the carrier recombination in the perovskite layer. The photovoltaic performances were associated with the uniform morphologies, the crystal growth and orientation in the perovskite layer inserted by MABr or FABr and DPPS. The stabilities of the photovoltaic performance depended on the degree of incorporation of MABr or FABr with the DPPS layer, which suppressed decomposition in the perovskite layer.

# Sciforum-047091: Conductive epoxy/carbon nanofiber coatings for scale control

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Calcium carbonate ($CaCO_3$) is one of the most common scaling minerals and has been a long-standing problem for many industries. Undesirable scale formation can clog wells and pipelines in the oil and gas industry, affect the efficiency in nuclear power plants, and is described as a major challenge in wastewater reclamation and in the development of geothermal energy. Since precipitation of $CaCO_3$ is pH-dependent, scaling calcium carbonate on conductive surfaces can be prevented electrochemically by applying anodic polarization. However, anodic polarization is restricted to materials that do not undergo corrosion at anodic polarization conditions. Thus, in this study, we propose applying a conductive coating to a metal surface to allow anodic polarization and inhibit surface scaling without corrosion taking place. An epoxy/carbon nanofiber (CNF) conductive coating was developed and deposited onto steel (SS316) surfaces. The anti-scaling performance of the coating under anodic polarization was investigated upon exposure to a 1.5 wt% $CaCl_2$ solution in contact with $CO_2$. The coating was tested at different potentials to find optimal conditions for scale inhibition. Potentials greater than 3 $V_{OCP}$ (open circuit potential) caused a degradation of the coating due to the oxygen evolution at the anode. At 1.5 and 2 $V_{OCP,}$ the coating remained intact and the precipitation of $CaCO_3$ was significantly reduced. The cathodic polarization of the coating was also investigated. Enhanced scaling and no coating degradation were observed during cathodic polarization, even at potentials as high as -5 $V_{OCP}$. In this study, we show that the polarization of steel coated with epoxy/CNF composite material can be utilized to either prevent surfaces from scaling or enhance scaling of pH-sensitive scaling minerals.

# Sciforum-049946: Does the supporting electrolyte affect the metal electrodeposition? The Hofmeister series applied to the copper plating

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The effect of various supporting electrolytes was investigated using saline species with fixed cation in order to check the effect of the anion. To enhance the specific ion effect a simple galvanic bath containing only the metal precursor was used, without any complexing agent, surfactant or organic additive. The Hofmeister series orders the ions depending on their ability to either salt out or salt in proteins. This specific ion effect has been the subject of several studies of great scientific interest, which have found remarkable outcomes in biochemical and colloidal systems [1]. According to some authors this effect is associated to the variation in solvation energy between the ions and the solvating water molecules. Ions are commonly distinguished between kosmotropes (order makers), that possess a large Gibbs free energy of hydration surface, a low polarizability, a small partial molar volume and decrease the solubility of nonpolar molecules ("salting out"). By contrast chaotropes (order disruptors) increase the solubility of nonpolar molecules ("salting in") and shows a lower Gibbs free energy of hydration surface, a large polarizability, and a greater partial molar volume. Part of the series, going from the kosmotropic to the chaotropic side, is: $SO_4^{2-} > NO_3^- > ClO_3^- > PF_6^-$.
In this work, we looked for a connection between the specific ion effect and the electrodeposition of copper. Copper was chosen because it is a commonly used metal employed in the galvanic industry and its deposition is relatively simple and straightforward. The relevance of the nature and properties of the investigated anions on the efficiency of metal deposition, the crystalline morphology and the kinetics of plating was monitored, at constant temperature. The study was sustained by electrochemical measurements (cyclic voltammetries and chronoamperometries) to make sure that no metal complexation was taking place and to evaluate the nucleation and growth mechanism; morphological characterization (SEM); crystalline analysis (XRD); deposition efficiency, measuring the film thickness (XRF).
This study aims to open new perspectives in the field of electrodeposition, both from the scientific and the application point of view, in order to provide green alternatives in the electroplating industry [2]. Indeed, if changing only the electrolyte could produce any improvement in the coating deposition, the use of organic additives and toxic compounds in a galvanic bath might be minimized, reducing their environmental impact. According to our preliminary measurements, we found differences in the morphology of the electrodeposited films, depending on the background electrolyte.
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# Sciforum-052043: Effect of surface roughness on the wettability of anodized and PTFE-impregnated aluminum surfaces

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The paper presents the method of producing layers on aluminum with different surface wettability . The hydrofiling, hydrophobic, and superhydrophobic properties have been obtained. Layers of porous alumina were produced by anodic oxidation on samples with different roughness profile, starting from smooth one to about Ra = 5; 10; 15 μm, and then impregnated in 10% aqueous PTFE dispersion. Mechanical surface treatment was carried out with the vibro-abrasive method. The nanoporous oxide layer was produced in a solution of sulfuric acid. The adsorption properties of the oxide coatings facilitate the impregnation process. Dispersion of PTFE was used for this purpose as a material with low surface energy. The structures of the layers were characterized by means of SEM. Roughness profiles of the samples were made by optical microscope. Wettability has been characterized by the contact angle. The roughness dimension was correlated with the wettability properties. The sample with Ra= 5 μm i 10 μm were characterized with the average contact angle about 152°i 159 °, respectively, so they showed superhydrophobicity. Estimations of surface energy by Smartdrop Test Inks have been done for anodized samples after abrasive blasting, without and with PTFE impregnation. Obtained results showed correlation with contact angle measurements. Potentiodynamic corrosion tests were also carried out in 0.5 M NaCl. The supehydrophobic anodic layer revealed good corrosion resistance compared to anodic layers.

