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INVITED SPEAKERS

Id-680

Assessment of Thin-Films for Thermo-chromic Application Using an In-Operando Approach

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Abstract: Thin-films for thermo-chromic application were tape-casted from pure vanadia, zirconium-doped vanadia and cerium-doped vanadia powders derived by wet chemistry synthesis from intermediate phase of vanadyl glycolate. We conceptualised a characterisation setup suitable for assessment of the thermo-chromic functionality reposing on in-operando grazing incidence synchrotron X-ray diffraction and Raman spectroscopy for structural evolution study of the films under isothermal conditions. The Materials Characterization by X-ray diffraction beamline goniometer demonstrated ideal performance combining flexible geometry, high resolution, and the possibility to accommodate the multi-channel equipment for in-operando characterisation, to continuously monitor the monoclinic to tetragonal transition in pure and doped vanadia phases, responsible for the transmission and reflection of light in the infrared part of the solar spectrum. Diffraction and spectroscopic results pointed out that the prepared films had a considerable level of chemical homogeneity, whereas spectroscopic results enhanced by a full-scale device allowed resolution suitable for thin-films with low-thicknesses. The fact that the transition temperature was lowered in average by 5°C suggests that metal ions doping in vanadia was successful from the structural point of view. Among doped samples, cerium-doped vanadia showed only minute phase separation, better tape casting and thermal treatment stability and consequently more favourable structure modification. Primarily on behalf of structural influence, the derived thin-films (especially cerium-doped vanadia) can derivatively be considered as candidates for materials with better thermo-chromic behaviour. Ultimately, the exploited diffraction/spectroscopic thermal in-operando setup enables comprehensive self-standing characterisation on nanoscale materials, including thermo-chromic films. This work has been funded by the projects UIP-2019-04-2367 SLIPPERY SLOPE of the Croatian Science Foundation and PZS-2019-02-1555 PV-WALL in Research Cooperability Program of the

Croatian Science Foundation funded by the European Union from the European Social Fund under the Operational Programme Efficient Human Resources 2014-2020.

Keywords: Smart Window, Thermochromic Transition, In-Operando GIXRD-Raman-f(T) Setup, Multi-Channel Characterisation, Vanadium Dioxide.

INVITED SPEAKERS

Id-681

Nano-Modified Epoxy: Effect of GO modification on Formation of Nacre-Like Structures

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Abstract: The upgrade of polymers by nanofillers (NF) is more marked in multicomponent systems where NF may induce formation of morphologies associated with synergic effects. The best performance is achieved with carbon nanoplatelets (CN), like graphene and graphene oxide (GO), due to good mechanical parameters and large specific surface, together with high potential for modifications. The effects of NF are even more complex in partially miscible systems, like epoxy thermosets, where best effectivity was found with impact modifiers attached to nanosilicate platelets through layered structures formed by a self-pinning mechanism. So far, formation of such structures has practically not been studied in CN-modified epoxy systems. Moreover, polymer chains-grafted GO with surfactant-like parameters has fair ability to form nacre-like structures. As a result, this work deals with the effect of various GO/impact modifiers combinations, including polymer chains-grafted GO in epoxy system. Understanding of formation of these effective structures is beneficial also for parallel formation of nacre-like interfacial layer in carbon-fibre composites. Suitably functionalized low-molecular-weight polymers, like aminated butadiene acrylonitrile copolymer (ATBN), aminated polybutadiene (ATB), polyoxypropylene diamine (APOP), and polyethylene glycol (PEG) were applied to prepare GO-polymer chains adducts. Their application in epoxy led mostly to formation of lamellar structures, differing mainly in distance between platelets, determined by degree and geometry of grafting, molecular weight and chain-packing. This structure is apparently more thermodynamically advantageous in comparison with exfoliated and other “ordered” geometry. The only exception is the structure found in the case of GO grafted with the most hydrophobic ATB which forms micelle-like arrays whereas dual modification with hydrophilic PEG and hydrophobic ATB leads to formation of lamellar “bundles”. Presence of lamellar structure together with spherical inclusions in the case of separate addition of aminated polymers and GO confirm in-situ formation of GO-polymer adducts as well. This was further confirmed by

absence of this morphology in the case of nonreactive reduced GO application. Addition of impact modifiers together with polymer-grafted GO led, practically in all cases, to modifications of self-assembled structures. Combination of GO-g-APOP with APOP even eliminates lamellar structure formation. Addition of ATB to GO-g-ATB led to block copolymer-like structures, while addition of ATBN caused formation of lamellar structure with “incorporated” rubber. This work was supported by Czech Science Foundation (Grant No 19-06065S)

Keywords: Graphene Oxide, Bimodal Grafting, Epoxy, Self Assembly.

INVITED SPEAKERS

Id-682

Covalent Functionalisation of Graphene by PAMAM Dendrimer and Its Implications on Graphene's Dispersion and Cytotoxicity

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Abstract: Functionalisation of graphene and its derivatives (e.g., graphene oxide) with polymers is receiving much attention lately, owing to their potential applications in CO₂ or heavy metal adsorption, energy storage, biosensors, and drug delivery. Among other, hyper-branched such as poly-(amidoamine) (PAMAM) dendrimers are highly reactive because of the presence of a large number of terminal functional groups, and therefore, they are particularly suited for functionalisation of graphene. Covalent functionalisation of graphene is indeed a very promising strategy due to the formation of stronger bonds that give rise to a stable nano-composite for various applications. Two major grafting approaches are employed for covalently grafting the polymers onto solid surfaces, namely *grafting-from* and *grafting-to*. In the *grafting-from* approach, the polymer is grown from the surface, whereas in *grafting-to* the polymer is end-tethered to the surface. Even though there are several experimental studies on the covalent functionalisation of graphene by dendrimers and its application, these are still limited when it comes to providing an atomic-level detail of the phenomena shedding light on the impact of changing the grafting approach or binding location. In this communication we move a step forward and present results of molecular dynamics (MD) simulations regarding the covalent functionalisation of graphene with PAMAM dendrimer by the two grafting approaches (*from* and *to*) for different binding locations (*top*, *edge*, and *top-edge*). The effect of the used grafting approach, the binding site, the surface area, and the dispersion are analysed in detail. In addition, the possible cytotoxicity of the dendrimer functionalised graphene is investigated by analysing its interactions with a typical lipid bilayer. These MD results pave the way for a more complete theoretical understanding of the key factors governing the covalent functionalisation of graphene and its and its implications on graphene's dispersion and cytotoxicity, which could lead to a development in the fabrication of graphene-based devices and their applications. Typical equilibrated snapshots of the graphene-dendrimer composites corresponding to various binding locations of the dendrimer from the two grafting approaches, considered in this study. The financial

