

POSTERS

Abstracts



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DETECTION OF NUCLEAR MATERIAL WITH MOISTURE CONTENT BY USING LIBS TECHNIQUE

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To improve the proliferation resistance in nuclear fuel recycling technology, it is crucial to develop an elemental analysis method of molten salt composition in real-time. However, the analytical performance is greatly influenced by its moisture content in molten salt. While spent nuclear fuel treatment processing has been produced for decades, this process conducts experiments within a hot cell due to high heat emitting nuclides and a radioactive environment. Therefore, many researchers have worked inside hot cell as harsh environment for monitoring the process. This method is simple, but a very dangerous activity due to the highly radioactive material inside. Hence, in this study, the effects of moisture content variation on the properties of the laser induced breakdown spectroscopy (LIBS) and its spectral signals were investigated using the molten salt composition with different moisture contents. The spectra of hydrogen intensity showed a higher peak position with increasing moisture content according to the laser power increasing. The work looked at using a pulsed Nd:YAG laser operating at a fundamental wavelength of 1,064 nm in 50 mJ power. In order to artificially add an exact amount of moisture to the KF-LiF-ZrF₄ mixed composition, two vials were used which are linked by tube. The vials were sealed with vacuum grease and high strength adhesive

Biography

Seunghyun Kim has completed his PhD from Chungnam National University in Korea and postdoctoral studies from Virginia Commonwealth University in USA. Currently, he is serving as the Senior Researcher of KORAD for spent nuclear fuel management.

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THE CONTROL MECHANISM OF NANO SiO₂/EPOXY COMPOSITE COATING ON SURFACE CHARGE IN EPOXY RESIN

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Charge accumulation on the surface of epoxy resin affects its insulation performance under DC voltage. In order to investigate the effect of surface coating on surface charge accumulation, epoxy resin was coated by nano SiO₂/epoxy composite, and the charge accumulation on the surface was studied by an electrostatic probe. The surface trap parameters were analysed by isothermal surface potential decay, and combining with the carrier mobility, the transport characteristics of surface charge and the control mechanism of coating were studied. The results suggest that the surface charge mainly accumulates near the electrodes, the main source of charge was injected from the electrodes. The surface charges near the anode were mainly caused by charge trapping, and the surface charges near the cathode were mainly caused by the adsorption due to the normal electric field. Surface charge accumulation could be suppressed by increasing the shallow trap density and carrier mobility on the surface of material, which could be achieved by coating with nano SiO₂/epoxy composite. It was found that, surface charge of epoxy resin could be suppressed effectively by coating of nano SiO₂ particles with content of 3 wt %

Biography

Youping Tu has received her BSc and MSc degrees from the Department of Electrical Engineering, Chongqing University in Chongqing, China, respectively in 1988, and in 1991. Currently, she is a Professor in the Department of Electrical Engineering at North China Electric Power University in Beijing, China. From 1991 to 1994, she worked in the Computer Application field in Hangzhou Heat Power Plant, Zhejiang Province, China. During 1994, she was a Research Assistant in the Department of Precision Instrument and Mechanics, Tsinghua University in Beijing, China. From 1994 to 1995, she worked in Ludao Company in Beijing, China. She was a Lecturer from 1995 to 2003, and an Associate Professor from 2004 to 2010 in the Department of Electrical Engineering at North China Electric Power University in Beijing, China. Her research interest includes insulation technology, overvoltage and protection for power system. She is the author of more than 100 technical papers

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HEAT EXCHANGER TECHNOLOGY AND APPLICATIONS: GROUND-SOURCE HEAT PUMP SYSTEM FOR BUILDINGS HEATING AND COOLING

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Geothermal heat pumps (GSHPs) or direct expansion (DX) ground source heat pumps are a highly efficient renewable energy technology which uses the earth, groundwater or surface water as a heat source when operating in heating mode or as a heat sink when operating in a cooling mode. It is receiving increasing interest because of its potential to reduce primary energy consumption and thus reduce emissions of the greenhouse gases (GHGs). The main concept of this technology is that it utilises the lower temperature of the ground (approximately $<32^{\circ}\text{C}$), which remains relatively stable throughout the year, to provide space heating, cooling and domestic hot water inside the building area. The main goal of this study is to stimulate the uptake of the GSHPs. Recent attempts to stimulate alternative energy sources for heating and cooling of buildings has emphasised the utilisation of the ambient energy from ground source and other renewable energy sources. The purpose of this study, however, is to examine the means of reduction of energy consumption in buildings, identify GSHPs as an environmental friendly technology able to provide efficient utilisation of energy in the buildings sector, promote using GSHPs applications as an optimum means of heating and cooling, and to present typical applications and recent advances of the DX GSHPs. The study highlighted the potential energy saving that could be achieved through the use of ground energy sources. It also focuses on the optimisation and improvement of the operation conditions of the heat cycle and performance of the DX GSHP. It is concluded that the direct expansion of the GSHP, combined with the ground heat exchanger in foundation piles and the seasonal thermal energy storage from solar thermal collectors, is extendable to more comprehensive applications.

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GOLDEN TREATMENT FOR BLINDNESS: THE USE OF GOLD NANOPARTICLES AS AN ENHANCED DRUG DELIVERY SYSTEM IN AGE RELATED MACULAR DEGENERATION

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Background: Age related macular degeneration (AMD) has fast become one of the leading causes of blindness in the developed world. There are number of effective bio-macromolecule therapeutics available to treat patients with AMD but due to their susceptibility to biodegradation these drugs are required to be administered at regular intervals via monthly intravitreal injections. This invasive procedure can be unpleasant for the patient and lead to detrimental side effects. Gold nanoparticle-based drug delivery systems have been emerging as an attractive alternative. Studies have shown that these nanoparticles can be used as drug depots that can control the release of drugs by exposing them to light.