# Sciforum-051807: Effects of decaphenylcyclopentasilane insertion and high-temperature annealing on $CH_3NH_3PbI_3$ perovskite photovoltaic devices

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The effects of a decaphenylcyclopentasilane (DPPS) treatment on perovskite solar cells were investigated. The DPPS layer was inserted at the perovskite/spiro-OMeTAD interface. The conversion efficiencies were improved by inserting the DPPS layer during spin-coating of $CH_3NH_3PbI_3$ and annealing above 190 °C. A cell fabricated at 220 °C had the highest photoconversion efficiency among the as-fabricated cells, and the conversion efficiencies of all devices remained stable over more than 8 months in air. In addition, a device fabricated at 190 °C had the highest efficiency following room-temperature aging. The DPPS treatment promoted fewer lattice defects and grain boundaries, which suppressed the leakage current and increased the short-circuit current density. The effectiveness of the DPPS on hole transport was also confirmed by ab initio molecular orbital calculations. These findings indicate that high-temperature annealing of devices treated with DPPS in chlorobenzene is an effective and easy method for improving the photoconversion efficiencies and stability of the $CH_3NH_3PbI_3$ solar cells.

# Sciforum-052103: Effects of GAI addition to $CH_3NH_3PbI_3$ perovskite solar cells inserted with decaphenylpentasilane

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Addictive effects of guanidinium [$C(NH_2)_3$, GA] iodide to $CH_3NH_3PbI_3$-based photovoltaic devices, fabricated at high temperature of 190°C in atmospheric air, were investigated. The addition of GAI and insertion of decaphenylpentasilane between the perovskite and hole transport layer improved the external quantum efficiency and short-circuit current density. X-ray diffraction showed that the lattice constant of the perovskite crystals increased by the addition of GA, and the surface morphology was improved by the GA addition. First-principles calculations on the density of states and band structures showed reduction of the total energy by the GA addition and the effectiveness of nitrogen atoms in GA.

# Sciforum-052101: Effects of zirconium or titanium addition on the microstructures and thermal conductivities of carbon/copper composite materials

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Carbon(C)/copper(Cu)-based materials with high thermal conductivity and good stability at high temperatures were developed by adding a small amount of zirconium or titanium, which have low enthalpies of alloy formation with C and Cu. The isotropic fine-grained nuclear grade graphite and felt type C/C composite, which were impregnated by Cu alloys, provided higher thermal conductivity at elevated temperatures than the original carbon materials. Microstructural analysis showed that the increase of thermal conductivity is due to the formation of metal compounds at the C/Cu interface. These carbon-based materials could be a candidate material for the plasma facing components of fusion devices.

# Sciforum-052111: Fabrication and characterization of ethylammonium-based perovskite solar cells added with Rb

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Perovskite solar cells are solar cells based on the perovskite crystals. The purpose of this study is to improve the conversion efficiency and stability of the perovskite solar cells by adding a small amount of ethylammonium (EA) and rubidium (Rb) to the $CH_3NH_3PbI_3$ compounds. Polysilane layers were also used to improve the stability. The co-addition of EABr and RbI provided an increase in carrier concentration and promotion of perovskite crystal growth, resulting in an improvement in conversion efficiencies and stabilities.

# Sciforum-049451: Glass surface roughness correlation with adhesion in polymer-glass hybrid injection molding

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Polymer-glass components can be fabricated using different processes nowadays. These processes have disadvantages due to the necessary large number of fabrication steps and restrictions in productivity, as well as due to the achievable component complexity.
Hybrid injection molding technology is a new approach which will enhance the possible options to use glass assembly of very complex multi-component products in a single step. In addition, it allows excellent final tolerances, as well as the reduction of finishing requirements. These are further enhanced by cost benefits resulting from their relative ease of assembly. However, there is still a lack of information of the polymer-glass hybrid molding process, since glass presents a fragile behavior when subjected to bending stress, behavior that occurs often during the filling the mold cavity process. Therefore, it is necessary to evaluate the behavior of the glass insert to the overmolding process, and the adhesion between the two materials that guarantees the tightness and resistance of the hybrid structure.
This research work focuses on investigating the correlation between the surface topography of glass, injection overmolding process parameters and polymer-glass interface. The primary approaches to provide maximized interfacial adhesion are via surface modification to create greater surface roughness. To this end, acid etchings based on hydrofluoric acid and other formulations were studied. In order to strengthen the adhesion of polymer to glass, silanes were applied as adhesion promoter. The effectiveness of the surface treatment was experimentally evaluated using surface analytical tools including optical microscopy, scanning electron microscopy and water contact angle. Adhesion was measured using the shear test in order to find the optimal match between processing parameters and bonding strength. As an outcome, the mold temperature, injection pressure, and surface roughness were found to influence bonding at the interface.

# Sciforum-052239: Influence of different substrates on the mechanical and tribological properties of cold spray ($Cr_3C_2$-25(Ni20Cr))-5(Ni25C) cermet coatings with the addition of solid lubricant

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Composite deposits produced by cold spraying have properties that make them often used in various industries such as aerospace and automotive mainly for application to machine elements. The advantage of the cold spray process is obtaining coatings that have excellent mechanical and tribological properties, as well as with the same phase composition as the feedstock powder. The ($Cr_3C_2$-25(Ni20Cr))-5(Ni25C) coatings were cold sprayed on the Al 7075 and 1H18N9T steel substrates using high-pressure cold spray system Impact Innovations 5/8 with robot Fanuc M-20iA. The tests of coatings using X-ray diffraction using a Bruker D8 Discover diffractometer methods allowed identification of the phase composition of the sprayed coatings. Characterisation of the microstructure was made based on observations carried out of the scanning electron microscope FEI E-SEM XL 30. The FEI TECNAI G2 TEM was used to investigate the coating microstructure in micro/nanoscale. The coating hardness test (HV0.3) according to the standard referred to as the Vickers hardness test at low loading force was performed using a device of the company CSM Instruments SA. The three-point bending test was performed with the INSTRON 6025 device. The abrasive wear tests were carried out using an ITEE T-07 tester and loose abrasive $Al_2O_3$ particles. The ball-on-disk tribometer T-21 under different loads and temperatures was used to study tribological tests according to the standard. The adhesion test was carried out by Positest AT-A device. The influence of different substrates on the mechanical and tribological properties of cold spray ($Cr_3C_2$-25(Ni20Cr))-5(Ni25C) coatings was observed. The coatings on the steel substrate revealed higher hardness HV0.3 and less removal material during abrasive wear tests with loose abrasive $Al_2O_3$ particles than that deposited on the Al 7075 alloy. The force required to crack the coating in three-point bending test was about 10% higher for the deposit sprayed on the steel substrate.

