Book of Abstract

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Disclaimer

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PLENARY SPEAKER

Id-2597

Interaction between Chirality and Magnetism in Hybrid Nanostructures

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Abstract: Chirality plays a critical role in a wide range of systems, from biology and chemistry to condensed matter physics and high energy physics. For example, in the biochemistry and pharmaceutical industries, enantiomer separation is a major issue, since enantiomers with a specific chirality often have different biochemical properties or pharmacological effects from their counterparts with the opposite chirality. Indeed, enantioseparation is an extremely important process in the pharmaceutical and chemical industries. However, despite intensive efforts, obtaining enantiomerically pure synthetic materials remains a challenge, as the cost of separation is relatively high and an extensive effort is required. We have reported a new effect of magnetization switching of ferromagnetic thin film without applying a magnetic or electric field but being induced solely by adsorption of chiral molecules [1] . The direction of the magnetization depends on the handedness of the adsorbed chiral molecules Here magnetization switching of ferromagnetic thin film is induced solely by adsorption of chiral molecules. The local magnetization switching is achieved by adsorbing the chiral molecules as a self-assembled monolayer on a gold-coated magnetic (Co) layer with perpendicular magnetic anisotropy. The direction of the magnetization depends on the handedness of the adsorbed chiral molecules. Owing to spin-selective electron transfer, the cobalt layer underneath the adsorbed chiral molecules becomes spin polarized, and hence magnetization direction is determined. Recent studies have suggested that charge redistribution in chiral molecules manifests an enantiospecific preference in electron spin orientation. Therefore it is possible that the induced spin polarization may affect enantio-recognition through exchange interactions. We have shown experimentally [2] that the interaction of chiral molecules with a perpendicularly magnetized substrate is enantiospecific. Thus, one enantiomer adsorbs preferentially when the magnetic dipole is pointing up, whereas the other adsorbs faster for the opposite alignment of the magnetization. The interaction is not controlled by the magnetic field but rather by the electron spin orientations, and opens prospects for a distinct approach to enantiomeric separations. The enantioselective interaction of chiral molecules and a magnetic substrate with perpendicular anisotropy provides a potentially generic chromatographic method for enantioseparation, which does not require a specific and costly separating column. As the observed effect depends on the electrical spin polarization and because this polarization depends on the global structure of the chiral molecule, this new method may also allow the separation of chiral molecules from a mixture of molecules, either chiral or achiral.

Keywords: Nanomagnetism, Spin Polarization, Separation of Chiral Molecules, Magnetic Thin Films.

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PLENARY SPEAKER

Id-2659

Quantum Computing with Silicon Spins

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Abstract: Quantum computers hold the potential to solve key tasks exponentially faster than classical computers. Classical transistor scaling achieved the integration of billions of Si transistors on-chip, making them so small that a single electron or hole can be trapped and held in place. The magnetic moment of such a trapped charge – the spin – is a prime contender for building scalable qubits out of classical Si transistors, thus making semiconductor spins a leading candidate for full-scale quantum computing. In this talk, I will present our recent progress on building spin qubits with holes in Ge/Si core/shell nanowires and Si fin FETs, pursued in the Swiss National Quantum Computing Program NCCR SPIN. Highlights include ultrafast qubits, taking only 1 ns to coherently rotate a spin from pointing up to down; operation of spin qubits up to 5 K, where vast cooling power becomes available, making possible integration of the classical control electronics; operation of a 2-qubit gate with highly anisotropic exchange, allowing for high fidelity gate operation while operating at high speeds; and finally a sweet spot combining both maximal coherence and maximal speed, thus opening new avenues for ultrafast and highly coherent spin-orbit qubits. These experiments are supported by laboratory instruments developed by our spin-off Basel Precision Instruments GmbH, including low-noise amplifiers, high-resolution voltage sources and cryogenic microwave filters and thermalizers.

Keywords: Quantum Computing, Spin Qubits, Silicon, Spin-Orbit Coupling.

Acknowledgements: This work was supported by the NCCR SPIN, the Swiss National Quantum Computation Program with Si Spins of the Swiss NSF, the Swiss Nanoscience Institute (SNI), the Georg H. Endress Foundation, and the EU H2020 European Microkelvin Platform EMP, TOPSQUAD and QLSI programs.

PLENARY SPEAKER

Id-2664

Biomass Conversion: The Raw Material of Tomorrow

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Abstract: The present talk aims at using vegetal biomass, as a source of sustainable raw material for fine chemicals, energy and commodity and high-added values products. Thus, wood, as well as, agricultural and industrial residues can be readily extracted and used as such, as starting chemicals or can be suitably converted to second generation functionalized synthons to be used, as sustainable raw material to face our needs in material science and engineering area. In fact, different strategies will be described:

(i) The first strategy consists of extracting first generation high added-values natural monomers, oligomers and polymers and the application of the high-purity extracted materials in the above-mentioned fields. In this context, typical examples could be the extraction of high-added values hemicelluloses for application as a food- or cosmetic-additive or the preparation of sugars for bio-ethanol, bio-surfactants...

(ii) Converting some original molecules into second generation starting molecules, in order to substitute the use of fossil resources. Thus, high-added values lubricants were prepared starting from sugar-based chemistry for the hydrophilic moieties of the surfactant, whereas vegetal oil-based molecules have served for the hydrophobic counterpart. The other example, could be the preparation of 2,5-dicarboxy furan and its polymerization with ethylene glycol, in order to synthetize the substitute of poly(ethylene terephthalate), destined for packaging of liquids.

(iii) Then, the functionalization of natural products extracted from vegetal biomass, thus providing them new added-values properties will be discussed. Thus, cellulose, the most abundant polymer in the earth is a hydroxy function-rich macromolecule, which is suitable to undergo several chemical reactions (esterification, etherification, urethane formation, silanation, etc.) leading to the preparation of active surfaces. This strategy involved the use of cellulose from various origins (several vegetal species, including annual plats residues and cotton by-products), different morphologies (fibres, beads, etc.), and at several sizes (from millimetres for fibres to nanometres for nanocellulose). Concretely, cellulose was grafted in order to be used as reinforcing phase in composite materials. The same way of surface modification yielded super-hydrophobic surfaces, antimicrobial in packaging applications, fire-proof, etc. Cellulose at nanoscale was also used as a binder in batteries which open the door of nanocellulose in energy area of application.

(iv) The last strategy consists in transforming the biomaterials into promising adsorbents for the adsorption of various kinds of inorganic and organic pollutants from contaminated water. The materials are transformed into nanocomposites, nanoparticles, bio-chars, activated carbons, etc. The adsorption process was studied under the variation of several experimental conditions in batch or dynamic mode. Experimental and theoretical (modelling) data exploitation will be given.

The common feature in all these strategies is the use of either wood or agricultural residues, which has two main advantages: rational valorisation of vegetal biomass, avoiding the concurrence of the raw material destined for food stream and using green conditions.

Keywords: Vegetal Biomass, Rational Valorisation, Cellulose, Nanocellulose, Medical Applications.

PLENARY SPEAKER

Id-2767

Effect of Preparation Methodologies on the Properties of ZnO QDs and Metal Halide Perovskites

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Abstract: Zinc oxide (ZnO) is one of the few oxides that show quantum confinement effects and ZnO nanostructures are one of the most versatile system with far-reaching perspectives However, the commonly used sol-gel approach provides ZnO nanostructures inherently alkali-metal contaminated QDs [1] featuring substantial imperfections in surface passivation, and substantially labile surface-coating ligand interactions [2], leading to a large number of traps. Recently, we have developed a novel one-pot self-supporting organometallic process to produce high-quality ZnO nanoplatelets [3] and QDs,[2] including organic-ligand free QDs inks [4]. These properties offer a promising alternative vs. currently used technologies for preparing high-quality and high electron mobility nanostructured ZnO materials via low-temperature solution processes. For example, low-temperature processed pure ZnO ETLs for planar heterojunction perovskite solar cells (PSCs) provided the champion PSC with a power conversion efficiency over 20% with negligible hysteresis, which is the state-of-the-art performance among reported non-passivated pure-ZnO-based PSCs [4]. Thus, this novel ZnO-based solar cells reached comparable performance to PSCs devices based on pristine SnO_2-ETLs [5]. Metal halide perovskites (MHPs) are promising semiconductor materials for photovoltaic applications due to the unique and tunable bandgap, high absorption coefficient and relatively simple synthesis methods [1]. Notably, the optoelectronic properties and the photovoltaic parameters of MHPs are highly sensitive to the adopted synthetic strategy. While the solution-based approach to MHPs is relatively versatile, it faces challenges such as limitations in both their compositional engineering and long-term storage. An alternative approach is the mechanochemical synthesis of perovskites by simply grinding the solid reactants that was pioneered by our group in 2015 [6]. The lack of the solubility limitation in mechanochemical synthesis allows to prepare MHPs that could not be obtained by wet methods. Another beneficial aspect of using this approach concerns superior storage stability of mechanoperovskite powders compared to their stock solution counterparts. We also demonstrated that the solar cells fabricated from mechanoperovskites exhibited superior photovoltaic performance compared to conventional devices made using the classical wet-chemical procedure [6]. Inherent features of MHPs are their softness, complex lattice dynamics, and phase transitions spectacularly tuning their structures and properties. In the course of our extensive studies on compositional engineering of MHPs by the incorporation into the perovskite lattice oversized cations, we revealed that δ-$AcaPbI_3$ (Aca = acetamidinium cation) exists at least in nine polymorphic forms, making it the most diverse polymorphic collection among known MHPs [7]. Strikingly, we also found a good correlation between the Pb⋯Pb distances and the pressure evolution of the band gap values in the δ-$AcaPbI_3$,

indicating that in 1D perovskitoid structures the contacts between Pb^{2+} ions are one of the critical parameters determining their properties.

Keywords: Halide Perovskites, Properties, Devices.

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PLENARY SPEAKER

Id-2782

Artificial Intelligence in Materials Science and Renewable Energy Research

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Abstract: Material science is an interdisciplinary field focusing on the discovery and design of new materials. Materials science studies the properties, structure, performance, and applications of materials. It combines principles from physics, chemistry, engineering, and biology to understand how materials behave under various conditions and how they can be used or modified for practical applications aiming to develop materials that meet specific criteria of strength, durability, weight, conductivity and reactivity. Materials science plays a crucial role in the development of new technologies, ranging from semiconductors and medical devices to aerospace structures and energy storage systems. In this talk, I will first discuss the main challenges in studying and discovering new technological materials in this field, and then focus on the use of artificial intelligence (AI) and related technological advances to face these challenges. Transitioning to more advanced, technology-driven approaches like integrating machine learning (ML), machine learning operations and large language models is essential to overcome these challenges. Artificial intelligence is revolutionizing materials science and engineering by accelerating research, development, and discovery processes. AI enables researchers to analyze vast datasets, predict material properties, leading to materials discovery and design using Machine Learning (ML) techniques, predictive modeling, process optimization and automation of experiments. I will provide real examples in energy storage and conversion: AI is being applied in optimizing materials for better performance in batteries, fuel cells, and solar cells, focusing on maximizing efficiency, capacity, and lifespan. Finally, I will discuss AI-Assisted Microscopy and Characterization and AI in Combinatorial Materials Science.

Keywords: Material Science, Artificial Intelligence, Machine Learning.

INVITED SPEAKER

Id-2578

Experimental and Computational Study of Fatigue Crack Growth in Austenitic Stainless-Steel Alloy 709 at Elevated Temperatures

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Abstract: This study presents experimental testing results and computational simulations of fatigue crack growth (FCG) in austenitic stainless-steel Fe-25Ni-20Cr (Alloy 709) at temperatures ranging between 550 and 700ºC. Steel alloy 709 is a material used in high-temperature structural applications, including coal-fired, gas-fired, and nuclear power plants. This material has outstanding mechanical properties under creep-fatigue loading, good thermal stability, weldability, and tensile strength properties. The potential power-plant applications of Alloy 709 include pressure vessels, core supports, and primary and secondary piping components. Characterizing FCG rates in Alloy 709 steels is of great interest at temperatures ranging between 550 and 700ºC. Considering the operating cycles for powerplants, structural components are expected to be subjected to fatigue loading waveforms, and FCG is a major failure mode to consider in design and service. FCG tests were conducted in Alloy 709 using compact tension C(T) specimens at R = 0.1, R = 0.5, and R = 0.7 load ratios. The FCG tests were performed on several servo-hydraulic test frames equipped with temperature-controlled furnaces. Crack growth rates were measured using several monitoring techniques. The crack length was monitored using a high-temperature extensometer, a direct-current potential drop (DCPD) system, and visual inspections using a traveling microscope. Post-failure analyses of crack surfaces were performed. C(T) specimens were tested at maximum applied loads ranging between 7 and 10 kN. In parallel with the experimental tests, a computational strip-yield model for creep-fatigue crack growth (SYM-CFCG) was employed to simulate crack growth under fatigue loading. The SYM-CFCG software predicts the development of plasticity-induced crack closure (PICC) near the tip of a growing crack. The PICC is used to compute the effective stress intensity factor range, which is the driving force for growing fatigue cracks. The crack plane is meshed with a number of one-dimensional elements placed both in the crack-tip plastic zone and behind the crack-tip on the entire cracked ligament. As the crack extends, the element ahead of the crack tip is removed cycle-by-cycle. SYM-CFCG software calculates crack opening and closing during a fatigue cycle, residual stresses at minimum load, and FCG rates based on the PICC phenomenon. The computation of the PICC allows the prediction of FCG rates at different R ratios. Predictions of crack length evolution as a function of applied load cycles are compared with the experimental results. In addition, predictions of crack growth rates per cycle versus applied stress intensity factor range are also compared with the experimental measurements. Excellent agreements between experimental data and SYM-CFCG predictions are obtained.

Keywords: Steel Alloy 709, Fatigue Crack Growth Rates, Strip-Yield Model, Compact Tension Specimen.

INVITED SPEAKER

Id-2590

Development of Amorphous Microwires with Graded Magnetic Anisotropy

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Abstract: Studies of magnetic wires have attracted great interest owing to outstanding magnetic properties, like the giant magnetoimpedance (GMI) or the magnetic bistability and related single domain wall (DW) propagation [1,2]. These properties make them quite attractive for a number of technological applications [1-3]. An important advantage of the glass-coated magnetic microwires prepared using the Taylor-Ulitovsky technology is that the wire diameter can be significantly reduced (an order of magnitude). Another advantages of such microwires are better corrosion resistance and mechanical properties. Therefore, such microwires are suitable for emerging applications including biomedicine, non-destructive control of external stimuli (stress, temperature) in smart composites, magnetic memories and logics, magnetic and magnetoelastic sensors or electronic surveillance [2,3]. Recently we observed that, the hysteresis loops Fe-rich microwires are substantially affected by the stress-annealing conditions (temperature or stress). In Co-rich microwires even conventional annealing at different temperatures produce similar modification of the hysteresis loops [2]. Therefore, we proposed simple method to prepare glass-coated microwires with graded magnetic anisotropy by annealing at variable temperature [2]. Previously, graded magnetic anisotropy was obtained by rather sophisticated method involving modification of the chemical composition during the sample preparation [4]. Magnetic materials with a graded magnetic anisotropy presenting controllable spatial distribution of the magnetic anisotropy can show unusual magnetic properties, like controllable nucleation or pinning of domain walls [2,4].We have studied the magnetic properties and domain wall dynamics in Fe-rich and Co-rich microwires subjected to stress-annealing. For the wires stress-annealed at variable temperatures we obtained a graded magnetic behavior with local hysteresis loops shapes and properties (coercivity, remanent magnetization) changing along the sample length. In the samples subjected to local stress-annealing we created an artificial source of DW injection allowing the manipulation of the DW dynamics. The observed stress-induced anisotropy could be related to the internal stresses relaxation after annealing and the interplay of compressive “back-stresses” arisen after stress annealing and axial internal stresses.

Keywords: Magnetic Wire, Magnetic Anisotropy, Hysteresis Loops, Domain Wall, Annealing.

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INVITED SPEAKER

Id-2593

Theoretical Study on In-Plane, Out-of-Plane, and Transverse Anisotropic Magnetoresistance Effects for Ferromagnetic Films

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Abstract: The anisotropic magnetoresistance (AMR) effect, in which the electrical resistivity depends on the direction of magnetization M, is one of the most fundamental characteristics involving magnetic and transport properties. The AMR effect has been observed for a variety of ferromagnets such as Fe, Co, Ni, Fe4N, and half metals, and has often been explained by using the electron scattering theory based on an extrinsic mechanism [1-7], in which the conduction (s) electron is scattered into the localized d states by nonmagnetic impurities. The AMR effect has recently been investigated for various directions of M. The AMR effects are, for example, in-plane AMR (IAMR), out-of-plane AMR (OAMR), and transverse AMR (TAMR) effects for ferromagnetic films. When the current flows in the [100] direction, the IAMR, OAMR, and TAMR mean that M lies in the (001), (010), and (100) planes, respectively. Quite recently, the IAMR, OAMR, and TAMR effects have been studied for CoxFe1-x films by using the first principles transport calculation with an intrinsic mechanism [8], in which the energy band structure depends on the direction of M. The calculation results have been verified experimentally [8]. On the other hand, the M direction dependences of IAMR [9], OAMR [10], and TAMR [11] have been experimentally measured at T=50 K also for Fe4N films. Here, the IAMR and OAMR exhibit the negative AMR with the twofold symmetry, whereas the TAMR shows the positive AMR with the fourfold symmetry. Such experimental results, however, have scarcely been analyzed theoretically. We note here that an experimental result of T dependence of the IAMR for T ≤ 35 K has ever been explained qualitatively by using the electron scattering theory with the extrinsic mechanism [3]. Our concern is therefore whether the present experimental results can also be explained by using the conventional electron scattering theory [7]. In this study, we analyze the experimental results of IAMR [9], OAMR [10], and TAMR [11] at T=50 K for Fe4N films using the electron scattering theory with the extrinsic mechanism. The theory is based on the two-current model with the s-s and s-d scatterings due to the impurities, where d is the localized d states with the spin-orbit interaction, exchange splitting energy, and crystal field energy [7]. We find that the calculation results of IAMR, OAMR, and TAMR agree qualitatively well with the respective experimental results. In addition, the peak structure of each AMR is considered on the basis of the probability density of the d states of the current direction.

Keywords: Anisotropic Magnetoresistance Effect, Spin-Orbit Interaction, Crystal Filed, Extrinsic Mechanism, Electron Scattering Theory.

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INVITED SPEAKER

Id-2602

Properties of Sn99Ag0.3Cu0.7-(ZrO_2/CuO/TiO_2) Composite Solder Joints

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Abstract: The “lead-free” change in the soldering technology caused the widespread application of the SnAgCu (SAC) solder alloys. The so-called low Ag content ones, like Sn99Ag0.3Cu0.7 (SAC0307) and Sn98.5Ag1Cu0.5 (SAC105), are more and more popular recently due to their excellent price and thermo-mechanical properties. The most novel solution to further improve the solder alloys’ properties is adding nano-sized ceramic reinforcement particles into the solder alloys. This procedure results in „nano-composite” solder joints. A wide range of ceramic nano-particles was already tested, like TiO_2, ZrO_2, Al_2O_3, Fe_2O_3, Si_3Ni_4, SiC, La_2O_3, etc [1]. The reinforcement particles improve the solder joints’ mechanical properties (shear force, yield strength, microhardness, etc.), with some Kelvin of change in the melting temperature of the alloy. It is generally accepted that mechanical improvement is caused by dispersion-strengthening mechanisms. The ceramic nano-particles are not soluble in the Sn solders, so they incorporate at the Sn and intermetallic (Cu_6Sn_5, Cu_3Sn, and Ag_3Sn) grain boundaries, where they promote heterogeneous nucleation. This results in the suppression of grain growth (at all phases) and decreases dislocation motions [2]. In the present study, the effect of three oxide ceramics (TiO_2, ZrO_2, and CuO) as reinforcements in 0.25 and 0.5wt% weight fractions was investigated on the quality and reliability of the composite SAC0307 solder alloy. The NPs were mixed into the solder paste homogeneously using a YX solder paste mixer for 10 min at 400 rpm. Standard spreading tests of the different alloys were done on FR4 laminates covered by Cu foil and Ag surface finishing over on it. Solder joints were prepared from the alloys and 0603 chip resistors by convectional surface mounting technology (SMT) on FR4-based printed circuit boards (PCB) with imm-Ag surface finish on the copper solder pads. The shear strength of the chip resistors was measured using a DAGE 2400 tester. The solder joints were loaded with 4000 hours 85°C/85RH% climatic test to investigate their corrosion resistance. Cross-sections were prepared to study the microstructure solder joints by scanning electron microscopy (SEM), and scanning ion microscopy (SIM). The results showed that NPs slightly decreased the wettability of the composite solders; considerable differences were not observed between the particles. The shear strength of the composite joints generally increased. Considerable grain refinement occurred in the composite solder joints (in the cases of Sn, Cu_6Sn_5, and Ag_3Sn as well), and the refined microstructure had a better load transferability. The novel CuO and ZrO_2 NPs performed not as positively, as TiO_2, so their application is questionable in soldering technology. TiO_2 NPs increased the corrosion resistance of the composite solder joints and suppressed the Sn whisker formation from them. Further results will be discussed in the presentation about the incorporation mechanism of the different NPs into the solder matrix and their effect on the reliability of the nano-composite solder joints.