support from FCT/MEC through national funds through Project UID/QUI/50006/2020 (LAQV@REQUIMTE) are acknowledged, as well as the computational facilities at IISc through SAHASRAT and TUE-CMS clusters.

Keywords: Dendrimers, Graphene, Covalent Functionaliza-Tion, Dispersion, Graphene-Based Devices.

INVITED SPEAKERS

Id-684

Carbon Quantum Dots – Known but Still Mysterious

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Abstract: While working with Nitrogen-rich carbon-based quantum dots (N-CQDs), some unexpected phenomena like (i) presence of Eigen/Zundel-like water structures in the Stern layer; (ii) extremely high water adsorption capacity (ca. 1.7 g/gCQD at 100 % RH), (iii) unusual shape of differential water adsorption enthalpy, entropy, and Gibbs free energy curves; (iv) high conductivity, (v) superhydrophilicity, and others, are possible to be detected. Carbon-based quantum dots (CQDs) are widely suggested as excellent carriers of drugs, genes or other bioactive molecules. Via their fluorescent properties, CQDs are among the most frequently employed biomaterials in theranostics. They allow for the real-time optical imaging of cells and tissues, facilitate intraoperative image-guided surgery, and fulfill the role of efficient and easy-to-track drug carriers. In addition to the fascinating photoluminescent properties, CQDs are water dispersible, chemically stable, cell-permeable, and fairly biocompatible or at least non-toxic to the cells and tissues. The benefits of low-cost, simple synthesis, and environmental friendliness are not to be underestimated. Two distinct approaches to the synthesis of CQD have been widely described: the graphitized quantum dots are synthesized from reduced graphene oxide as a precursor, and the amorphous ones, which are obtained mainly via the hydrothermal treatment of carbon-rich molecular precursors. The carbon source for the latter method can be inter alia carbohydrates, gelatin, soy milk, bovine albumin, polyacrylamide, and many other. Nitrogen-rich precursors, such as aminoacids, peptides, or proteins, allow us to obtain specific CQDs. The undisputable advantages of nitrogen-containing carbonaceous quantum dots (N-CQDs) are their extremely low toxicity and outstanding biodegradability, and thus, they appear to be ideal tools for biomedical applications. However, to use them and fully understand their properties, one has to answer some questions: what about their surface chemistry? What kind of functionalities causes their fluorescence? Can we modify their properties? In the literature, there are no answers to these questions. However, surface chemistry is the key factor in understanding the observed phenomena, like high water adsorption capacity and surface ionic conductivity. A new experimental method called the

“evaporating droplet ATR technique” is proposed to perform this. The technique enables the observations and characterization of selected coatings i.e. diffusive or Stern layer above the surface of tested materials, via controllable removal of water and thus selective uncovering of the hidden layers. By confirming surface functionalities, one can easily modify their character and thus explain unexpected phenomena mentioned above.

Keywords: Superhydrophilicity, Stern Layer, Carbon Quantum Dots, Surface Functionalities, H₂O Adsorption.

INVITED SPEAKERS

Id-687

Laser-Mediated Fabrication of Nanoparticles for the Decoration of Nanofibrous Membranes and Their Usage in the Oil/Water Separation Sector

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Abstract: The inadequate water and wastewater management are causing a progressively devastating environmental impact, with oil pollution being one of the most difficult to combat causes. This is because, during oil manufacturing, usage-life, and disposal, the oil usually gets in contact with water forming tight emulsions and hydrate formations that remain in the water sources causing short- and long-term toxic effects over local ecosystems, contributing substantially to the downturn of life in general. Given such a problem, the scientific society has developed different strategies to recover water from oily polluted sources like flotation, gravity separation, adsorption, electrocoagulation, flocculation, coagulation, and membrane filtration. Among these options, membrane filtration stands above the rest because its production is economically accessible and has a low carbon footprint, and the membrane-based systems are very versatile. Nowadays, such versatility lies in incorporating solutions from the nanotechnology sector, like the employment of nanofibers to exclude the free passage of oil droplets by the size sieving effect combined with the incorporation of nanoparticles (NPs) over their surface to improve their antifouling and self-cleaning properties. Although these nanomaterial-based solutions are very appealing, especially considering that nanofibers' size and porosity can be easily controlled by electrospinning, some issues are still connected to manipulating their superficial properties with the aid of NPs. These obstacles include the need of large amounts of NPs to load the membranes' surface, the extensive NPs leaching due to an improper attachment over the membranes, and ultimately, the restricted superficial modification options derived from the limited element composition of NPs offered by the current NPs synthesis methodologies. This talk focuses on solving these issues by the employment of pulsed laser sources. In brief, these instruments can efficiently lead to the production of ligand-free NPs either by laser photoreduction/oxidation in liquids (LPL) or reactive laser ablation in liquids (RLAL). On the one hand, in LPL, the laser is used to irradiate a liquid solution containing NPs