Method: Three studies which are done *in vitro* and *in vivo* models to test these drug delivery systems were presented and analysed.

Results: These studies demonstrated successful application of gold nanoparticles, *in vivo* and *in vitro*, in releasing multiple biologics for ocular therapeutics using polymer-coated gold nanoparticles (AuNPs) inside an agarose hydrogel as therapeutic depot. Hydrogel infused with gold nanoparticles when exposed to light could release pre-loaded therapeutics.

Conclusion: Although success was shown using gold nanoparticle delivery systems *in vivo* and *in vitro*, human trials must be considered along with longer term studies before these techniques can be implemented. The method can potentially reduce the number of intravitreal injections required.

PREDICTION OF TENSILE DEFORMATION BEHAVIOR OF AL-LI ALLOY 2060-T8 BY COMPUTATIONAL HOMOGENIZATION-BASED CRYSTAL PLASTICITY FINITE ELEMENT METHOD

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In current study, computational homogenization-based crystal plasticity (CP) modelling was presented to determine the deformation behavior of a novel third-generation AL-Li alloy 2060-T8 at room temperature, strain rate of 0.01s^{-1} and various loading directions. The computational homogenization strategy used a representative volume element (RVE) which describes the real microstructure of AA2060-T8 sheet to consider the in grains deformation behaviour. Besides, a periodically boundary condition was modified to consider both deformation induced anisotropy and the geometrical anisotropy. The initial microstructures and micro-textures of the AA2060-T8 sheet were determined by EBSD measurements, as well as used to build up the RVE model. The material parameters used in CP modelling was determined from the stress-strain curve obtained from the tensile test at strain rate of 0.001s^{-1} and loading direction of 30° with reference to rolling direction. The results obtained from computational homogenisation strategy keep a remarkable agreement with the results determined from experimentation. In conclusion, the computational homogenization based CPFEM is able to predict the deformation behavior and capture the anisotropic response of AA2060-T8 sheet at various deformation conditions.

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APPLICATION OF SUPERELASTIC SHAPE MEMORY ALLOY (SMA) IN CIVIL INFRASTRUCTURE FOR SEISMIC HAZARD MITIGATION

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Shape memory alloy (SMA) is a smart material that has a great potential for various civil engineering applications. The novelty of this material lies in its ability to undergo large deformation and return to its undeformed shape through stress removal (superelasticity) or heating (shape-memory effect). In particular, SMAs have distinct thermomechanical properties, including superelasticity, shape-memory effect and hysteretic damping. These properties could be effectively utilized to substantially enhance the safety of various structures. This presentation will cover the fundamental characteristics of SMAs, the constitutive material models of SMAs and the factors influencing the engineering properties of SMAs. The outcomes of several SMA-based research projects will be discussed including the reinforcement and repair of structural elements, bracing technology and the development of kernel components for seismic devices such as dampers and isolators and their performance-based seismic design. This presentation will synthesize existing information on various SMA types and their applications which is intended to motivate researchers and practicing engineers and extend the use of SMAs in novel and emerging applications.

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WAVE SCATTERING BY MANY SMALL IMPEDANCE PARTICLES AND CREATING MATERIALS WITH A DESIRED REFRACTION COEFFICIENT

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The theory of acoustic and electromagnetic (EM) wave scattering by one and many small impedance particles of arbitrary shapes is developed. The basic assumptions are: $a \ll d$, where 'a' is the characteristic size of particles and 'd' is the smallest distance between the neighbouring particles, is the wavelength. This theory allows one to give a recipe for creating materials with a desired refraction coefficient. One can create material with negative refraction: the group velocity in this material is directed opposite to the phase velocity. One can create a material with a desired wave focusing property. Equation is derived for the EM field in the medium in which many small impedance particles are embedded. Similar results are obtained in for heat transfer in the media in which many small particles are distributed. The theory presented in this talk is developed from our previous papers published.

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ADSORPTION ONTO APATITES AND APPLICATION TO BIOMATERIALS

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Calcium phosphates (CaP) have been widely used in the medical field as synthetic bone substitute and as carrier for targeted delivery applications. The apatite materials are similar to the bone mineral phase in terms of composition and biological properties and have the ability to form strong bonds with the bone tissues. Thus, it is needed to gain better understanding on the CaP biomineralization process as well as their interaction with biological environment in the living systems. This study aims at investigating under various conditions, the adsorption of polyanionic biomolecules onto synthetic CaP nanocrystals, in order to elucidate the effect of mineral active ions and the role of the functional groups in the uptake and release processes. The results revealed that equilibrium conditions were mostly reached within a short time of contact, attesting of the high surface reactivity of the apatite crystals. Biomolecules containing active end groups interact strongly with apatite crystals and are generally characterized by higher adsorption parameters, leading to isotherms Langmuirian in shape. Inversely, weak interaction occurs for simple molecules; the evolution of the loaded amount adsorbed for the latter, as a function of its remaining concentration in solution, conformed to the Freundlich-type isotherm. Furthermore, the process was irreversible with respect to dilution, while the adsorbed molecules were displaced when active species were added to the medium. A deep investigation of the uptake-release onto/from apatite surface indicated that adsorption for dilute solutions could be described as an ion-exchange process involving the functional groups of the molecules and the ionic groups at the apatite surface. For concentrated solutions, the interaction appears to be reactive and the adsorption process could then be described as a multifactor phenomenon. The present study indicated that control of the loading and release capacity of CaP materials is required to design drug delivery systems that meets the clinical needs.