Keywords: Reflow Soldering, Nanoparticles, Composite Solder Alloy, SAC0307, Corrosion.

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INVITED SPEAKER

Id-2603

Resistive Switching Memory (ReRAM) through Bio-materials

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Abstract: Sustainable growth strategies and economies are pushing for environmental friendly, green technologies. Green computing is one such emerging technologies. A green ReRAM, based on bio compatible and biodegradable materials is an important component of green computing. In this context we present our studies on the resistive switching properties of some of the interesting biomaterials and biodegradable composites. We have fabricated ReRAM devices using bio materials like plant extracts, animal milk, bio-nano composites of Gelatin, Chitosan and cellulose etc with the incorporation of suitable nano particles [1-8]. All devices are well characterized and studied in detail for conducting and resistive switching properties. We report on the unexpected resistive switching memory behaviours in raw cow milk and other plant extracts. Fat and ion content of milk plays an important role in the morphology, transport, and switching of these animal milk based devices [9]. While the bio-ReRAM parameters are not comparable to the state of art inorganic ReRAMs in the literature, yet, one can see a great emergence of the bio compatible and biodegradable ReRAM developments. A definitive cycling dependence is observed, which is a major problem to be understood and calls for further optimization of these devices.

Keywords: ReRAM, Biomaterials.

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INVITED SPEAKER

Id-2605

On the Theory of Transition Radiation of a Charge in a Waveguide Filled with an Anisotropic Magnetodielectric Medium

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Abstract: This article is devoted to a review of the author’s theoretical works related to the transition radiation of a charged particle moving uniformly perpendicular to the axis of a waveguide of arbitrary cross section completely or partially filled with both unmodulated and periodically modulated anisotropic magnetodielectric medium. The posed problems were solved by the analytical method developed by the author in his early works. Transverse-electric (TE) and transverse-magnetic (TM) fields of radiation in a waveguide are considered. Analytical expressions for the energy of transition radiation in the above problems are obtained. It is assumed that the modulation depths in the case of modulated filling are small values. The frequency regions of “weak” and “strong” interaction between the radiation wave and the modulation wave are considered, and the features of transition radiation are clarified when the first-order Wulff-Bragg condition is satisfied. As a result of the study the following main results were obtained:

1. It is shown that if in the waveguide there is an anisotropic magnetodielectric filling and certain condition is met, there will be no modes with the first index in the radiation. This is explained by the fact that the moving particle enters a node of the electromagnetic field and there is no interaction between the particle and this mode.

2. When a certain condition is met around a certain frequency a sharp maximum appears in the spectrum of transition radiation which determines Cherenkov radiation. The width of the maximum is proportional to the particle velocity.

3. When a charged particle passes uniformly through an anisotropic magnetodielectric plate in a waveguide perpendicular to its axis transition radiation in a certain frequency region does not leave the plate and a trapped radiation effect occurs. Also, Cherenkov radiation does not propagate outside the plate in the waveguide.

4. It is shown that the fields of transition radiation during uniformly passage of a charged particle through the periodically modulated along coordinate anisotropic magnetodielectric waveguide filling perpendicular to waveguide axis present a set of spatial harmonics with different amplitudes.

5. It is shown that the width of the frequency region of strong interaction between transition radiation and periodically modulated anisotropic magnetodielectric filling is small and proportional to the modulation depths. It has also been shown that in the region of strong interaction the peak of Cherenkov radiation does not appear in the spectrum of transition radiation, since the conditions for its occurrence are not satisfied.

Keywords: Waveguide, Anisotropic Magnetodielectric Filling, Transition Radiation, Cherenkov Radiation, Periodically Modulated Filling, Frequency Region of Strong Interaction.

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INVITED SPEAKER

Id-2609

Assessment of Soil Activity Levels from Decommissioning Area of a VVR-S Nuclear Research Reactor

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Abstract: The paper presents the methodology for evaluating the levels of soil activity in the area possibly affected by decommissioning activities of the VVR-S Nuclear Research Reactor from National Institute for Research and Development in Nuclear Physics and Engineering, Romania. Gamma spectrometric analyses of the soil samples sampled from the surface and depth were carried out in order to obtain information about possible recent contamination from radioactive dust in the air as well as from unknown past "accidents". The analysis was performed both before reactor decommissioning began (year 2006) and after its completion (year 2020) to demonstrate that the non-restrictive release criteria under the regulatory body regime for land from decommissioning area are met. Activity levels of anthropogenic and natural radionuclides do not exceed the exclusion levels imposed by the basic domestic safety standards in force. It can be stated that the reactor operation and decommissioning did not generate contamination of the surrounding soil.

Keywords: Soil Contamination, Reactor, Decommissioning.

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INVITED SPEAKER

Id-2629

Direct Observation of Spin Exciton in Superconducting Oxypnictides by Andreev Spectroscopy

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Abstract: We have studied superconducting (SC) oxypnictides Gd(O,F)FeAs and (Sm,Th)OFeAs (the 1111 family) of optimal and underdoped compositions and $T_c \approx 25$–54 K. In the Fermi surface, hole barrels near the Γ point and electron barrels near the M point are coupled by a nesting vector **Q**, at which the imaginary part of the dynamic spin susceptibility $\mathrm{Im}[\chi(\mathbf{Q},\omega)]$ shows a spin-resonance peak at position $\omega_R(0) < [\Delta_L(0) + \Delta_S(0)]$ [1]. In order to study the SC energy parameters we used incoherent multiple Andreev reflection effect (IMARE) spectroscopy of SC–thin normal metal–SC (SnS) nanojunctions. SnS junctions were formed by a planar “break-junction” technique [2]. IMARE causes an excess current at I(V) curve of SnS junction at any bias voltage *eV*, zero-bias conductance peak, and a subharmonic gap structure (SGS) in the dI(V)/dV-spectrum at bias voltages $V_n(T) = 2\Delta(T)/n$, n = 1, 2, …. The positions of the latter directly relate with the SC gap magnitude at any temperature until T_c. We reproducibly observed two distinct SGS’s and directly determined two SC gaps in the 1111 compounds, with characteristic ratios $2\Delta_L(0)/k_BT_c \approx 5.2$, and $2\Delta_S(0)/k_BT_c \approx 1.5$, those remained almost constant within the wide range $T_c \approx 25$–54 K [3]. Beyond to the parent SGS of the large SC gap, the dI(V)/dV spectra of SnS junctions showed a satellite fine structure below T_c caused by an emission of bosons (existing in the SC state only) with characteristic energy ε_0 by electrons during IMARE [4–6]. The positions of the fine structure satisfied the formula $V_n(T) = [2\Delta(T) + k\varepsilon_0(T)]/n$, k = 1, 2, … In the spectra of the most qualitative junctions we observed a multiple bosonic resonance with $k \le 4$ [5]. For Gd(O,F)FeAs and (Sm,Th)OFeAs with $T_c \approx 50$ K the boson energy $\varepsilon_0 \approx 10$–13 meV. Under doping variation, ε_0 was scaled with T_c together with $\Delta_L(0)$ and $\Delta_S(0)$ [6]. At $T << T_c$, ε_0 does not exceed the indirect SC gap $\Delta_L(0) + \Delta_S(0)$. We directly measured the temperature dependence of the boson energy. $\varepsilon_0(T)$ weakly decreases with temperature and does not resemble the $[\Delta_L(0) + \Delta_S(0)]$ temperature trend [6]. In the framework of 5-orbital $s^\pm$-model, we calculated the $\mathrm{Im}[\chi(\mathbf{Q},\omega)]$ dependences using the experimental $\Delta_{L,S}(T)$ IMARE data. We showed the temperature behavior $\omega_R(0)$ agrees well with the experimental $\varepsilon_0(T)$ [6]. Therefore, the observed bosonic mode could be a spin exciton, which indicates an important role of spin fluctuations in the Cooper pairing in the SC oxypnictides.

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Keywords: High-Temperature Superconductivity, Multiple-Gap Superconductors, Superconducting Order Parameter, Electron-Boson Interaction, Spin Resonance.

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INVITED SPEAKER

Id-2637

Spectroscopic Study of $K_{0.8}Fe_{1.7}(Se,S)_2$ Selenides in the Superconducting and the Normal State

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Abstract: Layered $K_{0.8}Fe_{1.7}(Se,S)_2$ selenides relate to the 122-Se family of Fe-based superconductors and show a natural phase separation, with an antiferromagnetic insulating 245-phase and superconducting (SC) 122-phase coexisting in the bulk [1]. Due to alkali metal, the SC properties of $K_{0.8}Fe_{1.7}(Se,S)_2$ rapidly degrade even in presence trace amounts of oxygen or water vapor. This feature strongly complicates any studies of the 111 family pnictides, and results to a lack of experimental data on the 122-selenides available to date. Using a “self-flux” technique, we have grown large $K_{0.8}Fe_{1.7}(Se_{0.82}S_{0.28})_2$ single crystals with $T_c \approx 25–27$ K, respectively [2-4]. For all the experiments, the sample mounting was made in a dry argon atmosphere. At 4.2 K, various types of tunneling structures were formed using a planar “break-junction” technique [2]. By measuring their I(V) and dI(V)/dV-characteristics within a wide temperature range, we have determined the main energy parameters of the 245 and 122 phases. In Andreev SnS-junctions (S – superconductor, n – thin normal metal) below T_c we for the first time observed an incoherent multiple Andreev reflection effect (IMARE) [5]. Using IMARE spectroscopy, we detected a single-gap superconductivity, directly determined the magnitude of the SC gap with characteristic ratio $2\Delta(0)/k_BT_c \approx 4.0\text{-}4.5 > 3.5$ [3,4], and its temperature dependence. Using tunneling spectroscopy of ScS and SnS-ScS structures (c – constriction), we measured temperature dependence of the supercurrent $I_c(T)$ and showed that it is consistent with Cooper pair concentration $n_S(T)$. For tunneling junctions of IcI-type (I – insulator) formed within the 245-phase clusters, the I(V) and dI(V)/dV-curves showed a dielectric gap (activation energy) $E_g \approx 47\text{-}51$ meV that remained almost constant with temperature in both, SC and the normal state. In the Fourier spectroscopy and ellipsometry probes, we obtained reflection spectra within the wide range 50–50000 cm^{-1}. Using the optical conductance and permittivity data obtained by Kramers-Kronig analysis, we determined the energies of characteristic phonon modes and interband transitions, as well as the magnitude of the dielectric gap about 50 meV, that agrees well with the tunneling spectroscopy data.

Keywords: High-Temperature Superconductivity, Fe-Based Superconductors, Superconducting Order Parameter, Tunneling Spectroscopy, Infrared Reflection Spectroscopy.

Acknowledgement: This research was funded by the RSF project number 22-72-10082.

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INVITED SPEAKER

Id-2640

Thin Porous Films: How to Control Microstructure and Electrical Properties?

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Abstract: Porous films of oxides and inorganic-organic hybrids are widely used in electronics, optics, sensors, etc. Particularly porous organosilica glasses (OSG) are used as an isolated dielectric with a low dielectric constant (low-k) in the semiconductor industry since the 45 nm technology node. OSG material contains a silicate network with methyl terminal groups located on the pore walls. These films can be obtained through plasma-enhanced chemical vapour deposition (PECVD) or chemical solution deposition (CSD). The letter techniques uses usually involve sol-gel reactions of metal alkoxides. The hydrolysis and polycondensation of these alkoxides lead to the formation of oxoalkoxide complexes, which are the true precursors of oxide phases. This fact offers several advantages, such as good stoichiometry control, a low temperature of oxide phase formation, the possibility to explore molecular self-assembly processes, etc. The evaporation-induced self-assembly (EISA) process was originally discovered by Brinker's group for the preparation of mesostructured silica thin films [1]. This process provides the formation of ordered pore structures with precise control over pore size. Pore walls can be reinforced by substituting inorganic silicon-oxygen bonds with organic ones. These suggestions can be considered as a starting point for the development of new low-k materials. We discuss the structure, electrical, and mechanical properties of periodic mesoporous organosilica films with various ratios of carbon groups between silicon atoms (methylene, ethylene, and benzene) [2]. We demonstrate that charge transport in porous films is governed not only by structural defects in the inorganic matrix (such as oxygen vacancies or divacancies) but to a large extent by pore interface behaviour (organic residues, adsorbed water, grain boundaries) [3], [4].

Keywords: Sol-gel, Thin Film, Porosity, Low-k, Microelectronics.

Acknowledgment: This work was supported by the Russian Scientific Foundation, grant № 23-79-30016.

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INVITED SPEAKER

Id-2644

Physical Phenomena in PZT Thin Films

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Abstract: Thin ferroelectric films are materials with unique properties suitable for various electronics applications. This is a highly nonlinear medium where many processes occur simultaneously, making the correct interpretation of physical phenomena and measurement data difficult and sometimes incorrect. In this report, we have conducted an analysis of methods that could provide a precise physical interpretation of experimental data obtained through commonly used measurement techniques, such as dielectric hysteresis, current-voltage dependencies, and others. We focus on the leakage current in ferroelectric thin films as it affects many electrical parameters of the films. The parameters, such as the remanent polarization and the coercive voltage, obtained from the hysteresis loop, do not reflect the true ferroelectric behavior of the material in the presence of leakage currents and dielectric losses. We will discuss this issue and describe techniques that provide the real value of the spontaneous polarization, the ohmic and relaxation components, as well as the correct estimation of the dead layer thickness in metal-ferroelectric-metal capacitor structures. Measurement of the leakage current is often conducted by applying a linear voltage sweep to a pre-polarized sample. However, the registered current value includes not only the steady-state leakage current but also transient current and the ferroelectric polarization recovery current caused by the rapid depolarization of pre-polarized film. To achieve a steady-state current, one may utilize a voltage step technique. We demonstrate that the steady-state leakage current in PZT films is controlled by the redistribution of oxygen vacancies under an external electric field and the formation of an induced p-n junction. Proposed experimental techniques and physical models can be useful for engineering Ferroelectric Random Access Memory (FRAM) and Microelectromechanical Systems (MEMS) devices based on PZT films.

Keywords: Ferroelectrics, Thin film, PZT, Hysteresis, Leakage Current.

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INVITED SPEAKER

Id-2668

High Entropy Alloys: Some Prospects and Problems

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Abstract: Novel high entropy alloys (HEA) show some excellent properties such as the fatigue, irradiation and corrosion resistance as well as outstanding catalytic performance. The broad compositional range of HEAs enables simple tunning of their properties by varying the contents of constituent elements. However, the understanding of their underlying physics is still limited which is detrimental to the design of HEAs and their application. Some problems hindering efforts to better understand their properties are the excessive uses of the mixing entropy and the rule of mixtures for their design and the prediction of their properties. The near absence of experimental insight into their electronic structure (ES) is especially harmful to their design since ES determines intrinsic properties of all alloys [1]. Thus, the identification of relevant features in ES responsible for the particular property would allow the design of new HEAs with desirable properties, which would also speed up the applications. Recently we have shown that photoemission spectroscopy (PES) can simply explain the evolution of properties in HEAs with different shapes of the electronic density of states (DOS) [2, 3, 4]. Here, in addition to showing the correlation between the PES spectra and the intrinsic properties of selected HEAs, we also show the correlation between the calculated (theoretical) DOS and that depicted from the corresponding PES spectra (experimental DOS). Despite some similarity between the shapes of theoretical and experimental DOS, there is a significant quantitative discrepancy between two DOSes in two HEAs ($Al0.5TiZrPdCuNi$ and $CrMnFeCoNi$) for which such comparison was possible [5]. This discrepancy can lead to the nonoptimal design of new HEAs as well as to the erroneous prediction of their properties. This emphasizes the importance of the careful experimental check of the calculated DOS in novel HEAs designed for specific applications.

Keywords: High Entropy Alloys, Electronic Structure, Photoemission Spectroscopy.

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INVITED SPEAKER

Id-2695

Raman and SERS Performances of PDA-coated Silver and Gold Nano-objects for Emerging Pollutants Monitoring

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Abstract: SERS detection is nowadays a very promising method for on-site, user-friendly monitoring of various organic dyes, pesticides, biomolecules and micro- and nano-plastics favoring a prompt environmental protection. With this perspective the need for stable, reusable, and efficient SERS sensing chips remains crucial for the possibility of label-free trace detection of organic molecules in real environments. Nowadays, the composites formed with polymers and metallic NPs have attracted great interest due to their multifunctionality and are potential alternatives for developing efficient and scalable SERS substrates. In this work we carefully studied the SERS properties of different SERS substrates made up of metal nano objects coated with an ultra-thin layer of polydopamine (PDA). PDA is a versatile biopolymer with great adhesive properties that spontaneously self-polymerizes from dopamine (DA) in weak alkaline media and in the presence of oxygen. Both gold nanostars (GNS) and silver nanospheres (AgNS) were used as metallic enhancing substrates realizing both colloidal and glassy solid SERS matrices. The solid glassy chips were decorated with the nano objects by means of self-assembled monolayer approach and subsequently covered by a thin PDA layer. A detailed characterization of the substrates morphologies has been carried out by TEM and SEM microscopies. The thicknesses of the different PDA layers were estimated by combining profilometry, AFM and ellipsometry measurements. UV-vis-NIR absorption measurements allowed to locate the main plasmonic resonances and monitor their changes with PDA coating. Both for colloids and solid substrates, the SERS responses of different standard Raman reported (Rhodamine 6G, Methylene Blue) were investigated at different PDA thicknesses in the range 0-10 nm. The decay of the enhancement factors allowed to monitor the behavior of average local electric field and to understand the role played by geometrical constraints, aggregation and/or chemical affinity towards specific analyte. The SERS performances were tested in terms of i) surface reproducibility by mapping the SERS signals at micron and millimeter scales, ii) stability over time and iii) enhancement factors. We have found that 1-2 nm thick PDA layers improve SERS performances especially towards Methylene Blue. On these bases possible applications in the detection of emerging pollutants like nano-plastics and antibiotics are discussed as well as the in on-site monitoring of food and beverage safety.

Keywords: Surface Enhanced Raman Spectroscopy, Nanoparticles, Plasmonic Resonances, Pollution Monitoring.