precursor molecules; the focused beam reaches enough energy to dissociate the solvent molecules for creating radicals, and the radicals reduce/oxidize the NPs precursors allowing the NPs formation. On the other hand, in RLAL, the NPs are formed by the ablation of a solid material immersed in a liquid solution of NPs precursor molecules. The ablation mechanism leads to the out-of-equilibrium conditions required to fuse elements from the solid target and the NPs precursor molecules in the liquid, resulting in nanoalloys that are otherwise virtually impossible to obtain. In the framework of wastewater treatment, employing these techniques has resulted in tremendous benefits, like the 3.9-fold improvement in oil/water separation performance over unmodified polymeric membranes, negligible decline through time, oil rejection rates above 96%, and the non-conventional possibility to degrade organic pollutants while recovering water. All these benefits at the minimal loading of ~ 100 ng/cm² over the membrane's surface. Unlike any other NPs, their ligand-free nature and controlled element composition and distribution are allowing the evolution of membranes into materials that recover truly clean water from oily polluted sources, improving their impact in the field.

Keywords: Femtosecond Laser Ablation, Nanofiber Membrane, Membrane Modification, Oil-Water Separation, Pollutant Degradation.

INVITED SPEAKERS

Id-697

Magneto-resistive Properties of Advanced Nanostructures Based on Graphene and Lanthanum Perovskite Films for High Magnetic Field Sensors Applications

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Abstract : An increasing demand of magnetic field sensors with high sensitivity and spatial resolution at micro-nanoscales has resulted in extensive investigations of physical phenomena in advanced materials and development of novel devices. For special scientific and industrial applications, the sensors with increased ranges of magnetic field measurement and operation temperature are required. Therefore, the search of novel materials and engineering of their nanostructures exhibiting extraordinary properties for high magnetic field sensing applications is of great importance. It has been demonstrated that nanostructured manganite films exhibiting negative colossal magnetoresistance (CMR) effect can be successfully used for the development of magnetic field sensors operating up to megagauss. The demand of magnetic field sensors with scaled effective volume resulted in the research of magnetoresistive properties of two-dimensional (2D) materials such as graphene [4]. The graphene exhibits Lorentz force induced positive magnetoresistance phenomenon and large linear magnetoresistance (MR) at high magnetic fields, however, at low field limit the MR is low due to classical quadratic dependence on the field. On the contrary, the nanostructured manganite films show significant MR values at low fields, however, shows tendency of saturation in high-field limit. In this report, the main focus is made on the investigations of magnetoresistive

properties of thin nanostructured ferromagnetic oxide films (manganites) and 2D materials (graphene). It is demonstrated, how tuning the nanostructure and chemical composition of thin lanthanum manganites results in a remarkable colossal magnetoresistance up to high fields. On the other hand, it is shown how change of a number of layers of 2D graphene results in increase of the magnetoresistance and the field range of its linearity. The results on the development of hybrid magnetic field sensor based on a combination of nanostructured manganite film and single/few-layer graphene are presented. It was shown, that the hybrid structure allows to increase the sensitivity of the developed hybrid magnetic sensor in a wide range of magnetic fields in comparison with single manganite or graphene sensors [6]. The ways to increase the magnetoresistance values and, as a result, the sensor's response signal and sensitivity by optimizing the manganite growth technology and graphene electrode configuration are demonstrated. Various design examples of the hybrid structure are demonstrated in order to allow local measurements of magnetic field distribution. The possibility to use hybrid manganite/graphene structure for measurements of magnetic field magnitude and its direction in respect to the sensor's plane is also demonstrated and discussed.

Keywords: Magnetic Sensors, Manganites, Graphene, High Magnetic Fields.

INVITED SPEAKERS

Id-705

2D Nanostructured Layered Double Hydroxides for
MRI and Anticancer Drug Delivery

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Abstract: Layered double hydroxides (LDH) are interesting and versatile materials for nanomedicine, particularly for diagnostic and therapy. They are made of bi- (M^{2+}) and tri-valent (M^{3+}) cations in octahedral coordination and surrounded by OH groups. The connected octahedra grow along *b* axis to form infinite 2D layers. The space between the layers is occupied by water and anions (A^{m-}), which stabilize the structure. The chemical formula of synthetic LDH is $[M^{2+}_{1-x}M^{3+}_x(OH)_2]^{x+}(A^{m-})_{x/m} \cdot nH_2O$. Various bioactive compounds (drugs, vitamins, proteins, nucleic acids, etc.) can be conveniently accommodated within the interlayer gallery. LDH are also known as anionic clays, since their chemistry and crystalline structure are similar to those of the natural mineral hydrotalcite. The hydroalcite, having CO_3^{2-} as anion, has been already commercialized by the European biopharmaceutical company Bayer, as antiacid and anti-pepsin agent, with the commercial name "Talcid®". The particular structure of LDH allows the design of a wide and varied range of new nanostructured (organic-) inorganic materials for biomedical applications. The main properties of LDH that make them appropriate for nanomedicine are biocompatibility, pH-sensitivity, controllable particle size within the nano range, large surface area, positive Zeta potential, homogeneous distribution of metal cations within the brucite-like layers, diverse functionality, etc. Yet, there are some challenges associated with LDH exposed to a biological system, particularly during intravenous administration, that is, the colloidal stability. This can be affected by the interaction between positively charged LDH surfaces and negatively charged proteins, which might cause a fast clearance by the immune system. To address this issue, LDH can be covered with proteins, biopolymers, or encapsulated in lipid-based nanocarriers, aiming to increase bioavailability, circulation time, biodistribution, and their accumulation in the targeted sites. Recent studies on biomedical applications of LDH, particularly for Imaging and drug delivery, proved the feasibility of inorganic LDH and organic-inorganic hybrids based on LDH as promising biocompatible and biodegradable nanomedicines with high diagnostic and therapeutic values.

Keywords: 2D LDH, Organic-Inorganic Hybrids, Cancer, Nanomedicine, Drug Delivery.