# Sciforum-052218: Influence of proton irradiation on positron annihilation parameters in nanoscale Zr/Nb metal layers

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Nanoscale multilayer coating (NMC) based on Zr/Nb layers before and after H+ irradiation was investigated using experimental techniques. Detailed studies of structural and phase state and defect structure of Zr/Nb NMC were performed using transmission electron microscopy methods, X-ray structural analysis, glow discharge optical emission spectrometry, and the Doppler broadening spectroscopy using variable energy positron beam. The thickness of the individual layers varied from 10 nm to 100 nm. Single-layer Zr and Nb coatings were also prepared to understand the annihilation parameters in the individual NMC Zr/Nb layers. The coatings with a total thickness of 1.05 ± 0.05 μm were irradiated with 1750 keV protons using Van-de-Graaff electrostatic accelerator EG-5 at JINR, Frank laboratory of neutron physics for 15, 30, and 120 minutes, the irradiation dose was 3.4·1015, 8.6·1015, and 3.4·1016 ions/cm2, respectively. A 33-μm aluminum degrader was used to achieve the required proton implantation depth. Analysis of the defect structure by DBS showed that in the whole range of energies of the implanted positrons, there is a tendency to decrease the DBS parameter's S value with an increase in the irradiation dose. In the studied NMCs Zr/Nb before and after the proton irradiation, one predominant center of the capture of positrons excess free volume near the interface in the zirconium vicinity is preserved. The research was funded by the Russian Science Foundation № 20-79-10343.

# Sciforum-051968: LDH coatings on AZ31 Mg alloy: characterization and corrosion performance

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Conversion coatings based on layered double hydroxides (LDH) are emerging as an environmentally friendly approach for corrosion protection of Mg alloys. LDH coatings can act as microcontainers for the encapsulation of corrosive species or inhibitors due to their hydrotalcite-like structure.
This study is focused on the effect of the source of ions on the LDH characteristics. In this study, different monovalent (Li) and divalent (Ca, Mn, Zn) cations with two different types of trivalent (Al, Fe) metal nitrates are investigated.
The coatings were fabricated by a two-step hydrothermal process. The morphology and composition of the coatings were characterized by scanning electron microscopy (SEM), X-ray diffraction (XRD) and attenuated total reflection (ATR) Fourier transform infrared spectroscopy (FTIR). Corrosion performance was assessed by electrochemical impedance spectroscopy (EIS). The water drop contact angle was also evaluated for each coating. Micrographs revealed that most of the coatings had a characteristic flaky morphology. The formation of hydrotalcite-like structures is confirmed by XRD and FTIR. The XRD peaks associated with the (003) and (006) planes are clearly observed in all coatings. The FTIR analysis confirms the incorporation of water molecules and nitrate ions in the intergallery spaces. Electrochemical measurements showed that the LDH coatings increased the impedance modulus at 0.01 Hz by at least one order of magnitude compared to the bare substrate. The water drop contact angle revealed a high grade of hydrophilicity of the manufactured coatings.

# Sciforum-052214: Mechanical and tribological properties of Ni/graphene nanocomposite coatings produced by electrochemical reduction method

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Dynamic progress of technology prompts the search for new, more functional materials. Composite coatings produced by electrochemical methods offer great opportunities in this field. The selection of the matrix material and the dispersion phase of the coating affects on properties of the final products.
The paper presents the results of research on nanocomposite nickel coatings with embedded flakes of graphene produced by electrochemical reduction method and their influence on the mechanical and tribological properties of produced materials.
Composite Ni/graphene coatings and, for comparative purposes, Ni coatings were deposited on a steel substrate. Flakes of graphene were used for the production of the coatings. The coatings were deposited from a Watts bath at different concentrations of graphene in the bath, namely 0.1; 0.2; 0.5 g/dm$^3$. The deposition process was carried out at current density of 3 A/dm$^2$, constant stirring speed of 300 rpm, bath temperature of 45 ° C, and deposition time of 60 minutes. The paper presents the characteristics of the used graphene. Results of morphology studies and surface topography of the coatings, as well as the structure of the produced coatings are exhibited. The mechanical properties of the produced coatings were tested by the Depth Sensing Indentation (DSI) method. Relationships of the loading force and relieving and displacement of the indenter during plastic and elastic deformation of the tested materials are presented. The Vickers hardness, Indentation hardness, and Martens hardness, as well as the modulus of elasticity and creep of the produced coatings are determined. The tribological tests were carried out using the ball on disc method.
The incorporation of graphene into the nickel matrix changes the morphology and topography of the surface of the produced coatings and increases the hardness and wear resistance of the coating material.

# Sciforum-052125: Microstructures and photovoltaic properties of polysilane-added perovskite solar cells

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Perovskite solar cells are being studied because of their high efficiencies, low cost, and easy fabrication process. However, there are some issues in terms of durability. In the present work, $CH_3NH_3PbI_3$ perovskite photovoltaic devices treated with a polysilane layer were fabricated and characterized. Decaphenylcyclopentasilane (DPPS) in chlorobenzene solution was spin-coated between the perovskite layer and the hole transport layer (spiro-OMeTAD), and the resulting device was annealed at 190 °C. The DPPS-treated devices had higher conversion efficiencies than the standard and they were stable in ambient air. Microstructural observations suggested that DPPS would work effectively like a bulk-hetero structure along with perovskite layers.