INVITED SPEAKER

Id-2731

Ultrafast Photo-induced Phenomena in Europium Chalcogenides

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Abstract: The ability of light to influence the fundamental parameters of the magnetic interaction in a medium is the focus of modern research in magnetism. In this lecture, we demonstrate a number of photo-induced phenomena in europium chalcogenides. Europium chalcogenides EuX (X = O, S, Se, Te) are intrinsic magnetic semiconductors with unique electronic, magnetic, optical and magneto-optical properties. The top of the valence band of the Eu2+ atom in these compounds is formed by 4f states, which contain 7 strongly localized electrons with a total spin of 7/2. The first empty 5d state forms the conduction band. When the light excites 4f electrons into the 5d band, a strong d-f exchange interaction appears. We report on an experimental study of ultrafast photo-induced phenomena in europium chalcogenides, which occurs when the sample is illuminated by light with photon energy exceeding the band gap. Pump-probe measurements of EuO-based ferromagnets by a time-resolved two-color stroboscopic technique establish optical spin orientation by the electronic transition 4f75d0 → 4f65d1 as a mechanism triggering collective magnetization precession in these materials [1]. Acting on the lattice 4f spins a photo excited 5d1 electron leads to the formation of giant magnetic polarons with a large magnetic moment. It is shown that in the antiferromagnetic EuTe at temperature 5K light generates magnetic polarons with a magnetic moment larger than 600 Bohr magnetons [2]. Rather efficiently magnetic polarons are excited in EuSe [3]. In this material the concentration of polarons is not saturated with an increase in the intensity of the pump light. Thus, EuSe can be completely transferred to a ferromagnetic state by the optical excitation of magnetic polarons. By time-resolved pump-probe technique the spin dynamics involving the growth of giant spin polarons in a EuSe is investigated. Photo-induced Faraday effect helps to unveil the excitation of magnetic polarons with an extra large magnetic moment in the intrinsic ferromagnetic semiconductor europium oxide EuO. The temporal dynamics of magnetic polarons with a record high magnetic moment up to 175·103 μB is disclosed at temperatures slightly higher the Curie temperature. A reversal of the magnetic hysteresis loops by the Photo-induced Faraday effect is detected, which is due to the relaxation of excited electron associated with a magnetic polaron from 5d minority spin state to 5d majority spin state. The decay times of 5 μs is determined revealing the polaron lifetime. The colossal magnetic moments of magnetic polarons and its temperature behavior are in good agreement with available theoretical predictions on EuO. This finding has a great impact on the efficient optical control of magnetic state in solids.

Keywords: Europium Chalcogenides, Photo-induced Magneto-Optical Effects, Magnetization Precession, Magnetic Polaron, Magnetic Semiconductor.

Acknowledgment: The support from the Russian Science Foundation (grant no. 24-12-00348) is acknowledged.

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INVITED SPEAKER

Id-2770

Eco-Friendly Carbon-Based Conductive Composites: Shaping the Future of Biosensors and Beyond

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Abstract: Sustainable electronics has emerged as a key trend in today's world, driven by the need for non-toxic materials and recyclable components that not only benefit the environment but also pave the way for innovative solutions. One promising application of these advancements is in the biomedical field, particularly in the development of modern electrocardiographic electrodes. Our research focuses on creating disposable electrodes that are both sustainable in production and thermally recyclable through incineration without leaving harmful residues. Here we present extensive research into modern sustainable electrically conductive composite materials dedicated to such an application. We have investigated the applicability of new matrices for electrically conductive composites in technologies like screen printing and flexography. We have investigated both established biopolymers and also other materials that have not yet been used in electronics. To ensure the functionality of the printed composites, we examined essential physical properties, including viscosity, printability, substrate compatibility, and electrical performance. Given the biomedical focus, we also evaluated cytotoxicity, and in line with sustainability goals, we assessed degradation behavior under environmental stress.

Keywords: Printing Composites, Printed Electronics, Sustainability, Recyclable Sensors.

INVITED SPEAKER

Id-2773

Mechanical Properties of Recycled Aggregate Concrete Incorporating Recycled Concrete Powder

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Abstract: This study explores the sustainable use of recycled concrete powder (RCP) from construction and demolition waste as a partial cement replacement in concrete. RCP was produced from recycled concrete aggregates (RCA). Mechanical properties (compressive and flexural strength) were evaluated to assess the mechanical performance of concrete. The results revealed that recycled aggregate concrete with 50% RCA replacement showed a reduction of 8.3% and 12.3% in compressive strength at 28 and 90 days of curing, respectively, compared to conventional concrete with 100% natural gabbro aggregates. Additionally, the inclusion of 15% RCP maintained comparable compressive strength compared to 100% Ordinary Portland cement-based RAC.

Keywords: Recycled Concrete Powder, Mechanical Performance, Recycled Aggregate Concrete.

INVITED SPEAKER

Id-2774

Electron Beam Attenuation and Energy Dissipation between 0 eV and Relativistic Energies

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Abstract: The status quo of quantitative nanoanalysis using medium energy electrons will be briefly reviewed, demonstrating the impressive progress which has been made over the past fifty years. This is in stark contrast to the understanding of the interaction of low energy electrons (LEEs) with surfaces which is rapidly gaining attention due to its importance for a variety of processes on the nanoscale: LEEs are not only essential for nanoscale analysis such as microscopy, CD metrology or attosecond physics but also act as agents inducing physico-chemical processes as in, e.g., electron lithography, electron beam induced deposition, astrochemistry and, last but not least, DNA-bond breaking induced by high energy ionising radiation striking biological tissue. Improvement in this field is complicated by the lack of benchmark experiments specifically designed to obtain information on individual physical parameters or processes. In the present talk, a recently proposed experimental approach will be described [1] in which the quantitative knowledge of the medium energy range is used to gain information about the (poorly understood) low energy range. This is done by using medium energy primary electrons as messengers of the depth of creation of low energy secondaries. Measuring the secondary electron intensity as a function of depth of creation, the attenuation law in the low energy range is quantified. In the case of polymethylmethacrylate, it is found that the attenuation law is non-exponential, but is rather made up of two exponential functions, corresponding to two different groups of electrons playing a role in the energy dissipation process. The attenuation lengths of both groups are measured and essentially agree with a theory used for decades in astrophysics —albeit with units expressed in nm rather than lightyears— and providing electron attenuation lengths in the range between 0 eV and relativistic energies.

Keywords: Lithography, Resists, Electron Beam, Attenuation.

Acknowledgment: Financial support by the Horizon 2022 Marie-Curie Actions Initial Training Network (ITN) EUSpeclab (Grant No. 101073486) and by the FP7 People: Marie- Curie Actions Initial Training Network (ITN) SIMDALEE2 (Grant No. PITN 606988) is gratefully acknowledged.

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INVITED SPEAKER

Id-2778

Electron Emission from Graphitic Surfaces in the Low-Energy Regime

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Abstract: The interaction of Low-Energy Electrons (LEEs; with energies ≤ 100eV) with solids and the phenomenon of Secondary Electron Emission (SEE) from surfaces are of paramount importance for a multitude of modern technologies, applications, and emerging scientific fields, such as Attosecond Physics. For over a century, both LEEs and Secondary Electrons (SEs) have been employed e.g. in microscopy, in particle detectors, and photovoltaic devices. In contrast, the creation of these very same LE-SEs can pose a nuisance, hindering processes like lithographic patterning, or leading to unwanted DNA bond-breaking in biological tissue. Due to their lower Secondary Electron Yield (SEY), Carbon-based coatings are employed in charged particle storage rings to mitigate the electron cloud formation affecting the Large Hadron Collider operation at CERN. Improving our understanding of the mechanisms governing SEE, as well as elucidating LEE-transport characteristics, is not only imperative for technological progress, but also for resolving fundamental questions about SE generation-ejection mechanisms. This presentation will illustrate various aspects – studied by means of different experimental techniques – of the interaction of electrons and photons with graphitic surfaces chosen for their anisotropic electronic response, making them prototypical systems for modern uniaxial 2D-layered Van der Waals heterostructures.

The discussed experimental methods include:

(I) (absolute) Total Electron Yield (TEY) measurements in the LE-range, exposing the relevance of the band structure in the observed signal [1,2];

(II) Single-electron spectroscopies such as Reflection Electron Energy Loss Spectroscopy providing insights in the involved excitation channels, and Secondary Electron Emission Spectroscopy allowing identification of contributing final states in the spectral response;

(III) (e,2e)-coincidence spectroscopy which detects correlated electrons pairs from the same scattering event, establishing a causal link in between the energy-loss channels and the resulting SE-spectrum and providing kinematically complete measurements to study the elementary mechanism of SE-creation and -emission;

(IV) Photo-Electron Emission Microscopy (PEEM) experiments allowing the study of the electronic spectral response as a function of the photon energy, light polarisation and delivering K-space-resolved information contained in their energy-filtered angular distribution. The influence of the electronic band structure on the SE-emission process is observed with all employed approaches. Using electron-pair spectroscopy the (π+σ)-plasmon feature in graphite was resolved with respect to the involved interband transitions, highlighting a strong final-state resonance. This resonance, a strong characteristic peak in the SEE-spectrum, remained unexplained until recently [3].

Keywords: Graphite, Low-Energy Electrons, Fundamentals of SEE, EELS, Secondary Electron Emission, Electron-Pair Spectroscopy, PEEM.

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INVITED SPEAKER

Id-2779

Self-assembly Formation of Water Soluble Nanoparticles Explored by Computational Techniques

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Abstract: Supramolecular assembly of different amphiphilic molecules allows to incorporate sensors into vesicular aggregates with high colloid stability and biocompatibility, which provides a good basis for creating sensory systems. The uses of colorimetric and luminescence techniques for the sensing are particularly attractive, since they can facilitate naked-eye or simple spectroscopic detection of biomolecules or water soluble toxicants. The development of sensory systems on the basis of supramolecular assemblies requires structure optimization on both molecular and supramolecular levels. It is well known that both the conformation and the electronic structure of dye molecules inserted into phospholipid vesicles are greatly influenced by their environment, which causes the sensitivity of dye molecules to phase transitions of phospholipid bilayers. Moreover, both conformational flexibility and hydrophobic or hydrophilic environment of a dye molecule have a major influence on its sensory function. We will demonstrate how computational modeling of self-assembling behavior of various phospholipid and dye molecules allows to clarify details of the microscopic structure of the modeled species, both at the atomistic and quantum mechanical levels. The cluster modeling will be shown to deliver valuable information on the structure of hydration of dye molecules incorporated into the formed nanoparticles, their inter- and intramolecular hydrogen bonding, and impact of nanomatrix on their tautomeric and conformational equilibria. Possible applications of the developed technique in analysis of nano-sized micelles will be also discussed.

Keywords: Quantum Chemistry, Molecular Dynamics, Clusters, Tautomers, Conformers, Hydrogen Bonding.

ORAL PRESENTATION

Id-2573

Base Excitation and Finite Element Simulation for Assessing the Risk of Acoustic Induced Fatigue

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Abstract: Acoustic induced vibration often give rise to high frequency vibrations that can be damaging to static and rotating equipment alike. In this paper, the vibration of steam inlet pipe to a turbine that drives a production-critical compressor is investigated. The pipe is hot (circa 230ºC), insulated and largely inaccessible. Due to production requirements, shutting down the compressor, removing the insulation and installing strain gauges on this line is not operationally feasible. A field-based approach was used to assess the risk of acoustic induced vibration to the pipe. Vibration measurements near a governor valve were recorded and were then used along with a finite element (FE) model and random vibration analysis to compute the stresses in the pipe. Furthermore, noise level measurements outside the pipe were also recorded and the sound pressure level inside the pipe was calculated and applied in a separate FE simulation of the pipework. In both simulations (using the noise as an input and using the pipe vibration as an input to the FE model), the resulting predictions were similar and indicated that risk is inadequate for long-term operations. The results of this investigation were used to justify the shutdown of the compressor and to initiate a measurement campaign to further assess the risk, confirm the root cause of the vibration and propose (short- and long-term) solutions.

Keywords: Vibration Induced Fatigue, Finite Element Analysis, Base Excitation, Random Vibration.

ORAL PRESENTATION

Id-2576

Exploiting Underlying Crystal Lattice for Efficient Computation of Multi-million Atoms Nanostructures

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Abstract: Atomistic modeling of nanostructures often leads to computationally challenging problems involving millions of atoms and tens of thousands of Coulomb matrix elements. We present a practical solution to this problem [1,2], where quasi-linear efficiency, both in time and memory, was obtained using the fast Fourier transform. Here, we present an updated version of our approach: a highly parallelized computer program [1], named Coulombo-Lattice [2] that eliminates the necessity of introducing an auxiliary basis set for the wave-function transfer to the computational grid. Here, we instead exploit the properties of the underlying crystal lattice and run calculations on a regular three-dimensional grid superimposed on the original, lower-symmetry lattice. Due to the removal of spurious interactions from other supercells, the resulting Coulomb matrix elements are, up to numerical precision, identical to those obtained by the direct summation O(N2) method. Yet, our code maintains O(N log N) scaling. We illustrate our approach by calculations involving up to 1.7 million integrals and a number of atoms reaching up to 2.8 million for the problem of dopant charging energy for a single phosphorus dopant embedded in a silicon lattice. Next, to emphasize the broad applicability of our code, we show the results for mixed zinc-blend/wurtzite lattice systems, also known as crystal phase quantum dots.

Keywords: Quantum Dots, Atomistic Calculations, Dopants in Silicon.

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ORAL PRESENTATION

Id-2650

Application of Ionic Liquid-Multi Walled Carbon Nanotubes-l-lysine Modified Glassy Carbon Electrode for Detection of Prednisolone

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Abstract: Prednisolone (PDN) is a corticosteroid drug that is used for treatment of a number of inflammatory conditions such as bronchial asthma and allergic reactions around the world. An overdose of PDN can cause adverse effects in the human body. Therefore, the development of analytical tools for PDN monitoring is vital. In this work, multi-walled carbon nanotubes (MWCNTs)-Ionic liquid (IL)-l-lysine modified glassy carbon electrode (GCE) sensor was developed for the determination of PDN using voltammetry technique. The IL based nanocomposites were characterized via scanning electron microscopy (SEM), transmission electron microscopy (TEM), Fourier transform infra-red (FT-IR) spectrometer, thermal gravimetric analysis (TGA) and electrochemical impedance spectroscopy (EIS) techniques. Under optimized experimental conditions, the newly fabricated electrode exhibited remarkable electrochemical performance with LOD (limit of detection) and LOQ (limit of quantification) of 0.0214 μM and 0.3016 μM, respectively, for PDN detection. In addition, the developed electrode also displayed a superior selectivity for PDN in the presence of the interfering substances. The fabricated MWCNTs-ILs-l-lysine-GCE exhibited a remarkable stability where the electrode retained 89 % of its first peak-current response with an estimated relative standard deviation (RSD) of 1.72 % after 4 weeks storage. Furthermore, the reproducibility the fabricated electrode was acceptable with RSD value of 3.0% for ten repeated measurements (n = 10). The proposed MWCNTs-ILs-l-lysine-GCE sensor was successfully employed for determination of PDN in aspelone syrup sample via differential pulse voltammetry (DPV).

Keywords: Nanofabrication, Sensor, MWCNTs, GCE.

ORAL PRESENTATION

Id-2651

New Requirements of Defence in Depth and Extension of Its Application

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Abstract: As states in the IAEA-TECDOC-1791, the defence in depth concept is not to be understood as merely limited to the request for the implementation of a number of consecutive barriers and protection levels, but is to be understood as the main general principle that leads to the formulation of safety requirements including requirements necessary to achieve the quality and reliability expected for the barriers and for systems ensuring their integrity. Thus, the application of defence in depth is not only limited in the reactor core, but also can extend to a wider range. In this paper, the application of defence in depth in the irradiated fuel water pool storage, electrical system, internal and external hazards of the nuclear power plant design are reviewed. Base on the study of the newest standard and codes, the design requirements of each level of defence in depth in the above systems are confirmed. The analysis of defence in depth design features of an advanced nuclear power plant in China are also show the application value of defence in depth in these extended regions.

Keywords: Nuclear Safety Standard, Defence in Depth, Extended Application of Defence in Depth.

ORAL PRESENTATION

Id-2674

Self-Propagating High-Temperature Synthesis in Ti-Ni Core-Shell Nanoparticles

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Abstract: Ti-Ni core-shell nanoparticles were fabricated using a combined gas aggregation source. They can be used as a source of heat for the brazing of nanostructured components due to the heat released during the self-propagating high-temperature synthesis. In-situ TEM experiments performed on nanoparticles during heating up to 1100 °C showed that the heating rate is a controlling mechanism for deciding the type of reaction occurring at high temperatures. While the heating at low heating rates results in a separation of Ni from Ti, a rapid increase in temperature leads to the formation of an intermetallic NiTi phase. TEM results were confirmed by molecular dynamics simulations.

Keywords: Ti-Ni Nanoparticles, Core-shell, High-temperature Self-propagating Synthesis, In-situ TEM, Molecular Dynamics.

ORAL PRESENTATION

Id-2691

Cementitious Coatings on Magnesium Alloys for In Vivo Passivation

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Abstract: Our recent studies demonstrate the effectiveness of cementitious coatings comprising water soluble phosphates including calcium, potassium phosphates and orthophosphoric acid. They were immobilized on reactive magnesium alloys by a facile dip coating technique to induce favorable reactions in physiological aqueous solutions for development of passive interphases at the implant surfaces. This novel approach is akin to the chemical conversion of corroding alloy surfaces, i.e. phosphatizing, in that corrosion is inhibited by the precipitating phosphate salt of the corroding metal ion. Yet this approach enables a more gradual and biomimetic conversion of the corroding alloy surface during the implantation stage, utilizing the leached cations to form a compatible interphase layer for enhanced bone bonding. These spontaneously crystallized surfaces that serve as both bioactive layers and passivating interphases on rapidly degrading magnesium alloys can be further enhanced by integration of biological macromolecules to the cementitious coatings.

Keywords: Magnesium, Corrosion, Cement, Biodegradation, Biocompatible, Phosphate.

ORAL PRESENTATION

Id-2717

Radiation Protection and Dosimetry in High Power Laser-driven Experiments

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Abstract: Extreme Light Infrastructure – Nuclear Physics (ELI-NP) research center is hosting a high-power laser beam system, with three outputs: 100 TW, 1PW and 10PW. The laser pulses are delivered towards the dedicated experimental setups, being focused on two types of targets: gaseous and solid ones. Internal dose constrains have been established as ten times lower than the legislative requirements. Monte Carlo – based simulation codes, active and passive dosimetry systems are building the complex system used to properly characterize high particles fields generated by the ELI-NP experiments. The active radiation monitoring system is foreseen to perform real time dose measurements outside of the experimental areas, meanwhile passive dosimetry is backing up the ultrashort pulses which might overcome the active detection limits. The scope of the current study is to present the dosimetry assessments performed for mixed high energy particle fields generated during laser-based experiments.

Keywords: Passive Dosimetry, High Power Laser, 10 PW, Radiation Protection.

ORAL PRESENTATION

Id-2733

Looking at Photocatalysis from a Different Perspective: Considering Hybridisation of Low Energy Waves with Visible Light for Organic Pollutant Removal

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Abstract: Visible-light-driven photocatalysis has garnered significant attention as a promising solution for effectively removing organic contaminants from water and creating hydrogen in an environmentally benign manner. Nevertheless, the use of this auspicious technology on an industrial level has been restricted due to the exorbitant expenses, suboptimal effectiveness, and challenges in retrieving and reutilising the photocatalyst. Thus, exploring the use of low energy waves on tailoring the physical, magnetic, optical, and electrochemical properties of fabricated photocatalysts is a promising possibility to explore. Moreover, designing photocatalyst nanocomposites that are low energy wave and visible light responsive, will open a door for the simultaneous use of the available green energy for the photodegradation of organic pollutants. Overall, the incorporation of low wave energy in photocatalysis offers significant opportunities for advancing the field and addressing pressing environmental and energy challenges. Continued research and development in this area will likely yield novel catalyst designs, improved process efficiencies, and expanded applications, ultimately contributing to a more sustainable and cleaner future.

Keywords: Low Wave Energy, Photocatalysis, Photocatalysts Design, Organic Pollutants Removal.

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ORAL PRESENTATION

Id-2772

A Study on the Development and Validation of an Integrated Steering and Driving Dynamics Model for an MR-Based K9 Howitzer Firing Simulator

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Abstract: This study aims to develop and validate an integrated steering and driving dynamics model for the K9 self-propelled howitzer, considering its steering and driving characteristics, as a preliminary step in the creation of an MR-based K9 howitzer firing simulator. The steering principles and characteristics of the K9 were analyzed to construct the dynamics model, and a CAD-based kinematic analysis was conducted. Additionally, steering dynamics factors required for the design of the VR physics engine were incorporated to enhance the accuracy of the developed model. Finally, an integrated model for both steering and driving was developed and validated using real vehicle measurement data to assess its reliability.