INVITED SPEAKERS

Id-715

Biodistribution, Pharmacokinetics and Toxicology Study of Highly Biocompatible and Biodegradable Ag₂S Near-Infrared Quantum Dots in Mice

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Abstract: Silver sulfide (Ag₂S) quantum dots have become attractive in recent years due to their biocompatibility shown in vitro and luminescence in the medical imaging window (700-900 nm). Our group is at the forefront of Ag₂S synthesis. In order to achieve optical detection coupled with gene/drug transfection, we have developed highly biocompatible and biodegradable cationic Ag₂S quantum dots. These nanoparticles were quite successful in the in vitro studies. In this study, we have analyzed the in vivo toxicity, bio-distribution, impact on the blood biochemistry as well as potential to obtain optical tissue images using commercial IVIS optical imaging instrument. The main objective was to learn the toxicity of different cationic Ag₂S quantum dots in vivo and while doing that build an experience on the in vivo investigation of quantum dots and investigate the utility of IVIS for near-infrared emitting quantum dots. For this purpose, we have synthesized cationic Ag₂S with biocompatible and biodegradable coating. Our results indicate that quantum dots enter the liver, spleen, and kidney, but not much to the heart or lungs. Surprisingly we have found out that they pass the blood-brain barrier and enter the

brain, as well. Blood analysis indicates that although the total protein level is not influenced much by the quantum dots, liver enzymes need to be tracked in future studies.

Keywords: Quantum Dots, Silver Sulfate, In Vivo Imaging System (IVIS), Blood-Brain-Barrier, Biocompatible.

INVITED SPEAKERS

Id-717

Ceramic Nanofibrous Structures for DNA Damage Detection

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Abstract: Ceramic nanofiber structures can be produced from a variety of techniques. Sol-gel electrospinning technique is very applicable and promising technology that allows to produce continuous ceramic nanofibers including TiO₂ [1]. Microstructure of the ceramic nanofibers can be altered by changing the calcination temperature. For instance, as-spun precursor Ti(IV) isopropoxide/PVP nanofibers are converted into crystalline TiO₂ nanofibers during the calcination process and crystal structure of the nanofibers can be transformed from anatase phase to rutile phase by just increasing calcination temperature and keeping all the other parameters constant [1]. Diagnosis of the diseases including cancer in early stage is very important for an appropriate treatment and healing process. Electrochemical methods are used for the detection of oxidation based damages on the DNA molecules [2-3]. Signal intensity should be enhanced for the detection of even low oxidation occurred on the molecules. Using nanofibers can allow more attachment of the DNA molecules on the surfaces that leading more communication of the electrode with the molecules during the measurement. So, more signals are obtained from the molecules. Using photoactive ceramic nanofibers can enhance the signal intensity more by using the proper wavelength of the light during the measurement. In this regard electrospun TiO₂ nanofibers which is a photoactive material have been produced with different microstructures and immobilized on the electrode system for the photoelectrochemical detection of DNA damages by focusing on guanine oxidation signal. Both single strand and hybridized double strand of DNA molecules were analyzed for the proper characterization of the damage on the genetic molecules. This study was supported by Scientific and Technical Research Council of Turkey (TUBITAK), under grant number 119M079.

Keywords: Ceramic Nanofiber, Sol-Gel Electrospinning, TiO₂, DNA Damage, Oxidation.

REGULAR SESSIONS

Id-690

Toxic Effect of Metal Nanoparticles on Ovarian Cells can be Prevented by Their Chemical Modification and Plant Molecules

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Abstract: The application of metal nanoparticles in modern society is growing, but their application is hampered by their general and reproductive toxicity. The possible approaches to reduce this toxicity could be the chemical modification of the used nanoparticles, as well as the application of some medicinal and functional food plants or their constituents. The aim of the present studies was to examine the direct influence of silver and titanium dioxide nanoparticles (AgNPs and TiO₂NPs), and unsupported and supported copper nanoparticles (CuNPs) of different morphologies, on ovarian granulosa cell functions, to understand the character and mechanisms of their action, as well as to determine whether their toxic effects could be mitigated by the chemical modification of the nanoparticles and some medicinal and functional food plants or plant isoflavones. It has been shown that the addition of these nanoparticles to cultured porcine ovarian granulosa cells is able to reduce the expression of markers of their proliferation, apoptosis, viability and hormones release. The addition of plant extracts (buckwheat, *Fagopyrum Esculentum*, and vitex, *Vitex Agnus-Castus*) and plant phytochemicals (resveratrol, diosgenin, rutin and apigenin) is able to mitigate and to prevent the action of AgNPs, TiO₂NPs and CuNPs on ovarian cell functions. The comparison of the activity of unsupported spherical, triangular and hexagonal CuNPs, as well as of spherical CuNPs supported on TiO₂, zeolite Y and activated charcoal, demonstrated that the morphology and support of CuNPs can affect, mitigate and even invert the toxic action of CuNPs on ovarian cells. These observations suggest some reproductive toxicity of metal nanoparticles, which should be taken into account for their application. Nevertheless, the adverse effects of these nanoparticles can be mitigated and prevented by modification of their morphology, support on inorganic substances and action of some medicinal and functional food plants or their derived isoflavones. This work was supported

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Keywords: Nanoparticles, Ovary, Toxicity, Proliferation, Apoptosis.