# Sciforum-052275: Ni-B/B composite coatings produced by the electroless deposition method

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The paper presents the results of research on Ni-B and Ni-B/B coatings produced by electroless deposition method on a carbon steel substrate. Three different contents of the dispersion phase in the bath were used.
The topography and surface morphology, as well as the structure characteristics of the produced materials are presented. The microhardness of the deposited coatings was tested. A scratch test and corrosion resistance tests of Ni-B and Ni-B/B coatings were carried out.
The conducted research allowed to determine the influence of the dispersion phase content in the bath on the properties of the produced coatings. The uniform incorporation of the particles of the dispersion phase into the Ni-B matrix was confirmed. The produced coatings are characterized by uniform thickness, compact structure, and good adhesion to the substrate. Incorporation of the boron particles into the Ni-B matrix increases hardness and surface development degree of the composite coatings compared to Ni-B alloy coating.

# Sciforum-049930: Optimization of the experimental parameters for the design PCL-ZnO electrospun fibers with tunable hydrophobicity

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In this work, a comparative study is presented that uses the electrospinning technique for the design and development of functional surfaces with a desired morphology in terms of wettability and corrosion resistance. With the aim to obtain the coatings with the best properties, a strict control of several input operational parameters (mostly applied voltage, flow rate, and collector distance) has been performed. In addition, a dual effect associated to the polymeric precursor concentration (polycaprolactone, PCL) and ZnO nanoparticles proportion has been also evaluated for showing a key role in the final properties. It has been demonstrated that the solution concentration has a significant effect on the structure in the final polymer obtained on the collector, being possible the formation of beads with a spherical shape or spindle-like beads at low solution viscosities. Moreover, the presence of the ZnO nanoparticles plays an important role in the wettability behavior of the electrospun fibers. Finally, in order to evaluate the coating morphology for the better performance, the following parameters, such as fiber diameter, surface roughness (Ra), corrosion rate, and wettability have been deeply analyzed.

# Sciforum-051966: Sol-gel synthesis of catalytic layers $Mo_2C$-WC on the alumina surface

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Ultrafine molybdenum and tungsten carbides are of considerable interest in various catalytic processes, including the conversion of methane and propane, the main components of associated petroleum gas. The development of a sol-gel technology for supported catalysts based on them will make it possible to switch to industrial production of catalytic membranes. As disperse systems, it is proposed to use dispersions of molybdenum-tungsten blue obtained using ascorbic acid.
Molybdenum-tungsten blue nanoparticles are formed as a result of the self-assembly process of building blocks. The formation of building blocks occurs with the partial reduction of molybdate and tungstate ions in an acidic medium using an organic reducing agent—ascorbic acid.
To obtain catalytic coatings by the sol-gel method, the initial dispersions were concentrated by evaporating the system in air. To create a coating on the surface of alumina, dip-coating was chosen; the contact time was 3 s. To achieve the specified content of the active component, the coating-drying cycle was carried out several times. To form the carbide phase, the samples were calcined in an inert atmosphere at a temperature of 900 °C. The catalysts were studied by SEM, ASAP, XRD methods.

# Abstracts

## S4. Coatings for Food Packaging and Preservation

## Invited Speakers

# Sciforum-054978: Postharvest Disease Control and Quality Maintenance of Fresh Fruits and Vegetables by Antifungal Edible Coatings

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Weight loss, physiological disorders, and postharvest diseases are the main causes of economic losses of fresh fruits and vegetables after harvest. Synthetic waxes, commonly amended with chemical fungicides, are currently often applied before cold storage or commercialization to reduce these losses. However, the continuous use of such agrochemicals is arising important health and environmental issues due to the presence of chemical residues on/in the fruit. Therefore, safe and cost-effective alternatives for postharvest preservation of horticultural products should be found and commercially implemented. Composite edible coatings (ECs), formulated with hydrocolloids (polysaccharides such as cellulose derivatives, alginates, pectins, gums, and peptides or proteins) and lipids (e.g., acylglycerols, fatty acids, natural waxes), have the potential to substitute synthetic waxes because they can regulate both fruit transpiration and respiration during storage. In addition, they can be formulated with specific food-grade antifungal ingredients to provide activity against pathogens that cause postharvest diseases. Thus, these resulting antifungal ECs can be a useful solution for both physiological and pathological issues causing postharvest losses. Antifungal ingredients of synthetic ECs can be low-toxicity chemical compounds and biological control agents (antagonistic strains of some bacteria, yeasts, or filamentous fungi). The former include natural or synthetic chemicals approved as food additives or generally recognized as safe (GRAS) compounds, such as some inorganic or organic salts (e.g., carbonates, sorbates, benzoates) and some essential oils, plant extracts, or antimicrobial peptides and proteins. Other natural ECs, such as chitosan or *Aloe* spp. gels, show inherent antifungal activity but can also be formulated with additional antifungal ingredients. Antifungal ECs can be applied after harvest as part of non-polluting integrated disease management (NPIDM) programs for postharvest decay control and quality maintenance of fresh fruits and vegetables.