Keywords: K-9 Self-Propelled Artillery, Steering Dynamics, Integrated Dynamic Model, Vehicle Measurement, Validation.

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ORAL PRESENTATION

Id-2780

Perpendicular Magnetic Anisotropy on Co/Pt Multilayers with Ru Spacers as TMR Sensor Applications

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Abstract: Magnetic Thin Films and their applications as magnetic sensors, which is the key as magnetic, electronic, and optical properties, play crucial roles in advancing technology in wild range using areas. The aim of our study is on magnetic materials which having perpendicular magnetizations. Perpendicular magnetic anisotropy which have data storage advantages for easy direction of magnetization (Out-of-Plane magnetization axis is advantageous). We can use Out-of-Plane magnetization on Perpendicular Magnetic Tunnel Junctions (p-MTJs) that have shown great potential in spintronics applications such as STT-MRAM and magnetic sensors in recently. They mostly rely on the perpendicular synthetic antiferromagnetic (p-SAF) structures based on thin Co/Pt multilayers, which exhibit large Perpendicular Magnetic Anisotropy (PMA) Energy and High Exchange Interlayer Energy. Field stability of the reference layer causes to p-MTJs that usually rely on p-SAF structures and have high coupling fields cause that capable of sustaining the reference system up to several kOe magnetic fields. Also, this study aims on RKKY interaction in Co/Pt p-SAF systems using as Ru spacer layer with different thickness to compare each other. The multilayer films were deposited at about UHV conditions by Magnetron Sputtering and Thermal Evaporation systems separately with Ru layers as buffer and cap layer about 100 Å, Pt 1,4 Å and Co 3,4 Å thickness. The magnetic properties and interlayer couplings were obtained at RT via Magneto-Optical Kerr Effect System (MOKE), Vibrating Sample Magnetometer (VSM) for Out-of-Plane magnetic fields. According to results, p-SAF systems could use as a pin layer for p-MTJs.

Keywords: Synthetic Antiferromagnetic Structures, Perpendicular Magnetic Anisotropy, Magnetic Multilayer Thin Films.

POSTER PRESENTATION

Id-2572

Viscoelastic Response of Sugar Beet Root Tissue to Mechanical Loading

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Abstract: Stress relaxation tests are an essential source of knowledge about the physical state of high water content agricultural products such as fruit and vegetables. The tests are of particular significance because their results make it possible to propose a model of studied material. Viscoelastic parameters are closely correlated with chemical composition, e.g. soluble solids content or acidity as well as texture features, e.g. hardness, springiness or chewiness. The aim of this study was to determine the sugar beet root flesh force response in the wide range of deformation velocities (quasi static and impact mechanical loading conditions). During the research the cylindrical samples of roots in the range of deformation velocities from 0.0002 to 1ms^{-1} were studied. The five-parameter generalized Maxwell model was used to describe the experimental stress relaxation curves. The relaxation times of the generalized Maxwell model decreased with the increase of deformation velocity. The relaxation times were related to the processes of gas and liquid flows in the intercellular spaces. The rapid decrease of both relaxation times was stated between deformation velocity of 0.0002 and 0.002 m^{-1}. It testifies to the existence of critical deformation velocity associated with the weakness of the root's tissue structure at the velocity mentioned above.

Keywords: Sugar Beet Root, Stress Relaxation, Maxwell Model.

POSTER PRESENTATION

Id-2579

The Directional Formation and Anti-corrosion Action of Self-Assembltd Siloxane Nanolayers on Copper Surface

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Abstract: The objective of this work was to examine the adsorption of organoysilanes on Cu as well as study the structural and anti-corrosive properties of an organosilane surface films. Adsorption of organosilanes with general formulae $R_nSi(OR')_{4-n}$ on the surface of copper from an aqueous solutions has been examined by quartz nanobalance (QCN), ellipsometry, and optical microscopy techniques. Organosilane molecules displace adsorbed water from the surface during adsorption. For the interpretation of adsorption data, Langmuir, BET, Flory-Huggins, multisite Langmuir, Temkin, Frumkin, and Freundlich adsorption approaches were used. The surface orientation of adsorbed molecules and the heats of adsorption of silanes moleculed was determined. and it was shown that silane molecules are found to be chemisorbed on the surface of copper. It was established that at the initial stage of the formation of organosilane films on Cu, the VS molecules are chemisorbed monomolecularly and then - polymolecularly. The capacitance of the monolayer, the magnitude of the "landing area" of vinylsilane molecules and other main adsorption characteristics of the adsorbate molecules were determined. With using infrared spectroscopy(FT-IR), atomic-force microscopy(AFM), and scanning electron microscopy (with energy-dispersive X-ray spectroscopy(SEM-EDS)) it was established that the adsorption of vinyltriethoxysilane (VS) on a copper surface from an aqueous solution results in formation of a uniform, self-assembled protective siloxane layer covalently bound with surface metal by Cu-O-Si bonds with layer thickness 0.5–0.8 μm. Film thickness can be controlled by variation of deposition conditions. The mechanism of formation of surface self-assembled layers on zinc is proposed. The mechanism of formation of surface self-assembled layers on zinc is proposed. It was carried out the study of corrosion and electrochemical behavior of Cu with the use of routine electrochemical andcorrosion techniques, the electrochemical quartz costal nanobalance, scanner-assisted electrochemical reflectomctiy, SEM-EDS. and X-ray spectral microanalysis Electrochemical and corrosion test results demonstrated that the presence of vinilsilane films on Cu led to the inhibition of metals dissolution. It is found that an ordered vinyl siloxane nanolayer with a thickness of 3-8 molecular layers causes efficient inhibition of uniform and localized corrosion of copper. The magnitude of local depassivation potential was 70 mV The exposure of metal samples with films for 720 h in the climatic chamber (RH 95%, t=60°C) illustrated the best protective capacity of the Cu + VS system. For this system, the proportion of corrosion damage of surface was 3% and the time before the appearance of the first defect was 242 h. The greatest protective effect is observed at a thickness of 3-8 molecular layers when the most compact film, which hampers the adsorption of chloride ions and substantially decreases the rate of their interaction with the surface copper atoms, is formed. An infrared spectroscopy study carried out after electrochemical and corrosion tests showed a high resistance of surface organosilicon layers to the action of corrosive electrolytes. It is shown that the vinyl siloxane nanolayer is preserved on the surface of zinc after 30 days of corrosion tests, which indicates its stability at exposure to water and corrosive components.

Keywords: Adsorption, Quartz Nanobalance, Metal Corrosion, Copper, Organosilanes, Coupling Agents, Adhesion, Self-Assembled Layers, Corrosion Inhibition.

POSTER PRESENTATION

Id-2587

Diffusion mechanisms in superabsorbent hybrid hydrogels structures usable as water and nutrients carriers/releasers

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Abstract: The need for new or with improved properties materials is felt more and more in all fields (agriculture and environment [1,2], medicine [3,4], engineering [5,6]), their immediate availability being a necessity for adapting to the rapid technological progress and to its consequences. Hybrid hydrogels, with stable structures that allow the use in multiple swelling-deswelling cycles and with biodegradable potential may represent an alternative for both near future need of water and environmental protection, also. Two types of hybrid hydrogels based on acrylic acid, sodium alginate and poly(ethylene oxide) have been obtained by electron beam of 5.5 MeV irradiation [7], in the dose range of 5 to 20 kGy and used in swelling experiments in two types of water (distilled and tap) and two types of nutrients solutions in order to follow the swelling dynamic and kinetics. Lyophilized hydrogels previously immersed in water and nutrients solutions have been investigated by SEM technique in order to correlate the frequency and dimensions of voids with the water diffusion in the material structure. Biodegradation experiments by burial of hydrogels in soil for one and two months were also done to estimate if their nature and behavior are adequate with the purpose of obtaining: water stress reducer and nutrients carrier with biodegradable properties. The increase of the irradiation dose has led to the obtaining of hydrogels increasingly stable in the swollen state. The addition of reaction initiator did not significantly change the hydrogels physico-chemical properties, that confirms the effectiveness of the irradiation treatment to induce cross-linking and grafting processes. The values of diffusional coefficients and swelling exponents/constants revealed the fact that some hydrogels immersed in the nutrient solutions presented simultaneous manifestation of water diffusion through the pores and polymeric chains relaxation phenomenon (non- Fickian diffusion) while others, obtained especially at irradiation doses lower than 20 kGy, swelled exclusively through the phenomenon of macromolecular relaxation (super case II). The results were confirmed by the SEM investigations carried out on lyophilized hydrogels in swollen state in each of the considered swelling media, that revealed differences in terms of pore structure, favorable to one or another of the diffusion mechanisms. The biodegradable potential of the studied hydrogels has been investigated following the mass loss after 30 and 60 days of burial in the soil and the change in cross-link density, that provides information about the state of the polymer structure. The hydration of the soil and implicitly of hydrogels in acidic solutions have led to the recording of more than significative mass loss accompanied by a high decrease of cross-link density after 60 days. The hydration in basic solutions has led after both 30 and 60 days to mass losses and changes in the structure of the polymer network above the average results. The tap water (used in many real situations for lands irrigation) and

the organic nutrient solutions may represent viable solutions for solving the problem of water and nutrients lack of soils.

Keywords: Hybrid Hydrogels, Electron Beam Irradiation, Diffusion, Biodegradability.

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POSTER PRESENTATION

Id-2591

Tuning of Second Order Phase Transition of NiMnGa Heusler-Type Glass-Coated Microwires

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Abstract. Studies of Heusler alloy have attracted considerable attention because of their suitability for many applications [1]. Different Heusler alloys can present magnetocaloric effect (MCE) [1,2], ferromagnetic shape-memory effect, half-metallic behaviour, and even superconductivity [1]. The conventional preparation method of Heusler alloys is arc-melting, followed by prolonged high temperature annealing [1,2]. The technological advance requires miniaturized of Heusler-type materials [2,3]. However, the use of conventional methods for the preparation of thin Heusler-type materials is limited by poor mechanical properties and complex processing of Heusler alloys [2]. Therefore, recently rapidly quenching technique has been successfully employed for the preparation of Heusler-type ribbons and wires [3]. Usually, the second-order phase transition temperature can be tailored by the chemical composition of the alloy [1,2].In the present paper, we present our last results on the tuning of the second-order phase transitions in Heusler-type NiMnGa glass—coated microwires by annealing. NiMnGa glass-coated microwires, with a metallic nucleus diameter from 10 up to 21 μm, have been prepared using Taylor-Ulitovsky method [3]. We annealed the microwires at temperatures ranging from 550 up to 750 °C. As-prepared Ni-Mn-Ga microwires exhibit a very weak magnetization at room temperature. However, annealed samples present ferromagnetic behaviour and second-order phase transition at nearly room temperatures. Additionally, the Curie temperature, Tc, is considerably affected by the annealing conditions (annealing temperature and duration). Mixing of glass-coated microwires annealed at different conditions allows tuning of M(T) dependence and hence obtain broader second-order phase transition. As discussed elsewhere [4] such expanding the temperature range over which a significant magnetic entropy change can be obtained is beneficial for the improvement of the refrigerant capacity.

Keywords: Magnetic Wire; Heusler Alloy; Hysteresis Loops; Annealing; Curie Temperature.

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POSTER PRESENTATION

Id-2592

Nonvolatile Memory Cells Based on Thin Film Disorder Chalcogenide Semiconductors

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Abstract: The mass production of many electronic devices like name- and SIMM cards, control units of gas, electrical power and water consumption, protection systems, computers, mobile phones etc., where the novelty of their consumer characteristics is connected with the necessity of coding and power independent of data storage, is considerably complicated because of the lack of reliable and durable thin filmed memory elements. Today solid-state analogies based on semiconductor integrated microcircuits are manufactured by means of highly precise and expensive technologies do not satisfy the modern technical and economic requirements of mass-production. Also, modern electronic circuits can only get so small before they are overwhelmed with heat problems. Encoding bits using the spin of electrons instead of the usual charge, promises to allow even smaller circuits because flipping the spin to change a bit requires much less energy than moving charge. But the known processes of flipping electrons' spins with external magnetic fields are inefficient and require very low temperatures, making such "spintronic" devices impractical. To solve these problems, we have investigated physical effects of memory and switching at the interface of chalcogenide thin films on the basis of tellurium and its alloys and have worked out the technological process to manufacture the nonvolatile memory cells which are wiped off by electricity. We were focused on possible conversion of a normal isolator (OFF state) into a topological one (ON state) by application of an external electric field that shifts different energies and induced a specific band inversion, which leads to a topological state. The tuning of topological behavior with electric field would leads to spin-separated, gapless states, that is as spintronic and superconducting effects at the room temperature. The finding opens the possibilities of converting normal insulating chalcogenide materials into topological ones via electric field and making multifunctional "field effect transistor" that could manipulate simultaneously both spin and charge carrier. Electron spin can be visualized as the notation of an electron in one of two ways, with the rotation axis pointing up or down. Just like the present or absence of an electric charge represents a bit equaling "1" or "0", a spin pointing up or down can do so as well. It has been discovered the main parameters (time of data recording and data storage, the number of erasable cycles, etc.) of these elements excel the analogues. The main differences of the worked out memory elements over the analogues:

1. During the manufacture of our memory elements we use a cheap thin filmed technology that one of the main «commercial» stimulus for its production.
2. Especial features of thin filmed technology make it possible to use various kinds of substrates when manufacturing the memory elements: from glass to flexible printed plates. It extend considerable

the field of their application: from business cards and electric money to the microcircuits of memory with 1 Mbit capacity and more.

3. By their functional possibilities the memory elements are the usual resistors with two dimensions of resistance. This simplifies considerably the operation of these elements and makes these irreplaceable for the application in such structures as code locks, safeguarding systems, electronics keys and various meters.

4. These elements of memory differ from the most famous analogue of ESD Company, USA by the utilization of the original physical principles and constructive especial features as well as by the application of new combinations that makes them competitive and patentable.

5. The main differences of these elements of memory are splendid electric and technical data in combination with high safeguard of work and information storage.

Above mentioned peculiarities of the memory elements make it possible to prophesy the large prospects of their application in various kinds of new generation electronics. These include areas such as high-temperature superconductivity, spintronics, and nano-electronics. For example, one can manufacture electronic circuits for use in quantum computing that have properties similar to conventional semiconductor devices, but on much smaller scales, and with substantially reduced power requirement and an extremely high speed of operation. The areas also include new electronic keys, extremely fast switches, electro-optical modulators, sensors, magnetic devices, magneto-resistive memory cells, energy saving cells for random-access memory (RAM) devices, and the like.

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POSTER PRESENTATION

Id-2594

Covalent Organic Frameworks for Homojunction SMOSCs and Electrode Materials

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Abstract: Covalent Organic Frameworks (COFs) became important targets in organic chemistry and materials science due to their high stability, high control of the structure and texture (pore size, porosity), tunability for specific applications, rational design by the combination of the geometries of different building blocks and powerful access by the multitude of specific reactions of organic chemistry [1]. COFs incorporating alternatively disposed donor and acceptor units which involve the segregation of donors and acceptors with the formation of superheterojunctions and the migration of charge carriers along donor and acceptor columns revealed outstanding optoelectronic properties [2], while COFs exhibiting cationic groups showed relevant applications in anions recognition and transport. [3]. In this work we report the synthesis and characterization of novel 2D COFs obtained either by Knovenagel condensation of aromatic trialdehydes with di- and tricyanomethylarenes (COFs I) or by the classic imine formation condensation of trialdehydes (e.g. 1,3,5-triformylbenzene) with aromatic diamines (e.g. *p*-phenylenediamine) decorated with pendant arms exhibiting terminal trimethylammonium groups (COFs II). COFs I are among the few examples of COFs which act as Single Material Organic Solar Cells [4] and the obtained PCE values (up to 0.5%) are close to the PCE values reported for other SMOSCs [5]. COFs II revealed good affinity for anions (including OH^-) and are important candidates for the fabrication of anion transport electrode materials.

Keywords: COFs; Homojunction SMOSCs, Anions Transport and Electrode Materials for Batteries and Water Electrolysis.

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POSTER PRESENTATION

Id-2598

Picosecond Ultrasonic Photoacoustic Emitter Based on Graphene-Decorated Gold Nanoparticles

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Abstract: Piezophotonic or light-to-pressure transducer materials exhibit tremendous potential across various disciplines and applications, embracing theragnostic ultrasounds and permeabilization of biological barriers for drug delivery or for gene transfection. Here, we report the photoacoustic response in the picosecond excitation regime of graphene and gold nanoparticles decorated graphene dispersed in a polydimethylsiloxane polymer (PDMS) matrix. This study is a missed tile in the photoacoustic of graphene and its derivate, explores and explains the possibility of controlling the photoacoustic emission by linking material science and photoacoustic. First, a novel decoration method was developed to nucleate Au nanoparticles of 25 nm on the graphene surface without reducing agent. The nucleate particle improves the dispersibility of the flake inside the polymeric matrix, increases the surface area in contact with the matrix, and prevents the flakes from restacking. This leads to a better intercalation of the polymer in the inter-flake space and a more uniform and efficient photoacoustic response. We observed that the picosecond excitation enforced by the stress confinement generates high-frequency waves, with bandwidths of -6 dB and -20 dB of around 70 MHz and 130 MHz respectively, and peak pressure > 5 MPa. Further, the presence of gold surface decoration leads to an increasing bandwidth at -6 dB up to 85 MHz and to a better dispersibility of the flake into the polymer matrix. Our results show an increasing frequency of ultrasound with the reduction of the thickness of the source that retains its value against a large increase of the laser fluence, up to 150 mJ cm $^{-2}$.This enables the possibility to operate at high pressure while keeping the same bandwidth. We experimentally show the possibility of tailoring the photoacoustic waveform by changing the temporal duration of the laser light, the geometry of the acoustic source, and the nature of the starting graphene absorber. The comparison between films with the same thickness and optical penetration depth clearly shows a positive effect on the frequency response in the presence of gold nanoparticles. Piezophotonic composites based on 2D graphene and decorated graphene are stable and easy to fabricate, the generated high frequency and high pressure are tremendous of interest and ready to be explored as physical methods to permeabilize cell barriers for genetic transfection, assisted drug delivery, and high-resolution imaging systems. The flexible decoration and fabrication method of the thin film, along with the generation of high-frequency and high-pressure ultrasound waves, represents a promising avenue for the use of physical methods to permeabilize biological barriers and develop high-resolution photoacoustic imaging systems.

Keywords: Graphene Composite, Gold Nanoparticles, Photoacoustics**,** Piezophotonic, High-Frequency Ultrasound.

POSTER PRESENTATION

Id-2600

Study and Characterization of New Dosimeter MAGIC-Glytaraldehyde

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Abstract: The gel dosimeter depends on the radiation polymerization process of the monomer. Thus, the polymer formed for a dose is represent by particles polymerized in the gelatin molecules. It has been reported that the accuracy of the dose measured by such detectors depends on the accuracy of the original signal recorded inside the polymer gel medium and the precision of the calibration equation. In 2020, a structural study of the MAGIC polymer gel provided information on the origin of the gel, such as the important role of gelatin at the beginning of the polymerization process and when cross-linked three-dimensional network would facilitate the fixation of PMA in the gelatin matrix that would prevent their diffusion into the solution. The latest information helped us to undertake this study to improve the cross-linking of the gel in order to increase the signal obtained by the images (CT-scan) for radiotherapy treatment. The objective of this work is the development of a new dosimetry system that is more efficient than the MAGIC polymer gel (Methacrylic Acid in Gelatin Initiated by Copper) based on the cross-linking of the gel and using X-ray computed tomography (CT-scan) in order to apply it to dosimetry during the 3D simulation of a radiotherapy treatment. The determination of the calibration curve describing the performance of the new gel called MAGIC-Glutaraldehyde as a dosimeter capable of translating the 3D distribution of the radiation dose was determined using irradiations ranging from 2 to 12 Gy on the new gel. A linear relationship of this gel was established and compared with the calibration curve of the MAGIC dosimeter. It was found that the best linearity corresponds to the MAGIC-glutaraldehyde gel. From this result, a structural study was undertaken in order to provide more information on the structure of this new gel.

Keywords: MAGIC-Glutaraldehyde, R-X, Scanner.