REGULAR SESSIONS

Id-699

Single-Atom Catalyst Based on Al-MOF for Oxygen Evolution Reaction

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Abstract: Recently we all are facing the inevitable fact of exploiting fossil fuels, which will affect us on many grounds. In particular, scientists explore alternative ways to replace fossil fuels with new eco-friendly modern power sources. Clean energy can be produced in reactions such as Hydrogen Evolution Reaction (HER), Oxygen Evolution Reaction (OER), or Oxygen Reduction Reaction (ORR), where advanced materials are used as an electrode. The most important parameters that have to be achieved by those materials are sufficiently low overpotential for the reactions and extraordinary durability. Metal-organic frameworks (MOF) are unique and intriguing structures due to their advanced and remarkable architecture –where repeatable big structures with many micro/mesopores form the structure. Therefore, for single-atom catalysis (SAC), many metals can be introduced to those channels and play a crucial role in catalysis. Nickel (Ni), cobalt (Co) and iron (Fe) are the main and the most promising candidates for efficient catalysts material, especially when connected with nitrogen (N) and phosphorus (P) atoms, which boost its performance. Nonetheless, the high-temperature pyrolysis can cause the elements to agglomerate and then form nanoparticles frequently covered with carbon shells – which significantly decrease the electrochemical activity of the materials due to the surface: volume ratio. To counteract this effect, the easiest way is to introduce catalyst metals after pyrolysis of MOF with a low-temperature process. Al-MOF which the main component is aluminium (Al) is an interesting type of MOF due to its 2D structure and easy way to remove Al from carbon structure. Therefore the 2D carbon matrix can be successively modified to form structures with hierarchical pore structure and very good electrochemical performance (no oxidation peaks for Co) and with overpotential much lower than commercial catalyst (RuO_2 ; less than 350 mV) for OER and similar durability.

Keywords: SACs, MOF, OER.

REGULAR SESSIONS

Id-700

**Development of High Active Material Based on Nickel Nanoparticles
on Cellulose Platform for Electrochemical Applications**

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Abstract: With the environmental problem increase and the depletion risk of fossil fuels, there is an urgent need for an efficient, clean and sustainable source of energy, as well as new technology associated with energy conversion and storage. One of the most promising approach to overcome these issue may be the overall electrochemical water splitting to hydrogen and oxygen to produce energy. Hydrogen evolution reaction (HER) and oxygen evolution reaction (OER) are basic reaction of this process. However, commercially used electrocatalyst are based on noble low earth abundance and expensive metals (e.g. ruthenium, palladium iridium). Therefore there is a need to develop new electrocatalysts based on non-noble metals, which will be cheaper and possess improved electrocatalytic properties. On the past few decades, remarkable efforts have been made to develop non-precious metal based electrocatalysts for HER and OER reactions. The earth-abounded transition metal compounds attract much attention of scientists due to economic advantages and their specific electronic structure. From all of the transition metal compounds, transition metal phosphides (TMPs) have gained exceptional attention in this field due the their electrochemical activity, high conductivity and stability, corrosion resistance and many more. In particular, nickel phosphides, which possess unique electronic properties, efficient electrocatalytic activities, and anti-corrosion features, have attracted significant research attention and are recognized as efficient and low-cost HER and OER catalysts. In this work different shapes of nickel phosphides on the platform composed of cellulose fibers will be discussed. Characterization methods results from transition electron microscope (TEM) together with energy-dispersive X-ray spectroscopy (EDS) analysis and scanning electron microscope (SEM), x-ray powder diffraction (XRD) as well as x-ray photoelectron spectroscopy (XPS) will be consider. All materials were examined towards electrochemical applications, such as HER and OER reactions or as active material in supercapacitors. Electrochemical properties, such as overpotential, Tafel slope and stability were evaluated. Prepared samples exhibit promising results towards electrochemical oxygen

and hydrogen evolution reactions. Results showed lowered overpotential value of cellulose modified with nickel phosphides compared to the ruthenium oxide, which is considered as reference material in OER. The conducted analysis showed a great potential of prepared samples to the electrochemical applications.

Keywords: Nickel Phosphides, Cellulose, Electrochemistry.

REGULAR SESSIONS

Id-703

Compressive Mechanical Performance of an Epoxy Adhesive Doped with CNT, GNP and CB Nanofillers

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Abstract: Nanocomposites draw attention from many various fields and areas of usage increase with the improvement of their properties. For this purpose, nanoparticles have been used to enhance mechanical properties. The presented experimental study covers the investigation discoveries that focused on the impact of various nanoparticles on based adhesive nanocomposites. In this paper, nanocomposites were fabricated by reinforcing the DGEBA epoxy (adhesive) with different kinds of nanoparticles as carbon nanotubes (CNT), graphene nanoplatelets (GNP), and carbon black (CB) under different mass fractions as 1wt.%, 2wt.%, and 5wt.%. Because working at the nanoscale is still tricky, specific methods use macroscopic characterizations to assess the good distribution of nanoparticles into the adhesive that depends on their dimensions and form, etc. Therefore, the mechanical properties of CNT/DGEBA, GNP/DGEBA and CB/DGEBA nanocomposites were examined under compressive loading regimes. The findings reveal that adding nanoparticles to adhesive has a significant impact on its behavior. For each case, at least three specimens were tested. Indeed, the nature of nanofillers (0D, 1D, 2D, 3D) and the quality of the interfaces between reinforcement and matrix determines the mechanical properties of composite materials, whether doped by micronic or nanometric reinforcement. The mechanical characteristics of carbon nanoparticle-charged nanocomposites can only be improved by using an optimal mass fraction and distribution as well as ensuring good nanoparticle/adhesive adhesion (interface) to adequately throw the nanofillers. The type of nanoparticle utilized in the adhesive has an impact on these criteria. However, if dispersion is poor, these properties may be lower than those of the polymer alone.

Keywords: Adhesive, Carbon Nanotubes, Graphene Nanoplatelets, Carbon Black, Mechanical Behavior.