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DEVELOPMENT OF BIOMATERIALS FROM RENEWABLE RESOURCES

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In recent years, the use of renewable natural resources have become the focus of research in supplementing and/or replacing traditional petrochemical products due to growing energy demands and environmental concerns. The utilization of lipids and other renewable resources has been considered to play a primitive role towards sustainable development due to their large scale availability, built-in-functionality, biodegradability and no net carbon dioxide (CO₂) production. In addition, a broad range of monomers can be obtained as a single feedstock. These attributes make lipids a good fit for the development of renewable biomaterials. This presentation will focus on the conversion of lipids, from various sources including waste streams such as waste cooking oil and lipids extracted from spent fowl, into monomers, biopolymers and biomaterials for packaging water remediation, biomedical and other applications. The ability for complete conversion of oils in just few minutes under solvent free conditions into monomers, biopolymers and bio-composites/nanocomposites is undoubtedly an attractive concept from both an academic and an industrial point of view.

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DEVELOPMENT OF TAILOR MADE PROPERTIES VIA ADDITIVE MANUFACTURING OF FUNCTIONALLY GRADED INCONEL 718

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Additive manufacturing (AM) technologies are known to allow the production of parts with an extreme degree of complexity, enabling design and functional part optimization. This study demonstrates novel way in development of programmed location dependant properties through the control of microstructure in 3D-printed metallic components. It is shown that AM thermal profiles can be used to manipulate preferred orientation of growing crystals as well as produce grains with different sizes, which affects the Young's modulus, strength and overall mechanical properties. The transitions in microstructure, texture, and properties in functionally graded components can be obtained at relatively small or large length scales, depending upon the functional gradient desired in a particular application. As a proof-of-concept, graded Inconel 718 was designed exhibiting core with coarse elongated and outside shell with fine grained microstructure which allowed the best trade-off between creep and fatigue performance and showed improved thermomechanical fatigue lifetime as compared to conventional Inconel 718 material. The developed herein graded component is represented as a composite material where elongated grains in preferentially textured core enable fatigue cracks deviation into positions perpendicular to the loading direction, hence providing no driving force to cause any crack extension. Application of such materials featuring tailor-made microstructural design and site-specific properties will allow for a more efficient use of resources and can be exploited in AM fabrication of complex components requiring challenging high-temperature mechanical performance.

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CRASHWORTHY PERFORMANCE OF BOMBYX MORI GLASS FIBRE/EPOXY HYBRID CYLINDRICAL COMPOSITE TUBES: EXPERIMENTAL

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This study investigated the failure behaviour, energy absorption response and loads carrying capability of glass fibre (GF)/ *Bombyx mori* (*B.mori*)/epoxy hybrid composite cylindrical tubes subjected to an axial quasi-static compression test. The reinforced cylindrical composite tubes were prepared using mandrel assisted hand lay-up technique. The specimen tested were three glass fibre cylindrical tube, each consisting of five layers of (GF), three *B.mori* fibre cylindrical tubes, each consisting of 15 layers *B.mori* fibre and GF/*B.mori*/epoxy hybrid cylindrical tubes, each consisting of three layers of GF, nine layers of *B.mori* fibres. The height of each tube was 50 mm tall, the thickness was 10 mm and the diameter was 65 mm respectively. The energy absorption and load carrying ability of the tubes were analyzed by measuring specific energy absorption, maximum peak load (P_{max}) and total energy absorption (TE) as a function of diverse fibre behaviour under compressive loading. Failure mechanism of the tubes was analyzed from high resolution photographs obtained during test. As expected, GF/*B.mori*/epoxy hybrid tubes performed better in load carriability and energy attenuation, while *B.mori* tubes performed better in progressive crushing failure behaviour. Deformation morphology suggests micro to macro cracks, tear propagation, delamination and collapse.

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DEVIATING ELECTRIC AND MAGNETIC FEATURES OF PROTONS, NEUTRONS AND ELECTRONS IN NANOSCALE MATERIALS ACCORDING TO TWIN PHYSICS

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Using the Heisenberg principle and the definition of complementarity as defined by Max Jammer, formalism is developed, based on the concept that determinate and indeterminate aspects of phenomena are mutually independent and that they occur joined in nature in such a manner that one of both dominates an observation and the other occurs as a small disturbance. Combining this starting point with relativity theory, space may be considered as a finite physical item, having an extremely low energy density and a potential equal to that of mass. Space and time are described separately in a mathematical similar way. The basic item in the theory is the Heisenberg-unit (H-unit), defined as a constant amount of potential energy. By using set theory, this unit can be supplied with complementary attributes of time, space and mark (a precursor of charge and electromagnetism). Only by interaction with another Heisenberg unit, potential energy can be transformed into physical items. The resulting complementary language represents a dualistic way of considering the universe and creates a bridge between large- and small-scale phenomena and so between quantum-mechanics and gravity. The laws of Maxwell emerge in an easy way. A series of elementary particles as well as the four forces of nature, neutron decay and gravitational waves is described. In this lecture a general overview of twin physics will be given with a few examples of described particles. We concentrate on results which are related to electric and magnetic features of protons, neutrons and electrons in nanoscale materials. Two of the four described types of electrons are characteristic for this material providing it with features being unknown in classical physics. Besides that, protons and neutrons are occurring without having a spin and instead of that having a short-distance magnetic field around.