POSTER PRESENTATION

Id-2604

Influence of SAC0307-Al_2O_3 Composite Solder Joints on Thermal Parameters of Power Electronics Devices

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Abstract: The effect of SAC0307-Al_2O_3 composite solder joint on the thermal properties of MOSFETs soldered onto MCPCB (metal core printed circuit board) was investigated. Metal core glass-epoxy substrates (MCPCB) with a thickness of 1.50 mm, covered with a 35 µm thick Cu layer, were used. A surface finish was prepared from a hot air leveling (HAL) Sn99Cu0.7Ag0.3 layer with a thickness of 1 ÷ 40 µm. MOSFET transistors were soldered in a batch oven with composite solder pastes. Al_2O_3 nanoparticles and nanofibers were used as the reinforcements of the joints. The concentration of the reinforcement varied from 0.125 to 1 wt%. SAC0307 (Sn99Ag0.3Cu0.7) was used as a reference sample. The thermal impedance Zth(t) and thermal resistance Rth of MOSFETs were measured. Furthermore, the wettability of the solder paste, void formation and the microstructure of solder joints were also studied. The results showed that Al2O3 composite solder joints influence the thermal parameters of mounted transistors. Al2O3 addition changes the microstructure of the solder joint, which can influence the thermal parameters of the solder connection and finally decides of MOSFETs thermal management.

Keywords: Composite Solder, Al_2O_3, Nano-Particles, Reinforcement, Microstructure, Thermal Behavior.

Acknowledgment: This work was partially supported by the National Science Center (NCN, Poland) project no. 2022/47/B/ST5/00997.

POSTER PRESENTATION

Id-2607

Evaluation of Hardness and Composition of SiCN Films Deposited by HWCVD Method

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Abstract: SiCN film has excellent properties such as high hardness, high wear resistance and high adhesion to substrates, so it is expected to be applied in various fields. In the semiconductor industry, it is used as a protection film for chips before packaging, therefore, the coating films requires a low-temperature process below 400°C. However, SiCN studies in our laboratory have mainly been carried out using high-temperature processes between 400℃ and 800℃, and there is not sufficient knowledge of the hardness of SiCN films deposited at low temperatures. The purpose of this study is to investigate the relationship between the composition and hardness of SiCN films deposited at low temperatures. The SiCN film was deposited using the HWCVD method. This is a method in which material gases are decomposed on a heated catalyst and radicals are generated. 2 sccm of HMDS ($HN[Si(CH_3)_3]_2$) diluted with 100 sccm of H_2 or NH_3 were used as material gases. The heated tungsten catalyst with a diameter of 0.3 mm was used and the catalyst temperature was heated up to 1700 °C, and the stage temperature (Ts) was varied from 150 to 350°C and SiCN films were deposited on Si(100). After that the composition of the SiCN films were evaluated using X-ray photoelectron spectroscopy (XPS), the hardness of SiCN films were evaluated using a nanoindentation measurements. The film thickness was measured by an ellipsometer. The relationship between the Si-O, Si-C, and Si-O bond ratios on the SiCN film surface with respect to the holder temperature for H_2 dilution and NH_3 dilution was investigated. The bonding ratio was calculated from the XPS Si2p spectra. It was found that in the case of H_2 dilution, as Ts, increases, Si-C bonds increase and Si-N and Si-O bonds decrease. It was also found that that in the case of NH_3 dilution, the bond ratio remains almost constant even as Ts increases. We also investigated the relationship between the hardness and Ts of the SiCN film formed using H_2/HMDS and NH_3/HMDS. It was found that in the case of H_2 dilution, the hardness increases as Ts increases and highest hardness as high as 23 GPa was obtained at Ts of 350°C. On the other hand, in the case of NH_3 dilution, the hardness is almost constant even if Ts changes, and it was found that the hardness is about 10 GPa, which is the same as that of the Si substrate. We investigated the relationship between the hardness and composition of SiCN films by varying the diluent gas and stage temperature (Ts) during the formation of SiCN films by HWCVD. It was revealed that the hardness of the SiCN film depends on the stage temperature and the bond ratios of Si-C, Si-N, and Si-O, and can be controlled. In order to obtain high hardness, it is necessary to have a higher ratio of Si-C bonds than Si-N bonds or Si-O bonds, and it should be Ts of 250°C or higher is appropriate.

Keywords: HWCVD, SiCN, Hardness, Thin Film, XPS.

POSTER PRESENTATION

Id-2608

Evaluation of Tritium Release from Contaminated HEPA Filters in Extreme Conditions

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Abstract: In this paper, the hazard of the radionuclide release into the environment from the filtration systems of a tritium laboratory during a fire event was analyzed. A dedicated experimental rig was designed, manufactured, and commissioned aiming to measure the tritium release during a simulated fire event. The new facility is constituted from: (a) Gas mixture generator, (b) Controlled heater of gaseous effluents, (c) HEPA filter attachment module, (d) Labile tritium collector with ethylene glycol, (e) Stable tritium labeled molecules oxidizer with Heat exchangers coupled at a Ciller, (f) Stable tritium labeled molecules collector, (g) Membrane pump, (h) Electronic thermometers and flow meters positioned on the route of gaseous effluents. Different dust types (plaster, brick, concrete, charcoal, and zeolites) were contaminated in a controlled manner with stable tritium (organically bound tritium - OBT) and labile tritium (HTO) compounds. The HEPA filters were loaded with mixed dusts with predetermined activity and composition. Using the test facility, the amounts of tritium released from the controlled contaminated filters were determined depending on the temperature and flow rate of gaseous effluents. The tritium release in gaseous effluents were measured by ethylene glycol sampling from each section of the tritium collectors. The measurement of the labile (HTO, alcohol, acids, etc.) and stable (T_2, HT, CH_xT_{4-x}, etc.) tritium chemical forms were realized using liquid scintillator counting method (LSC). Finally, the residual tritium from the filter material was measured by total combustion technique. By analyzing the activities and the tritium species released in the gaseous effluents, correlated with the activities controlled uploaded on the HEPA filters, the potential environmental impact of a fire accidentally generated in a tritium laboratory was evaluated.

Keywords: Tritium, Tritium Release, Contaminate Dusts, HEPA Filter, Total Combustion.

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POSTER PRESENTATION

Id-2619

Novel 9,9’-Dispiro- and Trispirobifluorene Building Blocks for the Access to Smart Supramolecular and Covalent Organic Frameworks

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Abstract. Porous organic materials became in the last two decades attracting targets due to their accessibility and outstanding properties [1,2]. Supramolecular Organic Frameworks (SOFs) are obtained under dynamic conditions and they are built via secondary bonds (hydrogen, halogen bonds, π-donor-π-acceptor complexes or hydrophobic contacts) between molecules, [1] while Covalent Organic Frameworks (COFs) are obtained using the multitude of methods developed in organic synthesis, either in dynamic conditions (e.g. imine formation) or by procedures which lead to robust structures (e.g. Suzuki-Miyaura, Sonogashira cross-couplings reactions) [2,3]. In this work we report the synthesis, structure and applications of SOFs and COFs obtained starting from unexplored tetragonal building blocks exhibiting dispiro- {dispiro[fluorene-9,1'-cyclohexane-4',9''-fluorene]; DSBF} or trispirobifluorene {trispiro[fluorene-9,1'-cyclobutane-3',1''-cyclobutane-3'',9'''-fluorene], TSBF} units. SOFs were formed by N---I halogen bonds in cocrystals of tetrapyridyl derivatives of DSBF and TSBF as halogen acceptors and the isomers (*ortho, meta* and *para*) of diiodotetrafluorobenzene (DITFB) as halogen donors and they were obtained by a mechanochemical solvent-drop grinding method (SCD) developed in our group for the access to halogen bond based SOFs. [4] The spectacular arrangements of the molecules in the supramolecular frameworks were revealed by single crystal and powder X-ray diffraction methods. The Sonogashira cross-coupling reactions of tetrabromo derivatives of DSBF and TSBF with 1,6-diethynylpyrene lead to the one-step formation of Pd@DSBF and Pd@TSBF hybrid materials (by the incorporation as nanoparticles of the reduced Pd species of the catalysts used in the Sonogashira synthesis of COFs) and these materials were successfully used as heterogeneous catalysts to carry out classic Suzuki-Miyaura cross-coupling reactions [*p*-methylbenzene boronic acid with several brominated benzene derivatives].

Keywords: SOFs; COFs, 9,9’-dispiro- and trispiro-bifluorene, N---I halogen bonds, Pd@PAF hybrid catalysts

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POSTER PRESENTATION

Id-2623

Electronic Lock with Remote Control

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Abstract: There are electronic cabinet locks for cabinets used in public areas.These locks can be opened with a card or touch keypad. In addition, they can be opened mechanically if desired. However, they must have a sealing feature for outdoor use. In addition, when the lock password is forgotten, the password must be opened again using the master key. However, the master key is often lost by customers. In order to solve this problem, the electronic lock has been developed to reset the password via Bluetooth and mobile application. IP66 sealing is also provided mechanically. In this way, it will have a high chance of competing with competing products.

Keywords: Electronic Lock, Bluetooth, Mobile App.

POSTER PRESENTATION

Id-2625

Two-dimensional Valleytronic Materials: From Principles to Device Applications

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Abstract: In recent years, with the successful experimental preparation of two-dimensional (2D) materials, such as monolayer graphene, group-VI transition-metal dichalcogenides (MoS_2, $MoSe_2$, WS_2 and WSe_2), and so on, the valley degree of freedom (local maximum/minimum on the valence/conduction band) has attracted wide attention from researchers. Valleytronics based on 2D materials [1] is a brand-new field which considered as the heart of next-generation semiconductor technology. It proposes to use the valley degree of freedom as an information carrier. Compared with traditional electronics, valleytronics has the advantages of low power consumption, lossless information and faster processing speed. The top priorities of valleytronics are the generation and detection of valley-polarized currents, as well as the design and fabrication of optical devices, which achieve circularly polarized light absorption and electroluminescence. In this poster [2], we aim to give an overview of the recent developments achieved in valleytronics based on various 2D materials. Sec. 1 starts from the backgrounds of 2D materials and introduces valley-polarized Landau levels in graphene and early theoretical proposal of valleytronic application. Sec. 2 discusses an example of perfect valley polarized current—valley Hall effect, which does not accompany electric current thus free from Joule heating. We will also review some of the experimental setups, which detect non-local signals to experimentally interpret valley Hall effect and inverse valley Hall effect. Sec. 3–5 explore various methods for creating and manipulating valley polarized current, such as trigonal warping effect, spin-orbit coupling, strain, external fields, line defects, etc. We mainly concentrate on the application of strain and line defects due to massive publications on these points. We also introduce a new member of ferroic family—Ferrovalley materials, which exist intrinsic valley polarization. Sec. 6–7 mainly discuss the theoretical background and recent experimental developments of the valley-dependent optoelectronic devices based on monolayer 2D materials and their van der Waals heterostructures. Valley dephasing/relaxation mechanism and its effect on optoelectronic devices are also included. Valley LEDs, valleytronic transistor, exciton Hall effect and valley Zeeman effect are the highlights in these sections. Finally, the last section draws a summary and presents some current dilemmas which are still discussing in the scientific world. Some further challenges are also proposed in this section.

Keywords: Two-Dimensional Materials, Graphene, Transitional-Metal Dichalcogenides, Valleytronics; Optoelectronics.

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POSTER PRESENTATION

Id-2626

Enhancing Microbial Resistance of Additive Manufactured Titanium Implants by Magnetron Sputtering of Nb-Cu and Ta-Cu Coatings

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Abstract: Currently, the challenges of additive manufacturing of individual medical implants-endoprostheses (orthopedic, dental) with increased resistance to bacterial and fungal infections are the focus of attention of scientists, surgeons and medical production specialists. Such implants could significantly reduce the risks of implant failure and the development of periprosthetic infections, as well as the patient’s recovery time after surgery. The combination of advanced selective laser melting (SLM) technology to fabricate patient-specific implants with controlled porosity and magnetron sputtering (MS) technology to deposit antimicrobial coatings on implant surfaces may provide a unique opportunity to produce customized implants with desired mechanical, bioactive and antimicrobial properties.The objective of this work was to analyze how the thickness of magnetron sputtered Ta-Cu and Nb-Cu coatings on porous scaffolds made of Ti6Al4V alloy by SLM and on substrates of solid gas-abrasive-treated Ti6Al4V alloy affect the specimens' antifungal and antibacterial effectiveness against Candida albicans and Staphylococcus aureus strains. This comparison with the substrates' ability to inhibit these strains is essential to provide targeted recommendations for selecting materials and MS parameters of bacterial and fungal-resistant coatings on medical endoprosthesis implants made of Ti6Al4V alloy. As a result of the work, the antimicrobial effectiveness of MS Nb-Cu and Ta-Cu coatings on SLM porous scaffolds and gas-abrasive treated Ti6Al4V alloy against Staphylococcus aureus and Candida albicans strains was evaluated. Scanning electron microscopy with energy-dispersive X-ray analysis confirmed the production of coatings of a given composition of 25 wt. % Cu and thicknesses of 2 μm and 10 μm on scaffolds with a porosity of 72% and on solid Ti6Al4V alloy substrates with an average surface roughness of 4.6 ± 1 μm. Thicker coatings showed superior antimicrobial activity; however, thin Nb-Cu coatings and uncoated alloy did not exhibit any inhibitory effect. The dynamics of the release of Cu ions from Ta-Cu coatings into physiological solution, analyzed over ten days using inductively coupled plasma mass spectrometry, corresponded to the growth of the inhibition zone. The results support the potential of these coatings in the development of additively manufactured endoprosthetic implants with enhanced antimicrobial properties.

Keywords: Antibacterial Coatings, Antifungal Coatings, Additive Manufacturing, Selective Laser Melting.

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POSTER PRESENTATION

Id-2627

Manufacturing of Biocompatible Coatings for Medical Implants Using Robotic Microplasma Spraying: Ensuring Coating Uniform Thickness and Specified Porosity

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Abstract: Currently there is global interest in the production of patient-specific implants with improved surface bioactivity. One of the ways to increase the bioactivity of an implant is to coat it with a biocompatible material, such as hydroxyapatite (HA), tantalum (Ta), titanium (Ti), etc. The use of thermal plasma spraying for these purposes is new and very promising, but it is associated with a number of challenges, including the formation of a coating of a given thickness and controlled porosity on the implant of complex shape. A new approach was applied in this work, namely the use of an industrial robot-manipulator to move a plasma source with automatic code generation to ensure the movement of the robot's end effectors along the planned trajectory. With regard to the thermal plasma spraying process, the main task performed by the robot arm is to move the plasma source with constant linear speed in order to expose the substrate surface to the plasma flow with the coating particles in a stable, consistent and repeatable manner. This means that during plasma spraying, the robot always maintains the same spraying angle (preferably 90°), spraying distance (a distance from the plasma source nozzle to the surface) and fixed distance (a step) that the source is displaced to bring the next section of the surface into the plasma flow. The objective of the work was to select the above parameters: speed, spraying distance and step for a certain material (Ha and Ti) and test a new control algorithm for a robot performing microplasma spraying of Ha powder and Ti wire on a titanium alloy implant. The parameters of microplasma spraying were selected based on the planning matrix of a fractional factorial experiment, the thickness and porosity of the coatings were studied using light and scanning electron microscopy, and the results were processed by using regression analysis. The results confirmed that the use of a new robotic manipulator control algorithm, which ensures precise maintenance of the recommended microplasma spraying parameters, makes it possible to accurately apply three-layer Ti/Ti/ Ha coatings to joint endoprostheses. The coating layers were evenly distributed over the surface of the implant and had different specified average thickness and porosity: 80 μm thick dense lower Ti layer with a porosity of 5%, ensuring reliable adhesion, no worse than 30 MPa; 100 μm thick middle Ti layer with 25% porosity and 100 μm thick top HA layer with 20% porosity. A patent of the Republic of Kazakhstan No 8714 for a utility model titled “Method of spraying multilayer coatings on implants made of titanium alloys” was received. The results of this interdisciplinary research are very promising for the development of robotic technologies for coating medical implants.

Keywords: Multilayer Coatings, Endoprostheses, Robot-Manipulator, Control Algorithm, Trajectory.

Acknowledgement: This research is funded by the Ministry of Science and Higher Education of the Republic of Kazakhstan (Grant No. AP19679327).

POSTER PRESENTATION

Id-2630

Mesoporous SiO_2-TiO_2 Submicron Particles with High Photocatalytic Efficiency for Degradation of Organic Substances under Solar and Artificial Light

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Abstract: Dyes present in industrial wastewater pose significant environmental concerns due to their persistence and potential toxicity. To address this issue, fibrous mesoporous silica particles coated with a titanium dioxide layer ($mSiO_2@TiO_2$) were employed in this study to facilitate the solar-light assisted degradation of Rhodamine B, a model pollutant dye. This composite material exhibited a high surface area of 698.8 m^2/g, as determined by Brunauer–Emmett–Teller (BET) method. The $mSiO_2@TiO_2$ particles demonstrated effective photocatalytic activity when assisted by hydrogen peroxide (H_2O_2), 97.5% of a 5 mL solution containing $3*10^{-5}$ M rhodamine B dye was degraded using only 2 mg of the photocatalyst. The influence of interfering anions, pH, and catalyst load on the degradation process was also investigated, providing insights into the optimization of the photocatalytic system. Importantly, it was observed that the $mSiO_2@TiO_2$ particles could be reused multiple times without experiencing significant efficiency loss. These composites present a promising and potential solution for mitigating dye pollution in industrial wastewater, thereby offering notable applications in the realm of environmental remediation.

Keywords: Photocatalysis, Dye Degradation, Mesoporous Silica, Titanium (IV) Oxide, Rhodamine B.

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POSTER PRESENTATION

Id-2633

Functional Borates and Fluoride Borates and Their High-Pressure Modifications

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Abstract: Due to the α–β phase transition at a temperature of 925 °C, the main method for growing nonlinear optical crystals of low-temperature modification of barium borate $\beta\text{-BaB}_2\text{O}_4$ (BBO) is crystallization from high-temperature solutions. The key point determining the actual structure and optical quality of crystals is the choice of a proper solvent. The possibility of using various solvents of the Na, Ba, B // O, F quaternary reciprocal system for growing BBO crystals has been examined [1]. Using a multi-punch hydraulic press "Discoverer-1500" of DIE type at a pressure of 3 GPa and a temperature of 900 °C, single crystals of a new polymorphic modification $\gamma\text{-BaB}_2\text{O}_4$ were synthesized [2]. A unique feature of $\gamma\text{-BaB}_2\text{O}_4$ ($P2_1/n$) (CCDC No. 2106970) structure is the presence of infinite double chains of edge-sharing $[\text{B}_2\text{O}_6]$ tetrahedra. Crystals of the fourth modification $\delta\text{-BaB}_2\text{O}_4$ with the assumed symmetry of $Pa\bar{3}$, have so far been obtained only as a product of the decomposition of barium-sodium metaborate $\text{Ba}_2\text{Na}_3(\text{B}_3\text{O}_6)_2\text{F}$ at a pressure of 6 GPa and a temperature of 900 °C (two other products of decomposition are NaF and NaBO_2) [3]. Regularities of electronic structure and band gap changing for four polymorphic modifications of BaB_2O_4 were studied. In the Na, Ba, B // O, F system new type of fluoride borates with the so-called 'antizeolite' structure has been discovered [4]. They are built of a positively charged $[\text{Ba}_{12}(\text{BO}_3)_6]^{6+}$ framework with channels along the *c* axis with a diameter of 5.68÷5.85 Å, formed by altering barium cubes and anticubes. Both cube and anticube cages are filled with various anionic groups, in case of $\text{NaBa}_{12}(\text{BO}_3)_7\text{F}_4$, with $[\text{NaF}_4]^{3-}$ and $[\text{BO}_3]^{3-}$ ones, respectively. Extensive effort has been, and is, directed to understanding the relationship between the composition, structure, and functional properties of borates with 'antizeolite' structure [5]. First experiments revealing their behavior at high pressure were carried out.