POSTER SESSIONS

Id-683

Triple Perovskite-Based Triboelectric Nanogenerator: A Facile Method of Energy Harvesting and Self-Powered Information Generator

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Abstract: A modified aqueous sol-gel reaction is used to synthesize a triple perovskite with a composition $\text{Sr}_3\text{Co}_2\text{WO}_9$ (SCWO). The structural analysis conducted at room temperature reveals the presence of the cubic phase with space group $Fm-3m$. The microstructure of the as-synthesized SCWO particles shows a different size of particles depicting a polycrystalline nature. Triboelectrification is a trending and unique concept in energy scavenging methodologies with flexibility in choosing from a variety of materials. This paves the way to evolve eco-friendly triboelectric energy harvesters as a replacement for the limitation of batteries. The outstanding dielectric properties and low loss make triple perovskite a promising candidate for TENG. A triboelectric nanogenerator (TP-TENG) was designed, which operates in vertical contact separation mode generating an electrical response of voltage and current of 300 V and 2.2 μA , respectively, for 10 wt% polydimethylsiloxane- $\text{Sr}_3\text{Co}_2\text{WO}_9$ (PDMS-SCWO) composite film. The power density of the rough surface TP-TENG was 30.5 $\mu\text{W}/\text{cm}^2$, which is much higher than the power density of 5.5 $\mu\text{W}/\text{cm}^2$ of plain surface TP-TENG. The positive and negative triboelectric layers of the TP-TENG were made up of aluminum and PDMS-SCWO composite film, respectively. Furthermore, the excellent flexibility and durability of TP-TENG make it suitable for sensing various gaits and information signalling (Morse code) in real-time applications, as well as for charging commercial capacitors.

Keywords: Triboelectric Nanogenerator, Perovskites.

POSTER SESSIONS

Id-691

**Enhancement of the Water-Resistance Properties of Cassava Residues
by Fatty Acid Addition**

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Abstract: Environmental problem of packaging usage is solved for a long time, which consist of incineration and landfill. However, the solutions cause of pollution increase, they approach greatly into global warming. In this research, the natural materials are applied. In addition, we use cassava residue as main material, the advantage of cassava residue can be renewable resources and abundant materials. Whereas, the drawback of cassava residue absorbs water dramatically. The cassava residue can be improved by fatty acids with coupling agent in order to increase efficient mechanical and water-resistant properties. Besides the incorporation of antioxidation can protect an electronic device packaging, it causes to damage packaging properties and protect the electronic devices.

Keywords: Cassava Residue, Antioxidant, Coupling Agent, Water Resistance, Biodegradable Packaging.

POSTER SESSIONS

Id-695

**Study of Diamond – Like Carbon Coatings for Biomedical Applications
Produced by Electron-Beam Physical Vapor Deposition**

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Abstract: The progress in biomaterials area for applications in biomedicine pose new requirements to their mechanical and tribological properties as enhanced hardness, excellent combination of high strength and low friction coefficient, high corrosion and wear resistance as well improved biocompatibility. Because of fast changes in the age structure in world scale, a number of people with damaged tissues which have to be replaced with artificial materials, increase. Main medical approach for past decades is use of metal nails, screws, splints as implants for damaged tissues replacement and stabilization of osseous structures which are not enough inert in human body and cause allergic reactions and side effects. That's why, research efforts are directed to development of biomaterials which are maximum close to the natural substance to assist restorative mechanisms of organism which accomplish above demands. Diamond-like carbon (DLC) is applied in optoelectronics, energy, touch-screen and display technology, lighting, composites, as and in biotechnologies. These materials are distinguished with high biocompatibility and hardness, chemical inertness and low friction coefficient and elastic modulus but their resistance to corrosion and wear are not enough for use as biomaterials for implants. A promising way to overcome this problem is deposition of special corrosion resistant coatings on based of DLC. In our work, the films on based of DLC were deposited on 304 L steel substrates at temperatures of 200 °C and 400 °C by electron-beam physical vapor technique. The obtained coatings are characterized by X-Ray Diffraction (XRD), Scanning Electron Microscopy (SEM) and Atomic Force Microscopy (AFM). Studies on the corrosion resistance were performed using electrochemical techniques conventionally applied to that purpose: measurements of the open circuit potential (OCP) and cyclic voltammetry. The resistance to corrosion of obtained DLC coatings was investigated in a medium corresponded to the fluids in human body. The developed diamond-like carbon coatings will reduce and remove the patient pain, side effects and various allergic reactions as well they will give guarantee for reliability and longer exploitation life of the implants. Besides, the deposited films

will decide important problems of the society related to achievement of more effective and safe treatment in patient by implants quality improvement. This work was supported by National Science Fund at Ministry of Education and Science, under Competition for financial support of Fundamental Scientific Investigations of junior researchers and postdoctoral students– 2019, project KP-06-M-37/1.

Keywords: Electron-Beam Evaporation, Diamond-Like Carbon, Biomedical Applications.

POSTER SESSIONS

Id-704

A Multi-Technique Approach to Characterize the Adsorption of Plasma Proteins on Layered Double Hydroxides

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Abstract: The administration of nanoparticles (NPs) either as such or carrying a therapeutic and/or contrast agent via intravenous way results in the formation of NP–protein corona, which influences their biodistribution and bioavailability. Recently, we showed that layered double hydroxides (LDH) NPs carrying manganese as contrast agent and fluorouracil as therapeutic agent proved to be an efficient theranostic nanomedicine, since it significantly increased the T_1 relaxation time in MRI while slowly releasing the drug in *in vitro* experiments. LDH in which magnesium was fully replaced by manganese (Mn:Al = 2:1, molar ratio) was prepared by co-precipitation at low supersaturation using manganese and aluminum sulfates as metallic precursors and then characterized for their composition, structure, texture, morphology, and oxidation states by appropriate techniques. Herein, we investigated the ability of these nanoparticles to be decorated with proteins, aiming to predict their behavior upon intravenous administration. In addition, we extended our study to LDH in which magnesium was partially replaced by manganese (Mn:Mg:Al = 1:1:1, molar ratio). First, protein-LDH interaction studies were performed by UV-Vis spectroscopy and polyacrylamide gel electrophoresis (SDS-PAGE) using a fixed bovine serum albumin (BSA) solution of 0.4 mg/mL at pH 7.4 and different LDH concentrations (0.5, 1, 1.5, and 2 mg/mL). The BSA concentration was selected as to permit proper band quantification following electrophoresis experiments. UV-Vis results showed up to 17.42% BSA adsorption after 2 h incubation at room temperature for LDH 1 mg/mL, with a maximum adsorption capacity of 69.68 mg BSA/g LDH. SDS-PAGE experiments showed the same trend for the same concentration of LDH, with up to 21.55% BSA adsorption after 2 h incubation (86.21 mg BSA/g LDH). However, we found that most of the adsorbed BSA was only loosely bound to the LDH surface, as washing of the protein-LDH complexes led to more than a 100-fold decrease in the quantity of adsorbed BSA (0.192% BSA adsorption - 0.77 mg BSA/g MgMnAl-LDH). This indicates that the “hard” corona (protein strongly adsorbed on LDH) is made of a low amount of proteins while most part of the BSA forms the “soft” corona (loosely