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DISCOVERY OF THE OSCILLATIONS IN THE RPV STEEL RADIATION EMBRITTEMENT KINETICS AS AN INDICATION OF NANOSTRUCTURE SELF- ORGANIZING AND SMART BEHAVIOR

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Influence of neutron irradiation on reactor pressure vessel (RPV) steel degradation are examined with reference to the possible reasons of the substantial experimental data scatter and furthermore nonstandard (non-monotonous) and oscillatory embrittlement behaviour. In our glance, this phenomenon may be explained by presence of the wavelike recovering component in the embrittlement kinetics. We suppose that the main factor affecting steel anomalous embrittlement is fast neutron intensity (dose rate or flux); flux effect manifestation depends on state-of-the-art fluence level. At low fluencies radiation, degradation has to exceed normative value, then approaches to normative meaning and finally became sub normative. In our opinion, controversy in the estimation on neutron flux on radiation degradation impact may be explained by presence of the wavelike component in the embrittlement kinetics. Therefore, flux effect manifestation depends on fluence level. At low fluencies, radiation degradation has to exceed normative value, then approaches to normative meaning and finally became subnormative. As a result of dose, rate effect manifestation peripheral RPV's zones in some range of fluencies have to be damaged to a large extent than situated closely to reactor core. Moreover, as a hypothesis, we suppose that at some stages of irradiation, damaged metal have to be partially restored by irradiation i.e. neutron bombardment. Nascent during irradiation nanostructure undergo occurring once or periodically transformation in a direction both degradation and recovery of the initial properties. According to our hypothesis at some stage(s) of metal structure, degradation neutron bombardment became recovering factor. Self-recovering section of RPV steel radiation embrittlement kinetics is an indication of material nanostructure self-organizing and smart behavior.

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NANO TRIBLOCK COPOLYMERS PREPARED BY ATRP FOR INSULIN DRUG DELIVERY

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For controlled release applications requiring frequent injection, weight loss of the polymer matrix is the most important parameter of degradation. To avoid accumulation of polymer in the body, the matrix should disappear within a reasonable period of time (depending on the application). Novel triblock copolymers of different ration of L-lactide were prepared by atom-transfer radical polymerization (ATRP). They were characterized by FTIR, ¹H NMR, and micro elemental analysis. Triblock copolymers were used to prepare IPN's which had fiber characteristic due to presence of L-lactide in IPN's composition. Using the coated fiber, IPN's reduced the burst effects of insulin. Insulin release from fiber IPN's could be potentially controlled by changing the content of PEG, molecular weight of PEG, changing ratio of PLA/PEG-SC-PEG, presence of Pluronic F-127 with the composition of fiber IPN's, pH medium, crosslinked agent ratio, and the number of coated layers. The morphology of the uncoated fiber IPN's was performed using Scanning Electron Microscopy (SEM). All those polymer networks were loaded with 50 IU of insulin. *In vitro* release showed that the longer the PLA chain length, would be slower *in vitro* release rate of insulin due to decreasing the hydrophilicity which reflected the swelling of fiber IPN's and *in vitro* releasing rate of insulin. The obtained data showed that the release of insulin decreases within the first two hours for fiber IPN's of some triblock copolymers depending on the composition and molecular weights. The release rate of insulin can be designed by choosing the suitable conditions. The results simply support that loading of insulin with prepared fiber IPN's can be used for controlling insulin release and the fiber IPN's with triblock copolymer are suitable for insulin delivery system for the controlled administration of insulin.

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CHARGE TRANSFER CATALYSIS TO ENHANCE METAL CHALCOGENIDE FILM ELECTRODE STABILITY AND PHOTO-ELECTROCHEMICAL CONVERSION EFFICIENCY

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Attachment of electro-active species to the surface of a given semiconductor (SC) electrode permanently affects its photo-electrochemical (PEC) properties. Depending on the charge of the electro-active species, the flat band potentials may be shifted up (more negative) or down (more positive). The shift value depends on the applied ion charge density at the surface. Up to 300 mV shifting has been achieved here. Moreover, the electro-active species behaves as charge transfer catalyst across the electrode/redox junction. This increases the charge (holes or electrons depending on the type of the SC) transfer rate between the SC electrode and the redox couple. By doing so, the SC electrode can become more stable to photo-corrosion. All such advantages can be gained simply by attaching the proper electro-active materials to the proper SC electrode. The attachment can be performed by either chemical linkage or more recently by embedding the electro-active material inside a polymer matrix. The new technique has been successfully applied to monolithic and to polycrystalline SC electrode systems. Monolithic n-GaAs electrode showed up to eight fold enhancement in conversion efficiency. Polycrystalline film electrodes, involving nano-particles of semiconductors (CuS, CuSe, CdSe, CdTe, and others), are globally known to be unstable and yield low conversion efficiency (in the order of 1.0% or less) under PEC conditions. Stability and efficiency of such new types of electrodes have been enhanced here by the new technique. Conversion efficiency values of 4.4, 8.0, 15.0% and 18.0% have been observed from CdSe, CdTe, CuS and CuSe film electrodes, respectively. Such values have not been reported for pristine metal chalcogenide film electrodes before. This presentation will show a critical survey of our results observed throughout the last 15 years, as compared to other literature. The new model proposed for the efficiency and stability enhancement will also be rigorously presented. Future prospects of this work will also be discussed.

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COMPARATIVE ASSESSMENT OF DELAMINATION CONTROL TECHNIQUES IN CONVENTIONAL DRILLING OF CFRP

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Composite laminates are used in many applications due to their extremely high strength to low weight ratio and corrosion resistance properties. Comparing to other materials composites laminates have different properties throughout their thickness due to the layered structure. When drilling such structures, internal defects like delamination occur, caused by the drilling loads and their uneven distribution among the plies. The composite laminates are difficult to machine due to the composite's anisotropic and non-homogeneous nature. Thus it is important to develop an innovative advanced drilling process to overcome the difficulties related in machining of composite materials. The focus of present work is comprehensive study involving experimental characterization and development of different techniques for controlling the delamination in conventional drilling process, such as back up plate and helical milling has also been conducted. The analysis shows that the helical milling yields lower delamination extent, thrust force, hole size variation and hole surface roughness.

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SMART MATERIALS AND STRUCTURES: STATE OF THE ART AND APPLICATIONS

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The world of materials is an exciting and challenging field of research since it has always played a dominant role in the evolution of human civilization. The demands from diverse industrial branches (aerospace, automotive, defence, etc.) on much more advanced materials has led to the development of a new generation of materials surpassing conventional structural and functional materials and thus, the era of smart materials has started. Typical smart materials retain the ability to change their physical properties in a specific manner in response to a specific stimulus input. However, there is still a blurry image over the types and potential applications of smart materials. Moreover, smart materials and structures research includes many technically diverse fields that it is quite common for one field to completely misunderstand the terminology and start of the art in other fields. The purpose of this study is to better define the smart materials and structures field, its current status and its potential benefits. Results are presented and discussed. Finally, in order to demonstrate the characteristics of one class of smart materials, a numerical example is proposed and results are presented.