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POSTER PRESENTATION

Id-2638

Manufacturing and Research of Ta and Ta-Cu Bioactive and Antimicrobial Coatings of Titanium Endoprosthesis Implants

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Abstract: The latest trend in manufacturing endoprostheses, which fuse with the patient's bone, is to develop implant surfaces with both bioactive and bactericidal properties. This dual functionality is crucial for preventing periprosthetic infections and expediting patient recovery. Achieving this is a complex challenge. Bioactive coatings need to be non-toxic to human osteoblast cells, promoting their accelerated proliferation and ensuring osteoinductivity, osteoconductivity, and ultimately osseointegration of the implant. Conversely, antimicrobial activity requires the coating to kill microorganisms without harming human cells, and it must also prevent the proliferation of bacteria and fungi. Thus, a balanced compromise in the material, composition, and structure of the coating is necessary to meet these opposing requirements. Multilayer Ta and Ta-Cu coatings show promise as candidates for such coatings. Ta boasts excellent biocompatibility and corrosion resistant properties, while Cu is known for its bactericidal effects. A significant consideration is the coating production method, given Ta's refractory nature. Additionally, factors as the elemental composition of Ta-Cu and the porosity and roughness of the coating surface are critical. This study aimed to use microplasma spraying (MPS) of Ta coating and magnetron sputtering (MS) of Ta-Cu coating with varying Cu content (wt.%) on medical titanium alloy substrates. The goal was to examine the microstructure and properties of these coatings to recommend specific compositions and deposition parameters. The research hypothesis posited that a two-layer Ta/Ta-Cu coating with a thin Ta-Cu top layer could provide antibacterial properties through Cu ion release. The cytotoxicity of the coating could be controlled by adjusting the thickness of the top layer and the Cu content. The main results and achievements of this work are as follows: using the proposed methods and selected deposition parameters, coatings of refractory Ta with the specified characteristics were successfully obtained. The MPS Ta coating exhibited a porosity of up to 20 ± 2%, pore sizes ranging from 20 μm to 200 μm, mean surface roughness of 16.4 ± 0.5 μm, and tensile adhesive strengths of 28.0 ± 4.9 MPa. The MS Ta-Cu coatings had Cu content at 25, 10, and 5 wt. %. In vitro studies showed that Ta coatings positively affected the proliferation and osteogenic differentiation of mesenchymal stem cells. Specifically, Ta coatings significantly increased the expression of osteoblast-specific alkaline phosphatase by 10% and enhanced calcium deposit development by 11% during advanced osteogenesis stages compared to uncoated Ti6Al4V alloy. Additionally, in vitro tests revealed that Ta-Cu coatings with 25 wt.% Cu exhibited excellent inhibitory properties against Staphylococcus aureus and Candida albicans strains. Thus, this study demonstrates the potential of the combined approach for producing antimicrobial and bioactive coatings for medical implants. However, further experiments are needed to make definitive recommendations.

Keywords: Osseointegration, Bacterial Resistance, In Vitro Test, Microplasma Spraying, Magnetron Sputtering.

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POSTER PRESENTATION

Id-2639

Additive Robotic Microplasma Spraying of Multilayer Bioactive Coatings

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Abstract: The expanding possibilities for using biomaterials are driven by the development of new materials and advanced technologies that enhance material potential. Zirconium (Zr) is a popular material for coating dental and orthopedic endoprosthesis implants due to its excellent biocompatibility and corrosion resistance. Plasma technologies, particularly thermal plasma spraying, hold promise for coating implants. However, the potential of thermal plasma spraying is limited by challenges in understanding how spraying parameters affect coating microstructure and properties. This work integrates advancements in determining optimal thermal plasma spraying parameters for multilayer Zr coatings on titanium implants with the development of innovative additive technology for robotic microplasma spraying (MPS). The primary goal was to create new control algorithms for a robot manipulator equipped with a microplasmatron. This setup aims to produce functional multi-layer coatings by precisely depositing materials layer by layer based on a digital 3D model of the part. The robotic arm also reconstructs the 3D model of the product through 3D scanning. In conjunction with developing new robot control algorithms, the research aimed to ensure high-quality coating of complex-shaped products while maintaining high productivity and functionality of the additive manufacturing components (i.e., microplasmatron, robotic manipulator, and 3D scanning system). Key research objectives included selecting materials, composition, porosity, and layer thickness for multilayer functional coatings. The primary criterion for evaluating the success of these choices and the overall technology was the bioactive properties of the coatings, studied in vitro using rat mesenchymal stem cells (MSCs). The main achievements *of this work* are as follows: using the new technology, a two-layer Zr coating was successfully applied to an elbow joint implant. The dense bottom layer had a porosity of less than 4%, while the porous top layer had a porosity of up to 25% with pore sizes up to 200 μm. The bottom layer provided excellent adhesion, and the coatings had a uniform and controllable thickness: 150 μm for the bottom layer and 250 μm for the top layer. The Zr coatings increased MSC proliferation by statistically significant 8% compared to the titanium alloy substrate and demonstrated superior corrosion resistance in saline compared to the uncoated titanium alloy. Regression analysis established a pattern of influence of MPS parameters on Zr coating porosity. This study demonstrates the advantages of using additive robotic technology for spraying bioactive coatings onto implants with complex shapes. The results are significant for implant manufacturers and researchers in the field of coatings, highlighting the potential for enhanced performance and durability of medical implants.

Keywords: Biocompatibility, Medical Implants, Robotic Arm, Control Algorithm, 3D Scanning.

Acknowledgement: This research is funded by the Ministry of Science and Higher Education of the Republic of Kazakhstan (Grant No. AP13068317).

POSTER PRESENTATION

Id-2641

Recycling of Waste Aluminium Foil as a Low-Carbon Feedstock Substitute

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Abstract: It takes four tonnes of bauxite to produce one tonne of pure aluminium. Processing these four tonnes of bauxite produces up to three tonnes of waste, some of it toxic. Production is energy and water intensive. In terms of recycling, aluminium is a very suitable material. To produce new aluminium, the sorted metal practically only needs to be re-melted. Recycling one tonne of aluminium material saves 95% of the energy needed to produce primary aluminium and nine tonnes of carbon dioxide emissions, in addition to four tonnes of bauxite. For aluminium, however, recycling of aluminium thin foils is highly problematic due to the frequent content of other impurities, but the produced amount of these materials is significant and it is necessary to design a recycling procedure for them. This research therefore focuses on the recycling of used aluminium foil. These foils often contain admixtures of other materials, mainly paints with which the aluminium has been printed, protective plastic foils and also paper foils. However, these impurities must be removed before the actual melting of the recycled aluminium. This is an important step in the recycling industry that cannot be skipped. For this reason, possibilities for removing the various impurities are being explored in cooperation with industry. As part of the research into the removal of these impurities, two methods of removal were proposed and tested based on their properties. These are thermal decomposition and wet removal using partitioning mixtures. The thermal decomposition will test the pyrolysis method and determine the removal efficiency for aluminium foils with paper and paint admixtures, where mechanical methods for the removal of the solid residue will be further investigated. The removal efficiency will be assessed based on the result of characterisation before and after thermal decomposition. This will include the determination of TGA, water content, ash content, volatile combustibles a chemical composition of organic substances. The second option for removing unwanted impurities will be tested by the wet separation method using partitioning mixtures. In this case, it is planned to use a mixture of solvents, acids and other solutions to maximize the removal of impurities. Aluminium foils containing paint and plastic films will be recycled by this method. The parameters monitored in the testing will be the composition of the separation mixture, temperature and time required for separation. The removal efficiency will be assessed based on the result of characterisation before and after removal method.

Keywords: Recycling, Waste, Aluminium, Foil.

POSTER PRESENTATION

Id-2643

Plastic Deformation of Bronze under water by Laser Radiation

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Abstract: The use of a powerful laser pulse with a duration of 10 ns creates a specific impact effect of a hydraulic pulse on the surface of a solid material, which significantly modifies the properties of the material. In this study, we used Nd:YAG Q-switched laser (wavelength λ = 1064 nm, the pulse energy was up to 0,6 J, the pulse duration was 10 ns).The radiation was focused on the surface of a bronze target, which was placed in a cuvette with water. The bronze sample was 8 mm thickness. The energy density of laser radiation was up to 32 J/cm², with a single pulse. Laser exposure was carried out on the surface of the target with and without an absorbing coating. The laser radiation exposure was accompanied by the formation of a plasma torch and significant damage to the surface. The samples were studied using New View 7300 optical profilometer. The surface profiles in the zone of laser radiation exposure were obtained and studied. With an absorbent coating, a noticeable depression up to 5 μm deep appeared in the area of the laser spot. Without an absorbent coating, the cavity depth is smaller and there are also a large number of micropores. This surface modification method can be used to create compressive stresses and increase the surface hardness of bronze alloys.

Keywords: Laser, Bronze, Plastic Deformation, Nanosecond Pulse, NIR Radiation.

POSTER PRESENTATION

Id-2647

In Vitro Testing of Microplasma Sprayed Titanium and Hydroxyapatite Coatings on Ti6Al4V Alloy Substrates: The Effect of Materials and Spraying Parameters on Coating Bioactivity and Corrosion Resistance

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Abstract: Currently, scientists and manufacturers of medical endoprosthetic implants are increasingly focusing on imparting bioactive properties to implant surfaces. The primary goal is to expedite patient recovery by accelerating the fusion of the implant to the patient's bone, thereby minimizing risks associated with implant failure and allergic reactions. Despite significant progress, there remains no consensus on the optimal materials, composition, and porosity of implant coatings that can reliably protect metal endoprostheses from corrosion while enhancing surface biocompatibility. Thus, new experiments are essential, with *in vitro* tests serving as the initial stage for assessing bioactivity. The goal of this work is to establish the influence of microplasma spraying (MPS) parameters on the porosity of coatings made from biocompatible materials and recommend an optimal coating composition that ensures both bioactivity and corrosion resistance of the implant. The study focused on Ti6Al4V alloy specimens, a widely used titanium alloy for endoprosthetic implants. Microplasma spraying was performed using hydroxyapatite (HA) powder and commercially pure titanium (CP-Ti) wires onto titanium alloy substrates that had undergone gas abrasive treatment. The MPS-004 microplasma unit, produced by E.O. Paton Electric Welding Institute (Kyiv, Ukraine), was employed for this purpose. The response of rat mesenchymal stem cells (MSCs), crucial for bone healing, to these coatings was studied. By selecting and adjusting MPS parameters, coatings with varied porosities and surface roughness were achieved. Key MPS parameters adjusted included electric current, plasma gas (Argon) flow rate, spraying distance, and wire or powder feed rate. Corrosion tests were conducted by obtaining Tafel curves in simulated saline. The results demonstrated that HA coatings significantly increased MSC proliferation by 13% compared to the titanium alloy substrate, while CP-Ti coatings showed an 11% increase. It was observed that porosity inversely affected the elasticity of CP-Ti coatings, with less porous coatings exhibiting better corrosion resistance. HA coatings were found to promote osteogenic activity and angiogenesis, both critical for implant integration. Regression analysis helped establish the pattern of influence of spraying parameters on coating porosity. A new three-layer coating approach is proposed to optimize implant biocompatibility and durability. This approach combines a dense titanium base layer, a porous titanium intermediate layer, and an HA top layer. This layered structure aims to balance the need for mechanical strength, bioactivity, and corrosion resistance, offering a promising solution for enhancing the performance and longevity of medical implants.

Keywords: Endoprosthesis Implants, Biocompatible Coating, Porosity, Elasticity.

Acknowledgment: This research is funded by the Ministry of Science and Higher Education of the Republic of Kazakhstan (Grant No. AP14869862).

POSTER PRESENTATION

Id-2652

Doping Effect on Ferroelectric/Piezoelectric Properties of Nb-Modified $BiFeO_3$-$BaTiO_3$ Ceramics

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Abstract: Lead-free bulk $BiFeO_3$-$BaTiO_3$ system with small amount of donor dopant, $0.65BiFeO_3$-$0.35BaTi_xNb_{(1-x)}O_3$ (BF35BTNb, where $x = 0.00 - 0.03$), has been investigated as a potential piezoelectric material due to its large electromechanical performance and high Curie/maximum temperature (T_C/T_m), as these are the primary desirable parameters for application in actuators. Large strain property (S = 0.2535% and d^*_{33} = 724 pm/V at a field of 3.5 kV/mm, d_{33} ~201pC/N at RT and S = 0.3416% and d^*_{33} = 991 pm/V at applied field of 3.5 kV/mm at 90 ^oC), d_{33} ~ 230pC/N at 90 ^oC and typical ferroelectric behaviors were obtained for $x = 0.01$ with maximum temperature (T_m) ~ 431 ^oC. It is believed that the excellent piezoelectric response could be attributed to enhance relative density, optimum grain size, lattice distortion and enhanced domain reorientation/switching due to donor doping. The excellent piezoelectric properties along with high T_m suggested that BF-35BTNb system is a favorable applicable material at elevated temperature for enhanced piezoelectric performance.

Keywords: $BiFeO_3$, Leadfree Piezoceramic, High Tc.

POSTER PRESENTATION

Id-2667

Synthesis of Metal-Organic Framework Compounds on PET Track-Etched Membranes for CO_2 Capture

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Abstract: Metal-organic framework compounds (MOFs) are nanoporous materials that have a number of unique properties, such as a large surface area, high porosity, strong bonds between the metal and linkers, which determines their increasing scientific and technological importance. MOFs are promising materials for applications in catalysis, gas storage, targeted drug delivery, gas separation, luminescence, lithium-ion batteries, water purification, carbon dioxide capture, photo- and electrocatalysis, and their applications are still increasing. MOFs are used in the form of powders or they are immobilized on various carriers (fibers, lattices, polymers, membranes). The properties of MOFs and carrier determine their areas of application. This study is devoted to the study of methods for obtaining MOF (HKUST-1) on track-etched membranes based on poly(ethylene terephthalate) (PET TeMs). TeMs differ from all other types of membranes in that they have a record small distribution of pore sizes, there are possibilities for precise control of the number of pores per unit area and pore size, channel geometry, which makes these membranes highly selective. Immobilization of HKUST-1 was carried out through the stage of coating PET TeMs with PVC nanofibers using the electrospinning method. Also, HKUST-1 was added to the polymer solution before electrospinning in different concentrations. After this, MOX was synthesized using the hydrothermal method on the resulting hybrid membranes. Synthesis conditions (time, concentration, temperature) have been optimized. Samples were characterized by methods of FTIR, Raman spectroscopy, XRD, TGA/TDA, SEM, BET analysis. Capture of CO_2 were evaluated by TGA.

Keywords: MOFs, HKUST-1, Nanofibers, Track-Etched Membranes.

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POSTER PRESENTATION

Id-2669

Skin Dose Assessment for Patients Undergoing Medical Radiography by LiF:Cu,Mg,P, BeOSL and Halide Film Passive Dosimeter Systems

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Abstract: The x-ray techniques used for diagnosis or interventional medical procedures are varied and involve factors that lead to the increase of the patient dose, irradiations over the investigated area, irradiation of the medical staff or doses below the amount necessary to obtain the relevant radiographic image. In addition to the methods used in the direct measurement of physical quantities involved in the patient dosimetry the dose estimation by passive dosimeters is recommended by radioprotection rules from medical radiology. In the current study the time-integrating solid dosimeters are used for the dose monitoring of the patients exposed to general radiography with x-rays. The dose monitoring techniques are following: LiF:Cu,Mg,P thermoluminescence, BeOSL optical stimulate luminescence and halide film. The goals are: dose estimation at the entrance surface in the isodose and its vicinity in clearly defined irradiation conditions; assessment of the dose given by the useful radiation behind the PMMA human body equivalent phantom; development of the x-ray irradiation plan in order to monitor the doses of patients undergoing medical x-ray investigations; dose intercomparison recorded by passive dosimeters; collecting a relevant number of data in order to increase the passive detectors effectiveness in procedures for patient dose monitoring. In the irradiation procedure of the passive dosimeters the XStrahl installation was used. The passive dosimeters were exposed to the following radiation doses: 1.0 mSv; 3 mSv at 30 kV and 0.4 mSv, 7 mSv, 10 mSv and 30 mSv at 70 kV. The dose values at the entrance surface were analyzed by comparison with the true conventional dose values given by the secondary standard laboratory in dosimetry. The dose values obtained at 75 kV were generally underestimated by TLD system with the exception of the 0.4 mSv dose which is overestimated in average with +20%, approximately. The TLD system response standard deviation in the irradiated area for the same true conventional dose differs from a dosimeter to another on average by at most ±7.5%. The estimated doses with the BeOSL system are in average higher by up to +12% than the true conventional dose values in the case of the particle beam generated at 75 kV while at 30 kV are underestimated on average per dose by approximately -16% and even -24% at 1 mSv and 3 mSv, respectively. The standard deviation of the BeOSL system response in the irradiated area is ± 5.5%, in generally. The doses estimated with the photodosimetric system are overestimated at the voltage of 70 kV by up to +7.5% with the exception of the dose of 10 mSv where the overestimation is on average up to +20%. At 30 kV, the estimated doses with the photodosimetric system are very close to the true conventional dose values. The photodosimetric system response standard deviation in the isodose is ± 5.23%. A special case is the dose of 3 mSv where the TLD and BeOSL system responses are underestimated with an error of approximately -28% and -24%, respectively while the average value of

the dose measured with the photodosimetric system is 3.06 ± 5.23% mSv. Although the dependence of the response of the passive detectors on the energy of the incident radiation is obvious, from the analysis of the research data it appears that the passive dosimetric systems can be used to estimate the doses characteristic of the patients' dosimetry within the uncertainty limits declared on the system, especially in the case of high voltages. The results must be improved. The estimation of doses can be affected by multiple causes resulting either from the design of the experiment, input data considered in the experiment, performance limits of passive detectors or the XStrahl x-ray generator.

Keywords: Skin Dose, Passive Dosimetry, Medical Radiography, Radiation Protection

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POSTER PRESENTATION

Id-2677

Study on Recalescence front Dynamics in Crystal Growth Processes

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Abstract: Theoretical analysis of the anomalous crystallization kinetics of supercooled melts based on experimental data in electromagnetic levitation facilities on Earth, in reduced gravity facilities during parabolic flights and in microgravity conditions onboard ISS has been carried out. We formulate a nonlinear nonstationary mathematical model of anomalous phase transformation kinetics, taking into account directional motion of the solidification front and the process of crystal nucleation ahead of the front. This process of simultaneous directional and bulk growth of the solid phase has been described using the first- and second-order kinetic equations for the crystal-size distribution function, the equation of thermal balance in the supercooled two-phase region, heat conduction equations in the solid and liquid phases, and appropriate boundary and initial conditions. In the theory, the non-stationary crystal growth rate and the motion of two-phase transformation boundaries "solid phase - two-phase region" and "two-phase region - melt" have been taken into consideration. The solution is based on a combined application of the saddle-point technique for calculating the Laplace-type integral and the method of solution expansion into series using a small parameter. The developed theory allows determining the crystal-size distribution function in the supercooled region, the laws of motion of the phase transformation boundaries, the dynamics of supercooling removal between these boundaries, and the temperature distribution in the whole system. Within the framework of the theory, the compressing effect of the two-phase region due to heat production by growing crystals and the anomalous (U-shaped) behaviour of the "recalescence front velocity - full supercooling" dependence is described. Critical supercooling determining microstructures in crystallizing material is found and compared with experimental data.

Keywords: Recalescence Front, Moving-Boundary Problem, Solidification, Nucleation, Crystal Growth, Supercooling.

Acknowledgements: This study was financially supported by the Russian Science Foundation (project no. 23-19-00337).

POSTER PRESENTATION

Id-2679

Validation of a UV-VIS-NIR Spectrophotometric Method for Determination of Sodium Benzoate in Water

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Abstract: Sodium benzoate is a widely used food preservatives and its determination receives much interest. This article describes the development and validation of a method using a UV-VIS-NIR Spectrophotometer at 225 nm to determine the mass fraction of sodium benzoate in water for the purpose of characterization of a reference material. The study was carried out in accordance with the ICH and EURACHEM guides using a primary reference material of sodium benzoate of purity 99.98±0.22%. The studied performance characteristics were the limit of detection (LOD), limit of quantification (LOQ), selectivity, linearity, accuracy, precision, recovery and bias. The results obtained were statistically analyzed and the method showed very good linearity in the selected calibration range. The LOD and the LOQ were found 0.19 and 0.57 mg/kg respectively. This method demonstrated very good accuracy ranging from 99.54 to 100.08% and precision, 0.39% RSD, signifying its high reliability in producing precise and accurate results. The validation results also revealed that the method is fit-for-the purpose of determination of sodium benzoate in water.