# Invited Speakers

## Sciforum-054980: Prickly Pears Bioactive Compounds Preservation by Edible Coatings

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Prickly pears, the fruits of *Opuntia ficus indica* L. Mill (OFI), are widely used for human consumption due to their rich variety of nutrients, namely sugars, minerals, fibers, and bioactive compounds (e.g., ascorbic acid, betalains, flavonoids, phenols) [1,2]. Since they are highly perishable, it is important to find alternatives for their preservation. Generally, prickly pears are refrigerated (5 ºC to 8 ºC), which may cause chilling injuries that lead to the appearance of pitting spots and browning, diminishing their shelf-life. Thus, the application of edible coatings as an alternative or complementary treatment to refrigeration emerges as a possibility to maintain prickly pears' quality.
In this context, the main objective of this work is to evaluate the effect of different edible coatings (alginate, pectin, corn starch, and chitosan) on the bioactive compounds' preservation of prickly pears. Fruits from two different varieties (orange and red) were submerged in the coating solutions (2 % w/v polymer), left to dry, and kept refrigerated (5 ± 2 ºC) for 5 weeks. To evaluate the effects of the different coatings, samples were analyzed every week for five weeks in terms of their bioactive properties (total phenolic compounds, antioxidant activity (DPPH assay), ascorbic acid content, betanin, and indicaxhantin content). Fruits without edible coatings were used as control.
The results indicate that edible coatings helped delay the bioactivity loss of the fruits over time. At the end of 5 weeks, the control revealed a decrease in ascorbic acid content of 50% when compared to the initial value, while the fruits coated showed decay of 30%. The uncoated fruits showed a loss of 84% in antioxidant activity, but the edible coatings chitosan and starch helped sustain the antioxidant activity, leading to a loss of only 25%. The uncoated red fruits with high content in betalains showed a loss of betanin and indicaxhantin of 46% and 58%, respectively. The use of chitosan and starch as coating material led to smaller losses of those pigments, with a decrease of 25% for betanin and 23% for indicaxhantin.
Starch and chitosan are the edible coatings that best prevent the loss of bioactive compounds from prickly pear under refrigerated conditions.

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## Flash Poster Presentations

# Sciforum-052249: Chitosan-based multicomponent antibacterial coatings to prevent biofilm formation for food packaging application

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The uncontrolled growth of biofilms and rise of antimicrobial resistance (AMR) cause significant damage in many industrial and public sectors, including food industry. The need of new and efficient antimicrobial materials which are able to kill or inhibit pathogen microorganisms calls for fast response from a research community. Chitosan (CS) is a widely used cheap polymer and is known for its intrinsic antimicrobial and non-toxic properties. In particular, chitosan films have found application as a packaging material to prevent food spoilage caused by foodborne pathogens and act as an eco-friendly alternative to petroleum-based materials. CS can be potentially combined with other antimicrobial components, which can both increase its mechanical and antimicrobial performance. One of the candidates is tannic acid (TA), which has been proven to be an efficient crosslinking agent with intrinsic antimicrobial action. To provide even more pronounced antimicrobial action, inorganic nanophases, in particular metal nanoparticles, could be incorporated or in situ synthesized and immobilized in the polymer matrix. This way, the inorganic component can promote the generation of reactive oxygen species (ROS). ROS, along with and the metallic ion release can work synergistically with the bioactivity provided by the organic polymer matrix, thus efficiently inhibiting the pathogen growth, without causing the resistance development. Thanks to the controlled mixing of two or more solutions containing the organic and inorganic phases, solution casting method could be used to create thin antimicrobial coatings on various surfaces.
These hybrid multi-component coatings were developed and characterized by several spectroscopic (e.g., FT-IR, UV-vis) and microscopic techniques (e.g., TEM). The resulting coatings are also subjects for further antimicrobial activity evaluation tests, synergistic antibiofilm, and antimicrobial coatings.

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## Flash Poster Presentations

# Sciforum-052216: Sustainable multifunctional biobased coatings from waste sources for paper and bioplastics

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Biobased polymers are materials of growing interest to prevent the environmental concern caused by fossil plastics contributing to Greenhouse Gases Emissions and their problem of being materials destined to exhaust. The use of biobased polymers often required additives or functional coatings to reach the same properties shown by traditional materials. In the framework of the ECOFUNCO project, the preparation and characterization of coatings based on active molecules extracted from waste of agro-food were studied. In particular, molecules as polyphenols, extracted from tomato waste using techniques such as microwave-assisted extraction (MAE) and chitin nanofibrils, were used. Chitin nanofibrils were obtained from the chemical treatment of shrimps and mushrooms and their subsequent mechanical defibrillation with high-pressure homogenization (HPH) or grinding. Biobased coatings were applied on different substrates, such as paper tissues and boards, for personal care and disposable products or bioplastic sheets for food packaging. Active molecules obtained from waste sources through chemical and physical treatments were used to produce water-based coatings (WBC) in the form of suspension or solution. Coatings based on chitin nanofibrils were applied in the form of gel on paper and bioplastics to ensure antibacterial properties, while polyphenols were applied on paper tissues to ensure antioxidant properties. In order to increase the compatibility between the WBCs and some plastic substrates, as well as the adhesiveness of these coatings, an innovative system including a biobased primer was considered. Treated substrates were characterized by analyzing the surface properties and functional properties, such as antimicrobial or antioxidant capacity, and observing improvements for all the examined substrates.

# Sciforum-052254: Capillary Valving Phenomenon and Surface Treatment for Improved Liquid Retention in Food Packaging

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Food packaging plays a crucial role in maintaining the freshness, quality, and safety of packaged food products. It protects the contained food from biological and chemical contaminants while being convenient for the customer and supplier. However, liquid residue (exudate) of liquid-exuding foods, such as red meat, poultry, and fish, is still a big challenge to plastic food packaging. Free-moving exudate in meat packaging trays gives an unsightly and unhygienic appearance and is perceived negatively by customers. The exudate also has adverse effects on the meat's quality and safety due to the increased water activity and facilitated microbial proliferation. Although various packaging solutions have been adopted to isolate the meat exudate, such as absorbent pad and open-cell foam, these additional non-recyclable parts are problematic to the recyclability of plastic packaging as these must be manually separated and usually are glued to the bottom of the packaging trays. Therefore, a new technique is introduced to isolate the meat exudate within fully recyclable single component plastic meat trays. This technique is based on the capillary valving phenomenon of liquid-holding wells within plastic packaging to improve their liquid retention. Wells integrated into the tray base undergo a localised surface treatment to improve their surface wettability and to enhance their liquid pinning effect. A contrast in wetting properties between the wells and the rest of the tray gives more stability and pinning to the liquid menisci on the well openings. This dramatically increases the liquid retention capacity even when the plastic meat tray is turned upside down. The new meat packaging trays offer equivalent capacity performance to current absorbent pads without the need for additional absorbent material. This innovative packaging tray can therefore be made from a single recyclable polymer, ensuring full recovery of the packaging and reducing the burden of plastic waste on the environment.