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THE MORPHOLOGICAL, STRUCTURAL, OPTICAL AND ANTIBACTERIAL CHARACTERISTICS OF CR₂O₃ NANOPARTICLES: A COMPREHENSIVE STUDY

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Calcination via thermal treatment using a precursor material is employed in the generation of Cr₂O₃ nanoparticles. Precursor materials included chromium nitrate in addition to a capping agent of polyvinylpyrrolidone. A range of analytical techniques: X-ray diffraction (XRD); energy dispersive X-ray (EDX); transmission electron microscopy (TEM); and Fourier transform infrared spectroscopy (FT-IR) were used to characterise the samples generated. The observation that the Cr₂O₃ nanoparticles results exhibited hexagonal crystalline structures was demonstrated by XRD analysis. The Cr and O in the Cr₂O₃ nanoparticle samples was confirmed as original materials using energy-dispersive X-ray spectroscopy and Fourier-transform infrared spectroscopy phase analysis. TEM results demonstrated that the different of calcination temperature from 500 to 800 °C resulted in an increase average nanoparticle size from 4 nm to 16 nm. X-ray photoelectron spectroscopy (XPS) analyses were used to investigate surface composition and valence state of the final nanoparticle product. Assessment of the optical energy gap using the Kubelka–Munk equation was achieved by utilization of diffuse UV-visible reflectance spectra, revealing that the energy band gap reduced with increasing calcination temperature: from 3.12 to 3.01 eV. Furthermore, increasing particle size was also found to be associated with increased photoluminescence as demonstrated by photoluminescence (PL) spectra. Lastly, antibacterial activity of the chromium oxide nanoparticle was assessed *in-vitro* using *Escherichia coli* ATCC 25922 Gram (-ve) and *Bacillus Subtilis* UPMC 1175 Gram (+ve).

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NEW POTENTIOMETRIC SENSOR BASED ON MOLECULARLY IMPRINTED NANOPARTICLES FOR COCAINE DETECTION

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Here, we present a potentiometric sensor for cocaine detection based on molecularly imprinted polymer nanoparticles (nanoMIPs) produced by the solid-phase imprinting method. The composition of polymers with high affinity for cocaine was optimized using molecular modelling. Four compositions were selected and polymers prepared using two protocols: chemical polymerisation in water and UV-initiated polymerisation in organic solvent. All synthesised nanoparticles had very good affinity to cocaine with dissociation constants between 0.6 nM and 5.3 nM. However, imprinted polymers produced in organic solvent using acrylamide as a functional monomer demonstrated the highest yield and affinity. For further sensor development, nanoparticles were incorporated within a PVC matrix which was then used to prepare an ion-selective membrane integrated with a potentiometric transducer. It was demonstrated that the sensor was able to quantify cocaine in blood serum samples in the range of concentrations between 1 nM and 1mM.

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SMART MATERIALS AND FUNCTIONAL CHARACTERIZATION OF SHAPE MEMORY ALLOYS

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Shape memory alloys take place in a class of adaptive structural materials called intelligent or smart materials by giving stimulus response to changes in the external conditions. These alloys exhibit dual characteristics, shape memory effect (SME) and superelasticity (SE) with the recoverability of two certain shapes at different conditions. These alloys are functional materials with these properties, and used as shape memory elements in many interdisciplinary fields such as medicine, pharmacy, bioengineering, metallurgy. This phenomenon is based on martensitic transformation, which is a solid state phase transformation and governed by the remarkable changes in internal crystalline structure of materials. Superelasticity is performed in only mechanical manner by stressing and releasing in the parent austenite phase region. Shape memory effect (SME) is performed thermally in a temperature interval depending on the forward (austenite \rightarrow martensite) and reverse (martensite \rightarrow austenite) transformation, on cooling and heating, whereas superelasticity is performed by stressing the material in the strain limit in the parent phase region and shape recovery is performed simultaneously upon releasing the applied stress. Shape memory effect is result of successive thermally and stress induced martensitic transformations, whereas superelasticity is the result of stress-induced martensitic transformation and performed in non-linear way, unlike normal elastic materials and exhibits rubber like behaviour. Loading and unloading paths are different in pseudo elasticity, and cycling loop reveals energy dissipation. The strain energy is stored after releasing and these alloys are mainly used as deformation absorbent materials in control of civil structures subjected to seismic events, due to the absorbance of strain energy during any disaster or earthquake. Thermal induced martensitic transformations occur on cooling with cooperative movement of atoms in $\langle 110 \rangle$ type directions by means of lattice invariant shears on a $\{110\}$ -type plane of austenite matrix which is basal plane of martensite. Thermally induced martensite occurs as the twinned martensite on cooling, and the twinned structure turn into the detwinned martensite by means of stress induced martensitic by stressing material in the low temperature product phase condition. In the pseudoelasticity, material is deformed in the strain limits in a constant temperature in parent phase region, and parent phase structures turn into the detwinned structure by means of stress induced martensitic transformation by deformation. Copper based alloys exhibit this property in metastable beta-phase region. Lattice invariant shear is not uniform in copper based alloys and cause the formation of unusual complex layered structures. In the present contribution, X-ray diffraction and transmission electron microscopy (TEM) studies were carried out on two copper based CuZnAl and CuAlMn alloys. X-ray diffraction profiles and electron diffraction patterns reveal that both alloys exhibit super lattice reflections inherited from parent phase due to the displacive character of martensitic transformation.