bound proteins), which is removed after washing. Indeed, FTIR spectroscopy performed after three washing steps confirmed the SDS-PAGE results. The spectra of samples displayed very weak bands at 1649 and 1545 cm^{-1} corresponding to Amide I and Amide II groups, respectively, of BSA strongly adsorbed on LDH. It has been shown that the hard corona defines the biological identity of the NPs, key aspect for the bench to bedside technological transfer. Protein corona formation was furthermore investigated through SDS-PAGE following incubation of 1 mg/mL LDH with three concentrations of rat plasma (10, 25, and 50%) at 37 °C for 1 h. Specific protein bands appeared for plasma incubated LDH, but were present neither in plasma nor in supernatant, suggesting the preference of the investigated LDH for less abundant plasma protein species. The results also confirmed the low concentration of serum albumin in the hard protein corona of LDH.

Keywords: Layered Double Hydroxides, Protein Corona, SDS-PAGE, Spectroscopy.

POSTER SESSIONS

Id-706

**Efficacy of Dental Materials in Terms of Apparent Mineral Density
Restoration Assessed by X-Ray Microtomography**

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Abstract: The initial stage of caries is characterized by demineralization of the enamel (both in the coronal and cervical parts) without cavitation. Such a pathology is called the white spot lesion. The present study compares the mineral density values of such a carious enamel and dentine in its vicinity with the apparent mineral density of the same tissues modified by two filling materials and an infiltrant that replaced using micro-CT. Five cases were considered ex vivo. We used human molars extracted for orthodontic purposes from patients at the clinic of the Rostov State Medical University (Rostov-on-Don, Russia) as samples. The Independent Ethics Committee of Rostov State Medical University approved the study, the patient provided informed consent. Imaging of the samples before and after treatment was performed using an Xradia Versa 520 device (Carl Zeiss X-ray Microscopy, Inc., USA). The high efficacy of laboratory micro-CT for carrying out such observations has been demonstrated. The composite filling was found to be very close in terms of the apparent mineral density to natural enamel as opposed to glass ionomer cement. Also, unlike the latter, the composite material showed a small amount of internal structural artifacts. When studying the effect of the infiltrant on the apparent mineral density of carious enamel and dentine bordering it, a significant negative effect of acid pre-treatment was observed. In none of the infiltration cases considered was the apparent mineral density of the modified enamel restored to its natural values. In one case the infiltrant reached the dentine and increased its apparent mineral density. To correlate the geometry of the caries area before and after treatment, a following protocol was established: determination of the surface of the entire tooth with calibration phantoms; conversion of the surface to the region of interest, determination of the surface from the obtained region of interest; combining three-dimensional models before and after treatment, registering one three-dimensional model

relative to another to correlate their spatial coordinates; study of mineral density by regions using virtual volumetric cylinders containing tooth tissue material. The careful research of the features of the dental treatments allows one to provide the dental clinician with the specific advice based on accurate microstructure and mineral density examination. The study was supported by the Government of the Russian Federation (grant 14.Z50.31.0046). Microtomography was carried out at the Nanocenter of Don State Technical University (<https://nano.donstu.ru>).

Keywords: Caries, Apparent Mineral Density, Micro-CT, Composite Material, Glass Ionomer Cement.

POSTER SESSIONS

Id-707

Mathematical Modeling of Indentation of FGM Coatings

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Abstract: Advanced mathematical model of nano- and microindentation of coating-substrate systems is proposed. The model is based on a contact problem on indentation of a coated elastic half-space formulated in terms of the linear theory of elasticity. Elastic moduli of coating assumed to vary with depth according to arbitrary continuous law, thus, functionally graded materials are modelled. The contact problem is reduced to the solution of dual integral equation which is solved in an approximated analytical form. The solution is valid for any relative thickness of the coating. Well comparison between the theoretical and experimental results is observed. Contact characteristics for coated and non-coated materials are analyzed. The model can be used to analyze the experimental results obtained from nanoindentation of thin coatings, for example, to evaluate the Young's modulus of thin coatings.

Keywords: Indentation, Contact, Modelling, Functionally Graded Material, Thin Coating.