# Sciforum-052221: ECOFUNCO "ECO sustainable multifunctional biobased COATings with enhanced performance and end of life options!

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The concern of plastic waste accumulation in the environment has promoted the research into sustainable alternatives to those products devoted to single use application, whose collection and recycling are difficult. In particular, hardly recyclable plastic-based multi layers materials can be replaced by fully compostable multi-layer plastic or by highly biodegradable cellulose-based materials. Cellulose is the most available renewable material on Earth and it would be beneficial for the environment to use it in consumer products, such as in personal care and disposable products for food (tableware), where hardly recyclable petro-based plastics are currently used. The limits to be overcome are the hydrophilic and low barrier properties typical of a non-woven fibrous system. For this reason versions of cellulose combined with poly(ethylene) are widely present on the market, and petro-based version of these products are currently preferred, despite their negative environmental impact.
Coating of cellulose or bioplastics with proper functional coatings, based on biopolymer and functional materials coming from agro-food waste streams, will allow improving their performances allowing them for replacing, effectively, petrochemical products in the personal care, tableware and food packaging sectors. The overall objective of project ECOFUNCO is to select, extract-functionalize molecules (proteins, polysaccharides, cutin) from highly available, low valorized biomass, such as tomato, legumes, sunflower. etc.. for the development of new bio-based coating materials to be applied on two different substrates (cellulosic and plastic based), with improved performances compared to currently available products and at the same time with more sustainable end of life options. The products developed in the project are in particular: Antimicrobial-antioxidant coatings based on chitin nanofibrills, and/or chitosan, functionalised microcrystalline cellulose (MC), for cellulose tissues (personal care), paper and cardboard (packaging for fresh products such as pasta, tableware), woven and nonwoven (sanitary), plastic substrates (bio-polyesters) for active packaging. Cutin based formulations for coatings water repellent (paper cups, service paper, etc.), water vapour barrier (packaging) and protective properties (non-food packaging). Protein-based barrier adhesive for multilayer food packaging (bio polyesters based), with sustainable end of life options (composting, recyclability). The ECOFUNCOconsortium consists of 17 partners from 8 European countries (Italy, Germany, Spain, Belgium, Croatia, Denmark, United Kingdom) and 2 Associated countries (Israel, Turkey) that gather the necessary infrastructure, knowledge, expertise, services, and industry value chain to reach the project's objectives and the expected impacts of the topic BBI 2018 R49-: Develop functional molecules for bio-based coatings outperforming existing solutions and meeting market requirements. In its vision of creating new value chains with and for the industry, the ECOFUNCO consortium benefits from a strong industrial and commercial involvement since 9 SMEs and 2 large companies collaborate with a total of 6 RTD institutions, one of them based on industrial memberships.
This project has received funding from the Bio Based Industries Joint Undertaking under the European Union's Horizon 2020 research and innovation programme under grant agreement No 837863.

# Sciforum-051147: Inclusion of pomegranate peel extract improves the water and microbiological barrier properties of gelatin/chitosan coatings for strawberries preservation

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Strawberry (*Fragaria x ananassa* Duch) is one of the most popular fruits in the world; however, since it is very perishable, its post-harvest life period is extremely short. The aim of this study was to develop a polymeric coating based on gelatin, a natural and non-toxic protein with wide application in the food industry, combined with chitosan, a natural polysaccharide with high antimicrobial activity, aiming to extend the shelf life of strawberries. To improve the active properties of this coating, pomegranate (*Punica granatum* L.) peel extract (PPE) was used as a source of phenolic compounds: the extract was obtained by ultrasound-assisted extraction of pomegranate peels in ethanol/water 60% (v/v), at 45 °C for 1 h. For the coatings formulation, gelatin and chitosan solutions were prepared in water and lactic acid, respectively, both at 1% (w/w). PPE was solubilized in a 60% (v/v) ethanolic solution, at 100 mg $mL^{-1}$, and added to chitosan (1 mL of PPE/50 g of polymer mixture), followed by gelatin mixture. The final ratio between polymers in GCE coating was 4:1 (gelatin/chitosan). To coat the strawberries, the fruits were sanitized and immersed in GCE for 2 min; control fruits were immersed in water. Fruit weight loss and decay control were monitored over 14 days. In the first 8 days of analysis, the decay control was reduced by 40% in the coated strawberries, when compared to uncoated strawberries; regarding weight loss, after 14 days of storage the coated strawberries lost about 15% less water than the uncoated ones. Thus, it can be said that the material developed presented satisfactory results as a barrier against water loss and against microbial contamination, helping to extend the strawberries shelf life.