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MICROSTRUCTURE CHARACTERIZATION AND EVALUATION OF MECHANICAL PROPERTIES FOR FRICTION WELDED EN-24 ALLOY STEEL

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Continuous-drive friction welding is performed on EN-24 steel rods in the present study. The effect of post-weld heat treatment on microstructure and mechanical properties of the as-welded rods is examined with the particular focus on three different regions of weldment such as weld interface (WI), heat affected zone (HAZ), and unaffected base zone; and the results are compared with that of base metal. The microstructural characterization at WI and HAZ revealed martensitic structure and fine pearlite and ferrite respectively, in as-welded samples whereas it changes after post weld heat treatment (PWHT) to tempered martensite and coarse pearlite with ferrite, respectively. Martensitic structure at WI of as-welded samples imparts high hardness at the cost of low ductility while tempered martensite at WI of PWHT samples causes substantial decrease in hardness with improved ductility. However tensile strength of weld joint is achieved nearly equal to that of base metal.

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NEW PROCESSING OF RE-BASED MAGNETIC MATERIALS

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Rare-earth transition metals permanent magnets are vital components in the rapidly-developing renewable energy sector, where the motors require strong magnets with the ability to operate at temperatures well over 100 °C. To achieve high coercivity, remanence and consequently high energy product at elevated temperatures, the addition of heavy rare earth (HRE) to the basic Nd-Fe-B composition is needed. On the list of critical raw materials published by the EC in 2014, HRE is on the very top of it. To drastically reduce the use of HRE, we focused on developing a new method, which should enable us to achieve the properties needed for high-temperature application with the lowest amount of scarce elements. With our new inventive technique, further transferred to pilot production, we could minimize the amount of HRE used, down to 0.2 at %, the improvement of coercivity was 30 % with minimal loss in remanence. The total saving of the HRE is 16-times less need of HRE for the same performance, which is a significant contribution to the world economy and clean environment. In studying the mechanism for such an improvement in coercivity without significantly decreasing the remanence, a detailed microstructure investigation was performed by using high-resolution transmission electron microscopy. The so-called core-shell grains were observed, the thickness of the shell varied from 150 to 200 nm. By using the electron holography imaging, we also observe the magnetic domains. Reconstructed phase showed the magnetic flux distribution and colour maps. The contour spacing was $\pi/2$. Besides the use of these newly developed high energy magnets for electric and hybrid cars and the wind turbine generators the important application is also as the source of the magnetic field in the development of the new magnetic cooling devices.

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2D MATERIALS, FLEXIBLE ELECTRODES AND SURFACES

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I will present three of our primary research topics, as each relates to 1D/2D materials, substrates and surfaces. Firstly, I will focus on our investigation of chemical vapor deposition (CVD)-growth, achieving localized, patterned, single crystalline or polycrystalline monolayers of TMDs, including MoS_2 , WS_2 , WSe_2 and MoSe_2 , as well as their heterostructures. We study CVD-growth and perform extensive material characterization to illuminate the role of dissimilar 2D substrates in the prevention of interior defects in TMDs, thus uncovering the conditions for anti-oxidation. We further demonstrate the epitaxial growth of TMDs on hBN and graphene, as well as vertical/lateral heterostructures of TMDs, uniquely forming in-phase 2D heterostructures. This research provides a detailed observation of the oxidation and anti-oxidation behaviors of TMDs, which corroborate the role of underlying 2D layers in the prevention of interior defects in TMDs. If the technique could be developed to be highly reliable and high fidelity, it could have a large impact on the future research and commercialization of TMD-based devices. The second research area concerns our development and application of flexible electrodes and energy storage toward wearable and multifunctional electronics. Here, we develop a facile fabrication technique utilizing vertically aligned carbon nanotubes (VACNTs), which enables high-throughput fabrication of flexible supercapacitors. We develop an innovative technique, which facilitates a stable charge/discharge under varied strains. Our structure shows a high flexibility and stability during stretching up to 20% and bending up to 180°. These flexible supercapacitors are promising for various flexible electronics applications. Lastly, we investigate and utilize smart polymer functional surfaces using dodecylbenzenesulfonate-doped polypyrrole (PPy(DBS)); we demonstrate a novel *in situ* control of droplet pinning on the polymer surface, enabling the control of droplet adhesion from strongly pinned to extremely slippery (and vice versa). The pinning of organic droplets on the surfaces is dramatically controlled *in situ*, presenting great potential for manipulation and control of liquid droplets for various applications including oil separation, water treatment and anti-bacterial surfaces. In addition, we demonstrate controlled lateral actuation of organic droplets on PPy (DBS) electrodes in an aqueous environment. We believe that our work represents a major advance in materials science and engineering, especially pertaining to those topics that involve functional and tunable surfaces.

MECHANICAL INVESTIGATION APPROACH TO OPTIMIZE THE HVOF FE-BASED AMORPHOUS COATINGS REINFORCED BY B4C NANOPARTICLES

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Fe-based amorphous feedstock powders used as the matrix into which various ratios of hard B4C nanoparticles (0, 5, 10, 15, 20 vol %) as a reinforcing agent were prepared using a planetary high-energy mechanical milling. The ball-milled nanocomposite feedstock powders were also sprayed by means of high-velocity oxygen fuel (HVOF) technique. The characteristics of the powder particles and the prepared coating depending on their microstructures and nanohardness were examined in detail using nanoindentation tester. The results showed that the formation of the Fe-based amorphous phase was noticed over the course of high-energy ball milling. It is interesting to note that the nanocomposite coating is divided into two regions, namely, a full amorphous phase region and homogeneous dispersion of B4C nanoparticles with a scale of 10-50 nm in a residual amorphous matrix. As the B4C content increases, the nanohardness of the composite coatings increases, but the fracture toughness begins to decrease at the B4C content higher than 20 vol %. The optimal mechanical properties are obtained with 15 vol % B4C due to the suitable content and uniform distribution of nanoparticles. Consequently, the changes in mechanical properties of the coatings were attributed to the changes in the brittle to ductile transition by adding B4C nanoparticles.