Keywords: Sodium Benzoate, UV-VIS-NIR Spectrophotometer, Validation, Linearity, Precision, Accuracy.

POSTER PRESENTATION

Id-2680

Improved Stability and Endurance in ReRAM Using Novel Organic-Inorganic Tandem Structure for Synaptic Computing Applications

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Abstract: Resistive Random Access Memory (ReRAM) has emerged as a promising non-volatile memory technology, offering advantages such as high density, low power consumption, and fast switching speeds. ReRAM operates on the principle of resistance switching, where the resistance of a dielectric material can be reversibly changed between high and low resistance states. In recent years, there has been growing interest in biodegradable electronics, including memory devices, to address environmental concerns and enable biocompatible applications. Biodegradable ReRAM combines the advantages of ReRAM technology with eco-friendly materials, potentially opening new avenues in sustainable electronics and biomedical applications. We present a novel approach to fabricating ReRAM devices using an organic-inorganic tandem structure, aiming to enhance device stability while incorporating biodegradable materials. We developed ReRAM devices with a bottom layer of inorganic metal oxides (TiO2, ZnO, and SiO2), topped with a layer of biodegradable chitosan polymer, and completed with a silver contact to form ITO/MO/Chitosan/Ag ReRAM device. The devices were fabricated using spin coating methods. Metal oxide nanoparticles were first spin-coated onto FTO substrates for 8 coating cycles, with drying on a hot plate after each cycle. Subsequently, chitosan was spin-coated and allowed to dry at room temperature. Chitosan, a naturally derived polysaccharide, was chosen for its biodegradability, biocompatibility, and potential to improve device characteristics. Comparative analyses were conducted between these tandem structures and traditional single metal oxide ReRAM devices. The results revealed that the chitosan/metal oxide tandem structure exhibited more stable switching behaviour compared to single metal oxide ReRAMs. Notably, the hybrid devices demonstrated improved endurance, maintaining consistent resistance states over 10000 switching cycles. Retention studies also showed enhanced stability of resistance states over 3600 seconds in the tandem structure. The improved performance of the organic-inorganic tandem structure can be attributed to the synergistic effects of the chitosan layer and the metal oxide layer. The chitosan layer likely acts as a buffer, moderating the electric field distribution and ion migration processes that govern resistive switching. This moderation effect could contribute to more controlled and stable switching events, thereby enhancing overall device reliability. These findings suggest that the organic-inorganic tandem structure has the potential to significantly enhance the stability and performance of current ReRAM technology. By incorporating a biodegradable component, this approach also takes a step

toward more environmentally friendly memory devices. Future work will focus on optimizing the thickness ratio of organic and inorganic layers, exploring other biodegradable polymers, and investigating the long-term environmental impact of these hybrid devices. This research contributes to the ongoing efforts to create high-performance biodegradable ReRAM for synaptic computing.

Keywords: Biodegradable, ReRAM, Synaptic Computing, Tandem Devices.

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POSTER PRESENTATION

Id-2681

Chitosan Based New ReRAMs for Green Computing

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Abstract: Green computing is emerging as an important component of sustainable growth strategy. Environmental friendly and biodegradable ReRAM makes it possible [1-9]. Here we propose new ReRAMs based on Chitosan blends and nano composites and discuss their switching characteristics. resistive switching memory (ReRAM). Two device classes, Class A (drop cast) and Class B (spin coat), were develop, using chitosan modified by incorporating the MEH-PPV polymer. Class A devices exhibited memory behavior upto 20 write/erase cycles atleast. No switching was observed in class B devices. MEH-PPV concentration variation in the chitosan has a significant influence on the memory and electric transport mechanisms observed in all of our devices. We also evaluated the resistive switching properties of chitosan polysaccharide doped with the green synthesized ZnO nano particles. A noticeable I-V hysteresis is observed, which suggests the presence of both a low resistance state (LRS) and a high resistance state (HRS) in the device, which is essential for a ReRAM. Ultimately, this study indicates that chitosa blends and nano composites holds promise in the development of environmentally friendly ReRAMs.

Keywords: ReRAM, Biomaterials, Chitosan.

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POSTER PRESENTATION

Id-2697

Harnessing PEGylated PLGA Nanoparticles for Drug Delivery of Cdc42 Inhibitor: Unveiling Anti-Cancer Efficacy in Colon Cancer Cell Lines

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Abstract: Cdc42, a conserved protein, plays a crucial role in cell adhesion, cytoskeletal structure formation, and cell cycle regulation. Overexpression of Cdc42 has been found in various cancer types, including breast cancer, testicular cancer, and colorectal cancer. In human CRC, high expression is observed in 60% of cases. Cdc42 inhibition can reduce colon cancer cell proliferation, migration, and invasion. CASIN, a small molecule inhibitor, has shown promising results in targeting Cdc42 in cancer cells. CASIN has several limitations in systemic administration such as side effects, rapid elimination of drugs, and low bioavailability. Targeting Cdc42 regulation by CASIN in cancer cells may be achieved through delivery using PEG-PLGA nanoparticles. CASIN-PLGA-PEG-COOH nanoparticles (CASIN–PLGA–PEG-COOH NPs) were prepared by nanoprecipitation technique and characterized for size, polydispersity index and zeta-potential, encapsulation efficiency, loading capacity and in vitro drug release study. HT-29, SW620, and HCT116 were selected for in vitro investigations. Cell lines were treated with increasing concentrations of CASIN–PLGA–PEG Np's. The cytotoxic effect of CASIN–PLGA–PEG Np's was evaluated through the CCK-8 cell viability test. In addition, cell migration assay (in vitro wound-healing assay) and Transwell invasion assay were performed. CASIN–PLGA–PEG Np's were smooth in the surface and spherical in shape, with a particle size of 86 ± 1 nm. It was determined that the encapsulation efficiency was 66±5% and the drug loading capacity was 5±1 %. The release of CASIN from PLGA-PEG-COOH nanoparticles occurred gradually and reached a maximum after 24 h. CASIN–PLGA–PEG-COOH NPs could effectively inhibit the proliferation of HT-29, SW620, and HCT116 cells. In addition, it was found that treatment of cancer cells with CASIN–PLGA–PEG-COOH Np's leads to a decrease in cell migration and suppression of their invasive potential. Indeed, PLGA-PEG serves as a shielded carrier for CASIN, providing a protective envelope that enables sustained drug release. The resultant nanoparticles demonstrate efficacy in curbing the proliferation and migration of colon cancer cells. Moreover, PEGylation enhances their ability to traverse dense layers of mucus, potentially facilitating the transport of CASIN. This dual functionality positions them as potent inhibitors of cancer advancement and promising contenders in the realm of targeted drug delivery systems tailored for combating colon cancer.

Keywords: PEG-PLGA Nanoparticles, Colorectal Cancer, Cdc42, CASIN, Targeted Therapy.

Acknowledgment: This research has been funded by the The Committee of Science of the Ministry of Science and Higher Education of the Republic of Kazakhstan, Grant No. AP14871939, and Nazarbayev University, Collaborative Research Project (CRP) Grant No.211123CRP1611.

POSTER PRESENTATION

Id-2698

A Study of in vitro Cytotoxicity of Fullerene- and Fullerenol-Dihydroquercetine Complexes: Possible Implications for the Treatment of Neurodegenerative Disorders

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Abstract: Currently, the body of evidence suggests that antioxidant and anti-inflammatory properties of various natural and synthetic chemicals, including fullerenes can play an important role in the treatment of neurodegenerative conditions. To target oxidative stress and neuroinflammation associated with the development of Alzheimer's disease (AD), we propose to use fullerenes and fullerene-like structures, which were shown to have anti-inflammatory and antioxidant properties *in vitro*. Fullerenes are the molecular formation of carbon in the form of a truncated icosahedron that has a mass of 720 a.m.u. The most symmetrical and most fully studied member of the fullerene family is fullerene (C60), in which the carbon atoms form a truncated icosahedron consisting of 20 hexagons and 12 pentagons. Polyhydroxylated fullerenes (fullerenols) are excellent free radical scavengers and there is a large number of reports on their reactions with reactive oxygen species. Besides, the positive effects of fullerenes on aging have previously been reported. However, the mechanisms of effects of these compounds on neurodegenerative processes have not been studied yet. Furthermore, a serious problem with fullerenes and fullerene-like nano complexes is water solubility which limits their practical application in the biological system. In this regard, we_have addressed a problem of poor solubility and poor stability in aqueous media of phytochemical complexes of fullerene (C60) and fullerenol (C60(OH)24 with flavonoid, dihydroquercetin (DHQ). The design and synthesis of the water-soluble phytochemical complexes of the compounds were based on the principle of nanoparticles, e.g biodegradable polymeric nanostructures, nanofiber-based sutures, gold nanorods, etc. which can act as either nano-formulation (micelles–formatting) or encapsulation agents. The supramolecular complexes [C60-DHQ] and [C60(OH)24-DHQ] structures were evaluated using neutron facilities. Based on the accomplished analysis using combined SANS-diffraction and neutron spectroscopy measurements on IN4 and IN1-Lagrange, the interaction formed between the nanocarbon and the phytochemicals is revealed, the structure, molar ratio of either C60 or C60(OH)24 with DHQ in their complex is verified and role of the structural water/hydrated shell was evaluated. Supramolecular donor (DHQ) –acceptor (C60) or C60(OH)24 complexes are formed. For the PRODUCT with a Molar Ratio of C60 to DHQ of 1 to 4, the following structure can be proposed: where Donor (DHQ) –Acceptor (C60) type of bindings and Van der Waals interactions between C60 host and DHQ guest play an important role in assuring highly stable complex. There is also evidence that the complex is surrounded by water

molecules generating the clusters of the complex with water. Furthermore, such clusters are further aggregated by aqueous clusters. We further tested the possible toxic effects of a fullerene-dihydroquercetine complex in cell culture experiments. CTX TNA2 and bEnd3 cell lines were used in this research. CTX TNA2 is an astrocyte type 1 and bEnd3 is a mouse brain endothelial cell lines. Both cell lines are widely used in neuroscience research. We have shown that [C60-DHQ] was non-toxic for both cell types in all ranges of tested concentration up to 20 µg/ml.

Keywords: Fullerene- and Fullerenol-Dihydroquercetine Complexes, Neurodegenerative Disorders.

Acknowledgement: This research was funded by the Ministry of Higher Education and Science of the Republic of Kazakhstan (AP23485236) and EU Marie-Curie Skłodowska ”PhytoApp” 0101007642 (to NA, BS, and TS).

POSTER PRESENTATION

Id-2699

Metals and Antibiotics as Aqueous Sequestration Targets for Magnetic Polyamidoamine-Grafted SBA-15

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Abstract: In this study, a magnetic generation-5 polyamidoamine (G-5 PAMAM) dendrimer-functionalized SBA-15 (mPSBA) composite was synthesized by coupling amine-functionalized silica (SBA-15-NH2) and amine-functionalized magnetic nanoparticles (MNP-NH2) with the G-5 PAMAM, before characterization and aqueous sorption of As (III), Cd (II), tetracycline, and iprofloxacin using the composite. The mPSBA characterization data exhibited the typical Si O Si infrared peaks from the SBA-15 backbone in addition to the acquired characteristic infrared Fe O and amide-I/II peaks from the MNP and G-5 PAMAM dendrimers, respectively. Post sorption infrared spectra showing shifts for the amide-linked groups indicated the likely points of contaminant attachment on the composite. Its thermal stability was lower than that of SBA-15 but higher than that of SBA-15-NH, while the XRD diffractograms of the backbone SBA-15-NH and MNP were unchanged in the final composite. The mPSBA composite was a better As (III) and Cd (II) adsorbent than SBAequilibrium achieved at 120 min.

Keywords: Magnetic Generation-5 Polyamido-Amine (G-5 PAMAM), Dendrimer-Functionalized SBA-15(mPSBA), Metals and Antibiotics.

POSTER PRESENTATION

Id-2713

Development of 3D Coffee Ring Structure on Soft Compliant PDMS Substrate and Interplaying Factors

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Abstract: Evaporation of particle laden droplets on a surface results in the formation of 2D ring like deposits on the contact line. Furthermore, evaporation of protein drops can also produce 3D dome-shaped coffee stain structures (CSS) as well. In this study, the “coffee-ring” patterns of bovine serum albumin (BSA) are investigated, which are formed by evaporation of the sessile droplets of BSA aqueous dispersion over a soft polydimethylsiloxane (PDMS) substrate. By varying the different factors such as substrate wettability, elasticity, and protein concentrations, we have found that the saddle CSSs are only formed when an intermediate-concentration (1% - 10% w/v) BSA drop evaporates over a soft (<10 MPa) and hydrophobic substrate with low stiffness (0.3 – 10 MPa). Real-time imaging of the complete formation process employing BSA drops doped with fluorescently labelled BSA proteins discloses a new formation mechanism that is based on the subtle interactions of time scales of solvent evaporation, solute dispersion, and interfacial “skin” formation. Moreover, the results confirmed that apart from 3D dome-shaped CSSs, the saddle-shaped CSS is formed by rapid “drainage” of the solvent film between the interfacial protein “skin” at the air-liquid interface. The soft substrate leads to the asymmetrical distribution of BSA proteins along the contact line and subsequently causes the interfacial protein “skin” to buckle in the direction normal to the substrate as it dehydrates. An additional discovery was the observation of the formation of a microscopically smooth thin protein film on the substrate beneath the drop. This discovery further inspires the proposed reversible hydrophilic patterning technique.

Keywords: Bovine Serum Albumin, Particle Laden Droplets, Coffee Stain Structure, Hydrophilic Patterning Technique, Fluorescently Labelled BSA Proteins.

POSTER PRESENTATION

Id-2722

Observations of the Novel Low Field Microwave Absorption in $Zn_xCo_{1-x}Fe_{2-x}Al_xO_4$ Ferrites

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Abstract: Nanocrystalline $Zn_xCo_{1-x}Fe_{2-x}Al_xO_4$ with particles size between 6 nm and 13 nm were synthesized were synthesized by glycol-thermal reaction under low reaction temperature of 200 °C. The as-prepared compounds were investigated by XRD, TEM, SEM, FTIR, Raman spectroscopy and ESR measurements. Structural, vibrational and electron spin dynamics are sensitive to particle size and Zn and Al concentrations. Broad ESR signals are attributed to dipolar-dipolar interactions and random orientations of magnetic anisotropy axes. Results show evidence of the novel low field microwave absorption, making $Zn_xCo_{1-x}Fe_{2-x}Al_xO_4$ compounds interesting for potential applications in low magnetic field sensors, magnetic field-controlled absorbers, spin valves etc.

Keywords: Low Field Microwave Absorption, Ferrites, Electron Spin.

POSTER PRESENTATION

Id-2723

Synthesis, Molecular Docking and in vitro α-Glucosidase Inhibition Potential of Novel Thiourea Derivatives Based on 3-Aminopyridin-2(1H)-Ones

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Abstract: One of the main therapeutic approaches to combatting diabetes is the slowing of postprandial hyperglycemia by reducing glucose absorption through the inhibition of enzymes that hydrolyze carbohydrates in the gastrointestinal tract. α-glucosidase is a key carbohydrate hydrolase that regulates blood glucose levels by specific hydrolysis of the 1,4-α-glycosidic bond, forming α-glucose. Inhibition of α-glucosidase activity could retard the absorption of glucose and decrease the postprandial blood glucose levels. α-glucosidase is a perspective target for treating diabetes. Currently, only three α-glucosidase inhibitors are used in clinical practice: acarbose, miglitol and voglibose. α-glucosidase inhibitors can be developed into effective therapeutic drugs for this disease. It is known that thiourea is widely used in the synthesis of heterocyclic compounds, and functional derivatives of the thiourea class exhibit a wide range of pharmacological effects, including the hypoglycemic effect. In vitro antidiabetic activity of the experimental substances was evaluated according to inhibition of α-glucosidase activity using established methods [1]. Acarbose at a concentration of 15 mM was used as the reference drug. Negative control was devoid of the experimental compounds. All samples were analyzed in triplicates. Inhibitory activity was expressed as a percentage (%) according to the degree of inhibition of α-glucosidase in comparison with the negative control. The IC50 was determined from the graph of enzyme activity changes depending on the sample concentration. The putative biological activity of the experimental substances was evaluated by molecular docking method using the AutoDock Vina program. Reactions with allyl-, acetyl-, and phenyl- isothiocyanate have been studied on the basis of 3-amino-4,6-dimethylpyridine-2(1H)-one, 3-amino-4-phenylpyridine-2-one, and 3-amino-4-(thiophene-2-yl)pyridine-2(1H)-one (benzoyl-)isothiocyanates, and the corresponding thioureide derivatives were obtained. Twelve thiourea derivatives were obtained and studied for their anti-diabetic activity against the enzyme α-glucosidase in comparison with the standard drug acarbose. According to the results of the conducted studies, it was shown that alkyl and phenyl thiourea derivatives show high and moderate antidiabetic activity, in contrast to their acetyl and benzoyl derivatives. The results of molecular docking show that the affinity of the interaction of the studied compounds with the selected protein receptors (PDB ID: 3A4A, PDB ID: 5NN8) approximately equal the affinity of the interaction of these proteins with acarbose used as a comparison. The lack of actual biological activity in the acyl derivatives of thioureas, despite the molecular docking showing very good docking results, can be explained by the poor solubility of these compounds under the conditions of the biological experiment with the enzyme α-glucosidase. Thus, the newly synthesized derivatives of thiourea based on 3-aminopyridine-2(1H)-ones are promising candidates for the further modification and study of their potential anti-diabetic activity.

Keywords: 3-Aminopyridin-2(1H)-Ones, Isothiocyanates, Thiourea Derivatives, α-Glucosidase Inhibition, Antidiabetic Activity, Molecular Docking

Acknowledgment: This research is funded by the Science Committee of the Ministry of Science and Higher Education of the Republic of Kazakhstan (Grant No. AP14871433).

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POSTER PRESENTATION

Id-2724

Synthesis of 1-(2,4,6-Trimethylpyridin-3-yl)Ethan-1-ol and Study of Its Hemorheological and Antifibrotic Activity

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Abstract: The aim of the study is to synthesize a synthetic derivative based on 3-acetyl-2,4,6-trimethylpyridine and to study its potential for hemorheological and antifibrotic activity. Hyperviscosity syndrome was reproduced *in vitro* by incubating blood at 43.0°C for 60 min [1]. Blood viscosity was measured on a Brookfield DV2T rotational viscometer at different spindle speeds (from 2 to 60 rpm). Studies of hemorheological activity were carried out on 15 female Wistar rats aged 12 weeks. After blood collection, the initial blood viscosity was determined from the laboratory animals, after which the blood samples were incubated with the test substances at a temperature of 43.0°C for 60 min, and then the viscosity was measured again. Blood was incubated with 1-(2,4,6-trimethylpyridin-3-yl)ethan-1-ol at a concentration of 10-5 g/ml blood. Pentoxifylline was used as a comparison drug [2]. Pulmonary fibrosis in rats was induced by intratracheal administration of bleomycin [3]. Animals of the experimental group received 1-(2,4,6-trimethylpyridin-3-yl)ethan-1-ol intragastrically daily at a dose of 50 mg/kg, starting 1 week after bleomycin administration for 2 weeks. Histological sections were stained with hematoxylin and eosin for general histomorphometric characteristics, Masson's trichrome to demonstrate fibrosis and identify collagen fibers, and Gomori silvering to detect reticulin fibers. 1-(2,4,6-trimethylpyridin-3-yl)ethan-1-ol was obtained by reducing the acetyl group of 3-acetyl-2,4,6-trimethylpyridine to an alcohol group in the presence of a 2-fold excess of sodium borohydride in an aqueous ethanol solution. *In vitro* biological screening under conditions of blood hyperviscosity showed pronounced hemorheological activity of 1-(2,4,6-trimethylpyridin-3-yl)ethan-1-ol, which significantly reduced blood viscosity compared to the control. *In vivo* study of the antifibrotic activity of 1-(2,4,6-trimethylpyridin-3-yl)ethan-1-ol in an experimental model of pulmonary fibrosis in rats showed a unidirectional anti-inflammatory and antifibrotic effect of 1-(2,4,6-trimethylpyridin-3-yl)ethan-1-ol, improvement of locoregional histoarchitecture of lung tissue. Under the conditions of this experiment, blood hyperviscosity is also formed in experimental pulmonary fibrosis induced by bleomycin. Since 1-(2,4,6-trimethylpyridin-3-yl)ethan-1-ol under the conditions of our experiment prevents an increase in blood viscosity both in the *in vitro* blood hyperviscosity model and *in vivo* in experimental pulmonary fibrosis induced by bleomycin, this compound can be considered promising for further preclinical studies. Thus, new derivative 1-(2,4,6-trimethylpyridin-3-yl)ethan-1-ol under experimental conditions demonstrates the potential for antifibrotic activity and hemorheological activity in blood hyperviscosity in vitro and in a model of pulmonary fibrosis.