# Sciforum-048168: Physical property analysis of cellulose/pectin biocomposites for food packaging

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The European Plastics Strategy sets a target of 2030 to ensure that only plastic packaging that is reusable or easily recyclable is used in the EU. As a result, lately, the interest in environmentally friendly and biodegradable food packaging has increased. Researchers are looking for materials that would meet the requirements of changing world. The use of biocomposites could be one of the ways to develop bio-based food packaging. Biocomposites are made of two or more different materials from which at least one is natural. Usually its biopolymers such as proteins, lipids, polysaccharides, etc. Thus, cellulose and polysaccharide pectin could be a promising biocomposite materials due to its availability, low cost, and mechanical characteristics. So, the aim of the research was to produce cellulose/pectin biocomposites by laminating prepared cellulose fiber plates with 5.0%–20.0% concentration pectin containing glycerol as a plasticizer and evaluate their properties. The solubility in water, water vapor permeability (WVP), and surface hydrophobicity of prepared cellulose/pectin biocomposites were evaluated and compared. It was observed that increased amount of plasticizer glycerol increases solubility in water, as well as WVP, but decreases surface hydrophobicity of cellulose/pectin biocomposites. The highest result of WVP was in biocomposite with 5.0% of glycerol while lowest with 1.0% glycerol. All of the analyzed cellulose/pectin biocomposites had partly hydrophobic surface and highest surface hydrophobicity was achieved in biocomposite with 16.7% pectin without plasticizer (59 °). Overall results show, that cellulose/pectin biocomposites could be a promising material in developing food packaging for dry food products.

# Abstracts

## S5. Coatings and Interfaces in Cultural Heritage Conservation and Preservation

# Invited Speakers

## Sciforum-054966: On the Different Strategies to Reduce the Decay of Stone-Built Cultural Heritage

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Deterioration phenomena of ancient and modern stone cultural heritage are natural and unrestrainable decay processes mainly arising from water percolation into stone building materials [1-11]. Thus, the application of hydrophobic/superhydrophobic coatings to stone surfaces is mandatory to protect them from the deleterious effects of water exposition.
Here, in order to avoid both natural and artificial stone decay, mainly due to the interaction with atmospheric pollutants (both gases, such as $NO_x$ and $SO_2$, and particulate matter) i) commercially available Si-based resins have been applied as protective agents [3,8,10,11], ii) new polymeric coatings have been synthesized with satisfactory water repellence and improved durability, thanks to the combined use of fluorinated and long alkyl chain monomers and without the use of any photo-stabilizers agents [2,4,5,6,7], and, finally, iii) hybrid coatings containing home-made $TiO_2$ and $SiO_2$ nanoparticles mixed with the commercial silane polymers have been tested to obtain complete buoyancy and self-cleaning properties [1,9]. Both natural stone materials (Carrara, Botticino, Candoglia marbles and Angera, Vicenza stones) and mortars (an air hardening calcic lime mortar, ALM, and a natural hydraulic lime mortar, HLM) have been used as substrate to be treated.
The results concerning the physico-chemical characteristics of the bare stones compared with those of the treated samples will be presented and discussed. In order to evaluate the stability of the applied coatings towards degradation induced by solar radiation and interaction with the atmospheric pollution, accelerated ageing tests under UV irradiation (also exposing the samples in a Q-UV tester cabinet) and exposure tests in a typical polluted urban environment have been carried out. For the samples characterization the following analyses have been performed: contact angle measurements, Scanning Electron Microscopy with X-ray microanalysis (SEM-EDS), Ion Chromatography (IC), colorimetric tests by Diffuse Reflectance Spectroscopy (DRS) followed by CIELab elaboration, porosity measurements, water absorption by capillarity and water vapor permeability.
The properties of the home-made and commercial hydrophobizing polymers in terms of macromolecular structure, molecular weights, thermal features, and water repellence were determined. Furthermore, the long-term behavior of these polymers was estimated by means of accelerated aging tests exploiting UV radiations. Their behavior over time was checked via Size Exclusion Chromatography (SEC) by evaluating $M_n$ and D data of aged polymeric samples and by Fourier Transform Infrared (FT-IR) spectroscopy: all the synthesized polymers seem to be unaffected by UV aging. Thus, the present stable resins were applied on both natural (marble) and artificial (mortar) stone substrates and their wetting properties together with their absorption by capillarity and water vapour permeability were successfully assessed and compared, showing potential features for cultural heritage protection.

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## Invited Speakers

# Sciforum-054970: The Identification of Green Pigments in Chinese Paintings

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Based on pigment analyses of many dated caves and murals as well as an investigation into historical records and inscriptions in China, it is proposed that the most popular green pigment for wall painting and architecture might be copper trihydroxychlorides rather than malachite. In order to extensively and noninvasively investigate the techniques of Chinese scroll paintings, an automatic hyperspectral scanning system was set up. Using this system as well as a macroscopic X-ray fluorescence technique, a number of important Chinese scroll paintings will be studied, a task funded by a national project. The project will result in the detection of sketches and outlines of patterns, and pigments will be identified and mapped to the painting. Furthermore, quantitative maps of pigments can be obtained, which provides vital clues about the painters' techniques and use of pigments.

## Invited Speakers

# Sciforum-054969: Nano Meets Heritage: Nanomaterials for the Conservation of Historical Buildings and Artworks

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The rapid changes in the environmental context that artworks and historical buildings are facing have forced researchers to investigate innovative strategies and materials for the conservation of historical artworks and buildings. The application of nanotechnology to the conservation of Cultural Heritage is an emerging field and has the potential to improve conservation practices. The flexibility in tailoring properties at nanoscale can enable optimization of their properties and functionalization for highly effective prevention of the degradation processes without damage or alteration of the historic substrate. In this talk, an overview of the most promising nanomaterials for conservation will be shown. In particular, laboratory results on the use of nanomaterials for cleaning (enzymes-modified with nanoparticles) archaeological textiles and self-cleaning nano-$TiO_2$ coatings for the protection stone surfaces will be discussed, together with on-site applications on historical buildings.