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VACUUM-FREE AND HYDROGEN-FREE GRAPHENE SYNTHESIS

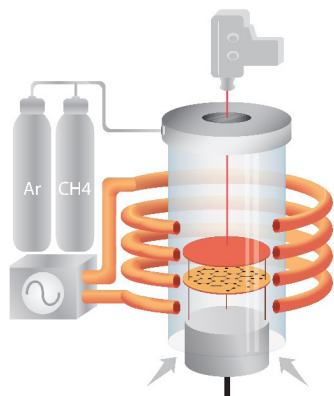
P Häberle¹, C Orellana¹, T Cunha², C Fantini² and A Jaques¹

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A modified method to grow graphene in a single-step process is proposed. It is based on chemical vapour deposition (CVD) and considers the use of methane as carbon source. Synthesis takes place in an open chamber without requiring the addition of gaseous hydrogen in any of the synthesis stages. The synthesis occurs between two parallel Cu plates, heated up via electromagnetic induction. The inductive heating yields a strong thermal gradient between the catalytic substrates and the surrounding environment, promoting the enrichment of hydrogen, generated as methane fragments, within the volume confined by the Cu foils. This induced density gradient is due to thermo diffusion, also known as the Soret effect. Hydrogen and other low mass molecular fractions produced during the synthesis process inhibit the oxidative effects and simultaneously reduce the native oxide on the Cu surface. As a result, high quality graphene is obtained, only on the inner surfaces of the Cu sheets, as confirmed by Raman Spectroscopy.

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DELIVERY OF DOCETAXEL TO BREAST CANCER CELLS EMPLOYING WATER SOLUBLE CARBON NANOTUBOLS: ENHANCED ANTI-NEOPLASTIC ACTIVITY AND IMPROVED PHARMACOKINETIC PROFILE

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In the present research, the aim was to synthesize aspartic acid tagged water soluble hydroxylated CNTs (CNTnols) and to deliver docetaxel to cancer cells with enhanced safety and efficacy. Various characterization studies like FT-IR and NMR spectroscopy were performed after synthesizing docetaxel conjugated aspartic acid derivatized CNTnols. Particle size analysis, zeta potential, PDI and FE-SEM were also used for characterization of the nanoconjugate. Release kinetics, cytotoxicity assay, cellular uptake studies and pharmacokinetics and other methods were used for evaluation of conjugate. From cell viability studies, it was found that there was 4.05 times decrease in IC50 values after conjugation showing the targeted action. Cellular uptake studies are in support with cytotoxic studies proving the enhancement in cellular uptake of docetaxel. Through pharmacokinetic studies it was observed that the half-life and bioavailability was increased by 6 and 4.3 times when compared to pure drug. It was found that the synthesised nanoconjugate was hemocompatible and offered low protein binding. All the findings are promising in nature and the nanoconjugate was considered as a novel carrier for delivery of anti-cancer drugs, especially belonging to bio pharmaceuticals classification system (BCS) class IV.

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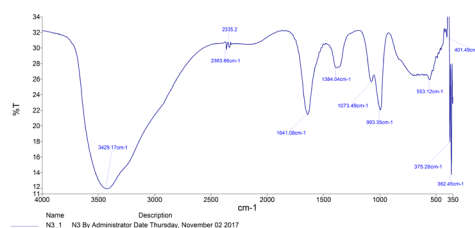
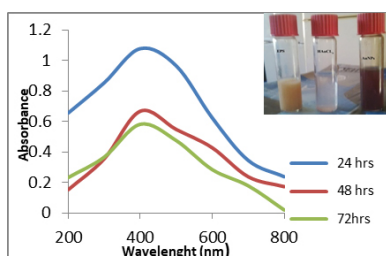
MYCOSYNTHESIS AND ANTIBACTERIAL ASSESSMENT OF GOLD AND SILVER NANOPARTICLES (NPS) AND FUNCTIONALIZED NPS USING BIOMOLECULES FROM PLEUROTUS OSTREATUS AGAINST SOME SELECTED MULTIDRUG RESISTANT PATHOGENS

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Biosynthesis and characterization of gold and silver nanoparticles (NPs) using biomolecules such as exopolysaccharide (EPS), cell free filtrate (CFF) and fruiting body extract (FBE) of *Pleurotus ostreatus* (PO) and antimicrobial potential of the biosynthesized NPs and functionalized NPs against some multidrug resistant bacteria was investigated. The silver NPs (SNPs) and gold NPs (AuNPs) biosynthesized using the biomolecules (EPS, CFF and FBE) were characterized using visual observation, UV-visible spectrophotometer, Fourier transform infrared (FTIR) and scanning electron microscope (SEM). Changes in colour from pale yellow and cloudy colour to dark brown and to purple and dark purple indicate the formation of SNPs and AuNPs. The intensity of the colour differs from CFF<EPS<FBE. The NPs had strong surface plasmon resonance (SPR) band at 500 nm and 400 nm after 72 hrs for AuNPs and SNPs. The NPs were polymorphic shape and aggregate. Hydroxyl, carboxyl and aldehydes were the major functional group present which may be responsible for the reduction, capping and stabilization of the NPs. The AuNPs and SNPs had antibacterial activity against the test pathogens and the zones of inhibition ranged from 9-27 and 8-29 mm. The ceftriaxone functionalized SNP and AuNP showed increased antimicrobial activity which ranged from 30-40 mm and 25-42 mm. Functionalization's of the NPs with antibiotics enhanced the antibacterial property of the NPs. In conclusion, this study demonstrated that biomolecules from *Pleurotus ostreatus* could be used for the production of stable SNPs and AuNPs with antibacterial activity against MDR pathogens. Functionalization improved the antibacterial potentials of the NPs.