POSTER SESSIONS

Id-708

Simplified Analytical Solution of the Contact Problem on Indentation of a Coated Half-Space by a Conical Punch for interpretation of Nanoindentation Tests

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Abstract: The present paper is devoted to the construction of the simplified analytical solution of the contact problem on indentation of an elastic coated half-space by a conical punch. The solution is constructed using the bilateral asymptotic method. For that purpose, kernel transform of the integral equation is approximated by a ratio of two quadratic functions and contains only one parameter. Thus, the approximated analytical solution is constructed in a significantly simplified manner in comparison with the general case in which the product of such functions was used. The obtained solution is suitable both for homogeneous (when elastic moduli are constant) and functionally graded (when elastic moduli change with depth) coatings. Such an approach allows us to obtain explicit analytical expressions for the distribution of contact stresses, the force-displacement and the contact radius - displacement dependences in a simplified form, convenient for engineering calculations. The dependence of the characteristics of contact interaction on the relative Young's modulus of the coating and relative coating thickness is analyzed. The accuracy of the obtained results is studied in details. Particular attention is paid to the investigation of the indentation stiffness, the most important characteristic used in experimental researches. The analysis showed high accuracy of the simplified expressions for the indentation stiffness, force, depth and contact radius for any value of relative thickness of the coating and even in a case when the elastic moduli of the coating and substrate differ more than by an order of magnitude. The simplified distribution of the contact stresses demonstrates high accuracy for relatively small ratio of the elastic moduli of the coating and substrate. The results of the work can be used to describe an experiment on nanoindentation of materials with coatings using either a conical or a pyramidal (Berkovich) indenter. The study was supported by the Government of the Russian Federation (grant 14.Z50.31.0046).

Keywords: Contact Problem, Indentation, Coatings, Analytical Solutions, Simplified Solutions, Conical Indenter.

POSTER SESSIONS

Id-709

Synthesis and Research of ZnO Nanorods for Applications in Nanoelectronics

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Abstract: Zinc oxide nanorods are often used as active elements of gas sensors, photodetectors, ultraviolet diodes, nanolasers, solar cells and other nanoelectronic devices. Unlike photosensitivity, the gas sensitivity of ZnO nanorods increases with the concentration of oxygen vacancies on the rods surface. Thus, obtaining nanorods ZnO with the maximum and minimum concentrations of oxygen vacancies is an important task. The number of oxygen vacancies can be controlled by changing the parameters of carbothermal synthesis and by using a thin-film sublayer. The photoluminescence spectrum of pure zinc oxide with an ideal crystal structure is one narrow peak at 375 nm wavelength. But in the spectra of real samples, so-called "green luminescence" often appears. The nature of green luminescence has remained controversial for decades. In early studies, it was explained with copper impurities, but were later presented strong evidence in favor of point defects such as isolated oxygen vacancies (~ 510 nm) or complexes of oxygen vacancies (~ 525nm), which are major contributors to gas-sensing properties of ZnO nanorods. The main aim of this work is to study the luminescence spectra and morphology of zinc oxide nanorods obtained by carbothermal synthesis at different temperatures (900-1100 ° C) with and without a thin-film ZnO sublayer on Si (001). It was shown that the growth of green luminescence intensity occurs in direct ratio to the synthesis temperature growth up to 1050 ° C on samples without a thin-film sublayer. At temperatures higher than 1050 ° C, horizontal growth begins to predominate over the vertical one. At the same time, the nanorods grew even at 1100 ° C on samples with a thin-film sublayer. The nanorods with the maximum concentration of oxygen vacancies were synthesized at 1100 ° C using the ZnO sublayer. Such nanorods are more suitable for use in gas sensors than rods obtained under other conditions. Nanorods with a minimum concentration of oxygen vacancies were

synthesized at 925 ° C without ZnO sublayer. Such nanorods are more suitable for the use for UV photodetectors and photodiodes. These claims have been confirmed experimentally. The results obtained made it possible to conclude that an increase in the synthesis temperature entails an increasing the number of oxygen vacancies in zinc oxide nanorods, and a thin-film sublayer helps to obtain more crystalline perfect structures at high synthesis temperatures and to increase the maximum possible synthesis temperature of ZnO nanorods. Prototypes of gas-sensitive elements and photodetectors were created, based on the obtained results. These prototypes showed high sensitivity values. A. L. Nikolaev acknowledge support from the Government of Russia within grant no. 14.Z50.31.0046. A. S. Kamencev acknowledge support from the Russian Foundation for Basic Research within grant no. 20-07-00637 A. The research was made in Research and Education Center "Materials", Don State Technical University (<http://nano.donstu.ru>).

Keywords: Nanorods, Zinc Oxide, Carbothermal Synthesis, Photodetectors, Gas Sensors.

POSTER SESSIONS

Id-714

New Graphene Structures for Energy Storage in Lithium-Ion Batteries

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Abstract: Shortage of oil resources and increasing concerns over environmental pollution, interests in electric vehicles and utilization of renewable energies like solar or wind are increasing. Growing demand for high-performance portable power, energy storage technologies have attracted great interest. Lithium-ion batteries are the most developed energy storage technology for various applications such as portable electronic devices, electric vehicles, and sustainable energy generation systems because of their attractive high gravimetric and volumetric energy densities compared with other energy storage technologies. New materials suitable for the production of lithium ion batteries are currently being investigated. Very popular in the field of electronics is graphene and its modification structures. In this work, we present a potential candidate for application in lithium-ion batteries. This new material with high surface area, large pore volume and high chemical resistance and mechanical and other properties that allow for their use as a building material for the electrodes. Important characteristics of the synthesized nanoparticles were investigated by X-ray diffraction (XRD), transmission electron microscopy (TEM) together with Energy Dispersive X-Ray (EDX) as its mode, Brunauer-Emmett-Teller (BET) method, thermogravimetric analysis (TGA) and Raman spectroscopy.

Keywords: Graphene, Lithium-Ion Batteries.

ALL SUBMISSIONS & TOPICS

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	714 - New Graphene Structures for Energy Storage in Lithium-Ion Batteries
Nanomedicine	704 - A Multi-Technique Approach to Characterize the Adsorption of Plasma Proteins on Layered Double Hydroxides
	705 - 2D Nanostructured Layered Double Hydroxides for MRI and Anticancer Drug Delivery
	706 - Efficacy of Dental Materials in Terms of Apparent Mineral Density Restoration Assessed by X-Ray Microtomography
	715 - Biodistribution, Pharmacokinetics and Toxicology Study of Highly Biocompatible and Biodegradable Ag ₂ S Near-Infrared Quantum Dots in Mice
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