## Flash Poster Presentations

# Sciforum-048741: Assessment of copper alloy corrosion inhibitors 1H-Benzotriazole and 5-Phelyn-1H-tetrazole and their nanoencapsulation via one-step synthesis: a comparative study by spectroscopic methods and microscopy techniques

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Metals are fundamental materials for industrial applications, architectural buildings and Cultural Heritage artifacts. Thus, corrosion of metals and alloys is a major global issue, involving a great waste of economic resources and negative effects on the environment and on human health. For instance, organic molecules used as copper corrosion inhibitors, i.e., 1H-Benzotriazole (HBTA), and solvents needed for applications on the metal surface are often toxic and harmful for the operators. Moreover, these substances can easily spread into the environment, thus causing eco-sustainability issues and fast loss of efficacy.

For this reason, more and more efforts are being made to develop less toxic systems for the application of chemicals and to explore new inhibitors with very high efficiency at low concentrations. Currently, in the fight against corrosion, the trend is to combine both active/passive protection by dispersing the inhibitor molecules inside a polymeric matrix as an anticorrosion coating. However, the direct addition of corrosion inhibitors to a coating formulation can involve various disadvantages, such as the undesired interaction between the inhibitor molecules and the polymers of the coating, preventing proper function. More importantly, inhibitor protection against leaching is not guaranteed. The concept of "smart coatings" can be further improved by confining inhibitors in suitable inert nanocontainers able to release them on demand in order to overcome already discussed critical issues and minimize the amount of active chemical agents.

In this work, the effectiveness of two organic molecules against the corrosion of the copper-based alloy B14 is evaluated: commercial 1H-Benzotriazole (HBTA) and non-commercial 5-Phynil-1H-tetrazole (PhTA). The effectiveness assessment of the two organic molecules in a chloride environment on the B14 alloy is performed by electrochemical techniques (PP, EIS). Scanning Electron Microscopy (SEM-EDS), Atomic Force Microscopy (AFM), X-ray Photoemission Spectroscopy (XPS) and Raman Spectroscopy are performed in order to investigate the corrosion inhibition mechanism. Afterward, silica nanocapsules (SiNCs) have been prepared via one-stage synthesis, incorporating the corrosion inhibitors. The morphology and structure of the SiNCs are observed by Scanning Electron Microscopy (SEM-EDS) and Transmission Electron Microscopy (TEM), and their porosity is determined by $N_2$ physisorption (BET/BJH). The loading capacity (L%) and the encapsulation efficiency (EE%), and the composition of composite SiNCs are evaluated by UV-Vis Spectroscopy and Raman Spectroscopy, respectively.

# Sciforum-052177: Green multifunctional coating for the protection of archaeological frescoes

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This work proposes a new coating product for the protection of archaeological frescoes, designed for simultaneously responding to the art conservation needs and to health and environmental regulations [1]. This study defines a formulation based on green components that combine many of the relevant properties for fresco conservation, such as the antimicrobial and antifungal activities, as well as the bacteriostatic and hydrophobic features [2, 3]. In detail, the coating was prepared in one-pot synthesis combining a chitosan-gel, produced in a water solution substituting acetic acid with the biomass derived azelaic acid, and silver nitrate ($AgNO_3$) solution, used as precursor of $Ag^+$NPs. As reagent for NPs precipitation, Sodium Hydroxide (NaOH) was substituted with Calcium Hydroxide ($Ca(OH)_2$) because more compatible with the substrate. Such a formulation was tested on mock-up fresco samples. The synthesized nanoparticles showed an enhanced hydrophobic activity as compared with the raw chitosan hydrogel. UV spectroscopy and TEM analyses were performed to determine the adequate concentration of silver nitrate and the better precipitation agent to use. According to the results, the most performing solution was achieved with $AgNO_3$ 0.1M, in terms of synthesis yield and size and shape of NPs obtained. The sol-gel formulation was, therefore, diluted 1:1 in a mixture of two solvents: isopropanol and glycerol (in proportion 1:1), to balance rheological properties and proper evaporation time.
The effectiveness of the new formulation was assessed by testing hydrophobicity of the fresco mock-ups surfaces (static water contact angle), colorimetric stability (ΔE), chemical stability (ATR), morphological changes (OM), and water vapor permeability of the treated specimens (UNI EN 15803) before and after application on mock-ups, as well as after artificial ageing. The new coating showed a synergistic effect rendering a minimized water absorption without compromising water vapor permeability, good colorimetric, and chemical stability.

# Sciforum-052192: Photo-enhanced Gd-$TiO_2$/PDMS nanocomposites for stone preservation

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**Abstract**
The protection of stone artefacts from different defacements (chemical, physical, and biological agents) is an essential event due to their historical value. Hence, many research groups have focused on developing nanocomposite materials with multifunctional protective features to protect building stones, especially with high porosity, and to reduce the high cost of maintenance of these materials. $TiO_2$ nanoparticles have been extensively used for self-cleaning applications, particularly, cleaning and preventing colonisation of heritage building material surfaces. However, this semiconductor displays a weak activity under visible light, which can be properly enhanced by doping with Lanthanide ions. In addition, their inert colours make it possible to elaborate transparent thin films. The present research work focused to develop photo enhanced nanocomposite coatings: pure and Gd doped $TiO_2$ nanoparticles with different doping amounts were mixed, with Polydimethylsiloxane (PDMS) used as a binder. Moreover, newly prepared coatings were applied on a very porous stone substrate (Lecce stone) in order to investigate the self-cleaning properties and the protecting ability towards the historic stones from dye pollution and micro-organisms colonisation. For this purpose, different analyses and tests have been performed on the coated stone specimens, such as chromatic measurements, static contact angle measurements, water capillary absorption test, permeability to water vapour, pencil hardness test, scanning electron microscope combined with energy-dispersive X-ray spectroscopy (SEM-EDS), optical microscope analyses, self-cleaning test, and biological experiments. In addition, the durability of the coatings was studied to evaluate the stability of the elaborated nanocomposites. Results showed that PDMS mixed with 0.1 mol% Gd-$TiO_2$ materials can be considered as a promising and durable candidate to protect highly porous heritage building surfaces.


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