Keywords: Synthetic Pyridine Derivative, Perviscosity Syndrome, Hemorheological Activity, Fibrosis, Antifibrotic Activity.

Acknowledgment: This research is funded by the Science Committee of the Ministry of Science and Higher Education of the Republic of Kazakhstan (Grant No. AP19677062).

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POSTER PRESENTATION

Id-2726

Measurement of L Shell X-Ray Fluorescence Relative Intensities of Elements with Atomic Numbers 62 to 75 at 13.5 keV Using Synchrotron Radiation

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Abstract: The relative intensities of L-shell X-ray fluorescence (XRF) of different elements are of interest in diverse fields. In this study, the relative intensities of L-subshell X-rays of the elements $_{62}$Sm, $_{64}$Gd, $_{68}$Er, $_{73}$Ta, $_{74}$W and $_{75}$Re were measured. Measurements were made at an excitation energy of 13.5 keV using synchrotron radiation from SESAME in Jordan. The emitted X-ray were detected by the SDD detector system. Intensity values were calculated using theoretical L-subshell cross sections and L-subshell fluorescence, and Coster-Kronig potentials recommended by Campbell. The experimental results showed reasonable agreement with the theoretically calculated values.

Keywords: L Sub Shell, X- Ray Fluorescence (XRF), Relative Intensities, Synchrotron Radiation.

POSTER PRESENTATION

Id-2727

Synthesis and Characterization of Nanoparticle Materials Based on Zinc Oxide, Silver, and Tin as Electrocatalytic towards the Azo Dyes

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Abstract: Nanocomposite materials based on Zinc oxide, Silver, and Tin (ZnO-(Sn/Ag)) are prepared using a simple hydrothermal method. The crystal structure, elements' structure, particle size distribution, absorbance spectra, and the electrical conductivity of ZnO-(Sn/Ag) nanocomposite are characterized. The electrocatalytic degradation of Acid orange 7 is investigated in the presence of nanoparticle materials. Incorporating suitable amounts of Ag ions and Sn ions into the zinc oxide nanoparticles boosts the electrocatalytic activity, in addition to boosting the optical bandgap energy and electrical conductivity. The ZnO-(Sn/Ag) nanocomposite materials are attractive in photocatalyst and electrocatalyst applications and could be used in antibacterial applications.

Keywords: Nanoparticle, Zinc Oxide, Electrocatalytic, Azo Dyes.

POSTER PRESENTATION

Id-2729

Measuring the Concentration of Heavy Metals and Radionuclide in the Soil of Jordan Petroleum Refinery and Al-Hussein Thermal Station, Zarqa City, Jordan

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Abstract: The concentrations of natural radionuclides and heavy trace metals were analyzed in topsoil samples collected from different zones in Jordan petroleum refinery and Al-Hussein thermal station, Zarqa city, Jordan. The concentrations of ^{40}K, ^{238}U, ^{226}Ra, and ^{232}Th were measured using gamma ray spectrometry, whereas the concentrations of Ba, Zn, V, Cr, Ni, Cu, Pb, Co, Cd, and As were measured using Inductively Coupled Plasma Mass-Spectrometry (ICP-MS). The concentrations of ^{40}K, ^{238}U, ^{226}Ra, and ^{232}Th were ranged from 126 ± 11.9 to 443.0 ± 18.9 Bq/kg, 70.0 ± 10.5 to 71.0 ± 14.2 Bq/kg, 33.95 ± 2.0 to 79.1 ± 2.6 Bq/kg, and 17.3 ± 2.8 to 57.4 ± 3.7 Bq/kg, respectively. Furthermore, the obtained results are below the world average and the background value of soil. The result of the concentration of heavy metal elements were in the order: Ba > Zn > V > Cr > Ni > Cu > Pb > Co > Cd > U > As. Average values of Ni (65.4ppm), Zn (99.32ppm), Cd (12.94 ppm), Cr (82.4ppm), and Co (14.42ppm) were higher than the background values in soil and the world average, while for Cu, Pb, and V their concentration rates were lower than the global average. According to our results, populations living close to the study region may be at risk of exposure to Cd, Co, Cr, Ni, and Zn through direct contact with contaminated environment. It is crucial to continuously monitor the levels of heavy and trace metals in this region to prevent any future health risks brought on by elevated levels of heavy metals. In addition, detecting heavy metals and analyzing pollution is significant in terms of managing possible dangers and limiting pollution surrounding residential area near oil refineries and thermal stations.

Keywords: Heavy Metals, Radionuclide, Jordan Petroleum Refinery, Zarqa City.

POSTER PRESENTATION

Id-2737

Evaluation of Mare's Milk-Derived Exosomes as Novel Therapeutic Carriers: Comparative Isolation Techniques and Quercetin Bioavailability Enhancement

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Abstract: Exosomes are cell-derived, membrane-surrounded particles that deliver bioactive molecules to various cells. Due to their small size, low immunogenicity, extended blood circulation, and involvement in cellular communication, they hold potential as effective drug carriers. Exosomes are present in various biological fluids, including mare's milk, a traditional drink in Central Asia. This study aims to compare exosome isolation methodologies and determine the stability of mare's milk-derived exosomes as potential therapeutic carriers. Three extraction methods – immunoprecipitation (IP), size exclusion chromatography (SEC), and total exosome isolation (TEI) [1-2] – were compared in terms of exosome characteristics, purity, and content. The isolated exosomes were then loaded with quercetin, and their ability to increase its bioavailability was tested *in vitro* and *in vivo.* A comparison of the three different methods of exosome isolation performed to evaluate the morphology, properties of the obtained exosomes and their applicability as drug carriers. The morphology assessment of the isolated exosomes performed using Transmission Electron Microscopy, shows that exosomes isolated using the different methods have morphologically dense vesicular structure. Nanoparticle tracking illustrating the size distribution of the particles shows the distribution of particles close to 100 nm. Particles isolated by SEC showed less variation in particle distribution than IP and TEI. No significant difference in the mean size of exosomes across the different isolation methods SEC, IP and TEI (110nm, 118nm and 131.5nm, respectively). Western blot using the membrane markers, MEFG-8 monoclonal, MEFG-8 polyclonal and CD63 antibodies performed to measure confirm the identity of exosomes present in each of the isolates. The protein content in IP isolate is shown to be the highest as measured by MEFE-8 and CD63 antibodies. The TEI showed a significant band against MEGD-8 monoclonal antibody, but no significant differences in other antibodies tested in comparison with SEC. However, for protein content, isolates from TEI showed the highest, followed by IP and then SEC. Total exosome isolation was identified as the most efficient method, producing high-quality exosomes. These exosomes were loaded with quercetin and compared to free quercetin and exosomes alone. Exosomes loaded with 80 μM quercetin significantly restored β-galactosidase activity and cellular viability in doxorubicin-treated cells, exhibiting similar potency to 160 μM free quercetin. In aged model animals, treatment with quercetin-loaded exosomes resulted in significantly less acute and subacute damage to the myocardium, kidneys, and liver compared to untreated control animals. In conclusion, the current study supports the concept of using exosomes as a potentially reliable form of a drug carrier. The results demonstrated that mare's milk-derived exosomes, can easily be absorbed by different tissues, and that their use as a drug carrier, presumably, increased the bioavailability of quercetin.

Keywords: Exosomes, Extracellular Vesicles, Quercetin, Ageing, ROS.

Acknowledgment: This research is funded by the Science Committee of the Ministry of Science and Higher Education of the Republic of Kazakhstan (Grant No. AP13067844).

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POSTER PRESENTATION

Id-2739

Adsorption of Heavy Metals from Aqueous Solutions by Moringa Oleifera Pods and Feldspar Clay Composite

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Abstract: Pollution removal from contaminated water is a vital step in environmental and human health protection. For impoverished countries, using biomaterials to remove heavy metals from polluted water is an environmentally benign and cost-effective strategy. In this study, *Moringa Oleifera* pod-Modified Feldspar Clay (MFC) was calcined after being modified with *Moringa Oleifera* pod. The efficiency of these adsorbents in aqueous solution adsorption of Pb^{2+}, Cu^{2+}, and Cd^{2+} ions were investigated as a function of pH, time, initial concentration, and temperature. The maximum adsorption capacities of Pb^{2+}, Cd^{2+}, and Cu^{2+} by MFC were $54.42\ mg\cdot g^{-1}$, $41.26\ mg\cdot g^{-1}$ and $35.16\ mg\cdot g^{-1}$, respectively. The Langmuir and Freundlich isotherm equations were used to analyze the equilibrium isotherm data. The adsorption process fit the second-order kinetics well in all cases, and the Langmuir isotherm equation fit the experimental data well. ΔG^0 values up to $-10\ kJ.mol^{-1}$ are coherent with electrostatic interaction between adsorption sites and the metal ion, physisorption.

Keywords: Moringa Oleifera, Feldspar Clay, Environment, Heavy Metals, Adsorption.

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POSTER PRESENTATION

Id-2742

In-Vitro Effectiveness of Photodynamic Therapy on RBCs with Encapsulated Rose Bengali by Silica Nanoparticles

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Abstract: Photodynamic therapy (PDT) is a promising treatment strategy utilizing photosensitizers (PS) and light to generate singlet oxygen, with Rose Bengal (RB) showing high singlet oxygen quantum yield. Effective delivery of RB to the target tissue remains a key challenge. Encapsulation techniques have been investigated to improve PS delivery, inhibit diaphorase-induced reduction, mitigate PS-related toxicity and minimize PS leakage, Silica nanoparticles (SiNPs) offer favorable characteristics for drug delivery in PDT and serve as promising delivery carriers. In this study, SiNPs were synthesized and employed as carriers for RB. The size and shape of SiNPs were determined using Transmission Electron Microscopy (TEM). A range of concentrations of RB were applied to RBCs in order to evaluate the cytotoxicity of both naked and encapsulated RB. This helped in optimizing the most effective concentrations and the exposure time required to induce damage under light (Intensity ~110 mW/cm^2). The results indicated that SiNPs-encapsulated RB exhibited superior efficacy compared to naked RB, with a concentration efficacy increase of +60% and an exposure time efficacy increase of +40%. This underlines the enhanced capability of encapsulated RB to eliminate the RBCs when compared to naked RB. The application of synthesized SiNPs for RB delivery improved the effectiveness of photodynamic therapy by augmenting RB bioavailability in target cells.

Keywords: Photodaynamic, Silica Nanoparticles, Rose Bengal.

POSTER PRESENTATION

Id-2743

Anti-icing Performance of Transparent Epoxy-based Nanocomposite Coatings

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Abstract: In recent years, transparent polymer coatings have become very popular due to their variety of applications. Such coatings are used, among others, on the surfaces of photovoltaic modules, glass facades of skyscrapers or aircraft elements. These coatings are exposed to external factors such as dust, dirt, snow, ice or UV radiation. Taking this into account, the coatings must meet the appropriate requirements, which, in addition to high durability, include self-cleaning and anti-icing properties. These properties can be achieved, among others, by improving the hydrophobic properties of the surface. The solution is based on the assumption that a strongly hydrophobic material can spontaneously remove accumulated contaminants together with water droplets, while at negative temperatures it maximally shortens the contact time of supercooled droplets with the surface and as a result prevents the formation of ice and reduces its adhesion. In the presented research, the hybrid epoxy-silicone resin was modified with organosilicon and mineral modifiers. These compounds provide high compatibility and reactivity with the polymer matrix and can be functionalized with low polarity functional groups, which direct the properties to hydrophobic and icephobic. The paper presents results concerning, wettability (water contact angle, contact angle hysteresis, roll-off angle), roughness, ice adhesion and freezing delay time. In addition, the influence of the modifications on the optical properties of the tested coatings was determined.

Keywords: Hydrophobicity, Anti-icing Performance, Transparent Coatings, Ice Adhesion, Surface Roughness.

Acknowledgment: The study was conducted within the project „Transparent coatings with enhanced self-cleaning and icephobic properties" financed by the National Centre for Research and Development, Grant agreement no. LIDER/15/0089/L-12/20/NCBR/2021.

POSTER PRESENTATION

Id-2750

Benzene Oxidation over Pt Loaded on Fly Ash Zeolıte X

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Abstract: The increased energy consumption implies an increased release of coal fly ash (FA) from thermal power stations in the environment. About 800 million tons FA per year are separated as a waste product from coal-fired power plants and this amount is expected to grow. Due to the chemical, mineral and textural nature of the fly ash, it is a suitable initial material for the synthesis of zeolite structures. Thus, on one side, a certain amount of FA will be utilized, and on the other hand, a low-cost starting material will be used to obtain a product with a high added value. Zeolites are well known for their unique properties, which give them many advantages in the catalytic processes - large specific surface area, high diffusion of reagents in the volume, ion exchange properties, etc [6, 7]. By melting the ash with an alkaline base, soluble aluminates and silicates are formed, which could be easily transformed into a zeolite phase. The zeolites obtained by this method, in contrast to the natural and synthetic zeolites, obtained from pure chemicals, contain significant amount of iron oxides together with traces of other active metals, which is a precondition for their good catalytic activity In the present study, zeolite X (FANaX) was synthesized from coal fly ash by a two-step high-temperature method. In order to follow the effect of different contaminants in the starting coal ash, zeolite X was also synthesized from pure chemicals according to a classical recipe (NaX). Iron was loaded on this reference zeolite with the amount which was contained in the coal FA. The final catalytic samples were obtained by wet impregnation of Pt nanoparticles on both types of zeolite crystals. The most active sample is Pt FANaX. The difference in the temperature at which 50 % conversion of benzene was reached between the Pt FANaX and the Pt-containing reference samples is 20 °C. The presence of stable redox pairs plays a key role in the Mars-van Krevelen mechanism, which is determined in Pt FANaX sample by the presence of Fe, Mg, Ca, Pt ions, making it more active. The loaded platinum is higher dispersed on the FANaX sample than on the Fe NaX one. The Pt dispersion also is a factor for the higher catalytic activity of the Pt FANaX sample. Additional reason for the lower activity of the Fe NaX sample is the blocked pores, which makes the diffusion of reagents and products of the oxidation reaction through the zeolite pores more difficult. The observed temperature for 100 % complete benzene oxidation over Pt FANaX is higher than this of Pt/Al_2O_3 catalysts and it is comparable with this of Au and Pd catalysts loaded on iron modified cerium oxides and Mn/Co binary catalysts and cobalt – cerium oxides. The advantages are the utilization of fly ash from one side and cheap source for the preparation of zeolite support from other side.

Keywords: Fly Ash, Zeolite X, Pt Nanoparticles, Catalytic Oxidation, Benzene.

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POSTER PRESENTATION

Id-2751

Modeling the Operation of a Gas Compressor Station to Minimize Fuel Costs for Protection against Surge Zone

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Abstract: Gas transmission through a pipeline network requires high pressure due to friction. As natural gas moves through a pipeline, it loses speed. To increase the pressure required for movement, it is necessary, that compressor stations are located along the main network. The same transported gas is used as fuel for the compressor station blowers, so about 3-5% is spent on gas compression. Therefore, when optimally planning a gas transportation route, it is necessary to optimize compression costs. We present research on the costs of fuel gas by compressor stations, using mathematical models of the operation of gas compressor units, to minimize the consumption of gas as fuel and present an optimization method with control of the number of revolutions of the supercharger and faucets for the safe process of transporting gas through a pipeline network [1]. Mathematical modeling of the described process made it possible to detect, technically unjustified, fuel gas consumption during the operation of gas compressor units at one of the compressor stations. The work proposes a method to minimize costs, which can be the basis for making recommendations to dispatch compressor unit engineers to load units to ensure gas flow with the required pressure and stable operation of the main network [2]. Minimizing this consumption is a challenge that has not only great financial implications for the industry; but also important environmental implications. This leads to the fuel cost minimization problem (FCMP). The construction of a special model to minimize the fuel cost in stationary mode is presented and used to solve FCMP [3]. Another dynamic programming approach is presented in [4], [5]. Taking into account and studying such diversity in search of global optimal solutions requires an in-depth study of its structure and principle of operation. We propose a solution to the problem of minimizing the fuel costs incurred by compressor stations. The problem of protecting the compressor from stopping in surge mode is one of the most important problems in the reliable and safe operation of compressor units.

Keywords: Gas Transmission, Gas Engine Compressor, Gas Compressor Unit, Region of Admissible Regimes.

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POSTER PRESENTATION

Id-2761

A Compositional Engineering and Phase Transitions of $DMA_xFA_{1-x}PbI_3$ Perovskites

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Abstract: Metal halide perovskites with a generic formula ABX_3 are promising semiconductor materials for photovoltaic applications due to the unique and tunable bandgap, high absorption coefficient and relatively simple synthesis methods [1]. However, one of the most demanding challenges nowadays is to face their instability under environmental conditions. One of the popular strategies to overcome this significant drawback is the incorporation of oversized cations into the perovskite lattice. For example, in case of methylammonium lead iodide ($MAPbI_3$) partial substitution of MA by guanidinium (GUA) cation can lead to materials with highly enhanced charge-carrier lifetimes [2] and stability [3]. In turn, in the triple-cation $GUA_xFA_xMA_{1-2x}PbI_3$ system, the introduction of large cations results in increased band gap energies as the amounts of GUA and FA increase [4]. In this study, we focus on dimethylammonium cation (DMA) as the oversized cation and develop mechanochemical synthesis and compositional engineering of double-cation A-site $DMA_xFA_{1-x}PbI_3$ perovskite materials along with an examination of their temperature-dependent polytypism. Powder XRD analysis of as-ground materials confirms complete miscibility across the entire substitution range, leading to the formation of one-dimensional δ-perovskitoid structures. Moreover, we revealed that the processing conditions have huge impact on the temperature-induced phase transitions and the formation of 3D polytypes. Specifically, the applied high rate of heating of the samples supports phase segregation, while the slow, gradual heating leads to single-phase materials. Interestingly, the slow heating results in the formation of a single black α-perovskite phase for material compositions up to 10% DMA, while in the fast heating a black α-perovskite coexists as secondary phase with the 4H polytype in compositions up to 30% of DMA. Thus, this work offers a comprehensive understanding of the effect of composition engineering and processing conditions on the phase transition to a given polytype in double A-cation $DMA_xFA_{1-x}PbI_3$ materials.

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POSTER PRESENTATION

Id-2783

Performing a n-type Doping of the Laser-Induced Graphene Using Urea and It's Characterization

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Abstract: For organic electronics, n-type polymers are costly and fabricating process are required specific equipment. In literature, n-type electrodes are fabricated through the manipulation of the graphene-based materials using specific tools like plasma treatment or using the hydrazine which it's very dangerous for human health. In this study, we will use the urea as a nitrogen source which it's cheap and has not a toxic behavior. At first, laser-induced graphene (LIG) films will be fabricated with the laser-inducing method with certain parameters. The following procedure dissolving the urea in DI water and combining with the LIG films. Combining process includes three steps; dipping, holding and heat treatment. After the heat treatment, films are evaluating with several characterization methods.

Keywords: Nitrogen-doped Graphene, Laser-induced Graphene, Chemical Properties.

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