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CALORIMETRIC MEASUREMENT OF INTERFACE ENTHALPY OF NANOCRYSTALLINE SILVER (I) OXIDE (AG₂O)

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The interface enthalpy of nanocrystalline silver (I) oxide (Ag₂O.nH₂O) was measured. Ag₂O.nH₂O nanocrystalline samples of varying surface areas and degrees of agglomeration were synthesized by wet chemical technique. Interface areas were estimated by comparing the surface areas measured by N₂ adsorption to the crystallite sizes refined from X-ray diffraction data. The interface enthalpy was verified by utilizing thermodynamic cycle, using enthalpy of solution measurements in 25% HNO₃ at room temperature solution calorimetry. The interface enthalpy of the nanocrystalline Ag₂O.nH₂O is (0.842±0.508 J/m²). This work provides the first calorimetric measurement of the interface enthalpy of nanocrystalline silver (I) oxide (Ag₂O.nH₂O).

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ELECTROSPINNED NANONPOROUS PTFE FILM BASED FILTER MEDIA FOR DUST COLLECTOR BAGS IN HIGH TEMPERATURE AND CORROSIVE ENVIRONMENT**Harishchandra A Sonawane, Naman H Barot, Charudatta R Prayag and T Gangopodhyay**

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Polytetrafluoroethylene (PTFE) membrane coated glass fabric is available as robust filter media for high temperature dust filtration. Since it is a membrane coated media, only pores left out contributes to the filtration. PTFE membrane can withstand temperatures up to 500 °F (260 °C). The process of creation of PTFE based nanofiber nanoweb using free-surface electrospinning technology on twill weave glass fabric as well as its stabilization by heat treatment has been developed with an objective of providing an effective high temperature resistant fine dust filter media which can be used with less energy consumption during operation because of high porosity. The developed nanofiber coated glass fabric retains air permeability to the extent of 50-70% and remains stable at 260 °C. The prototype of dust collector bags were fabricated and subjected to filtration, mechanical and industrial trial. Filtration efficiency study clearly shows the improvement in filtration efficiency by 90% with respect to neat fabric and 30% more as compared to marketed product. The mechanical study reveals that the coated media has better strength as compared to non-coated or bare glass fabrics. The industrial study shows that the commercial product has filtration efficiency about 65-70% while the nanonporous PTFE coated media has efficiency of 85.3 %.

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NANOFIBER BASED WATER FILTER CARTRIDGE

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Polyamide 6 nanofibers are prepared by free surface electro spinning process in which a cylinder or wire electrode partially immersed in a polymer solution. A thin web layer of polymer is deposited over substrate fabric i.e. melt-blown polypropylene. Additional padding of spun-bond polypropylene coated with low molecular chitosan and nanoparticles is given as protective layer for the nanofibers and as heavy metal removal agent. Surface morphology of deposited nanofibers was determined with the use of a scanning electron microscope. The results show that this nanoweb is capable of removing all the suspended particles from the contaminated water samples. The turbidity test measurement shows that the turbidity limit of filtered water was well within acceptable limit of 1 NTU and below the permissible limit of 5 NTU in absence of any alternative source, which is as per the Indian Standard IS 10500:2012. Filtered water showed excellent results of turbidity removal. Bacteriological water analysis carried out to evaluate bacterial removing efficiency. The filter water was subjected to test the heavy metal removal by atomic absorption spectroscopy shows effective removal of chromium, cadmium, lead, arsenic and iron.

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INTERFACIAL ENGINEERING IN HETEROSTRUCTURES AND NANOTECHNOLOGY FOR RAPID PROTOTYPING OF ETHANOL SENSOR

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A trace amount of human breath is a mixture of ethanol, pentane, acetone and other volatile compounds. These originate from metabolic processes occurring in the organism, environmental exposure, dietary sources and alcohol intake. For example, volatile organic compounds (VOCs) in human breath have already been linked to a condition of lung cancer, diabetes and other diseases. Our interest is in the detection of ethanol vapours at sub ppm level to high level in human breath. The aim is to develop an alcohol breath analyzer to be used by the common man. The device for this kind of application should be reliable, sensitive, and operable at room temperature and easily complementary metal-oxide-semiconductor (CMOS) integrated. This paper presents batch fabrication and rapid prototyping of selective ethanol sensor. The sensing mechanism is based on the interface engineering of heterostructures. The sensing materials consist of TiO_2 and porous silicon (PS) and technique used is resistive sensing. Sensing data was also collected from single layers like PS and TiO_2 . The limit of detection was in sub-ppm level and the sensing response was repeatable and reproducible. The sensors operate at room temperature and were mounted onto transistor outline (TO), dual in-line (DIP) packages. These devices can form a basis for development of breath alcohol analyzers to be used by traffic policemen. This work highlights the significance of the interface formed between metal oxide and porous silicon and how this can be formed into a prototype for a social cause.

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EFFECT OF SYNTHETIC CONDITIONS ON THE TEXTURAL PROPERTIES OF GLUCONIC ACID COATED MAGNETIC IRON OXIDE NANOPARTICLES

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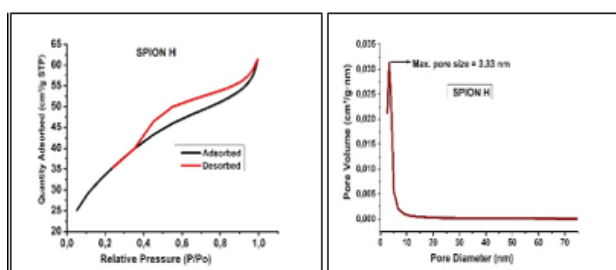
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Applications of magnetic iron oxide-based nanomaterials are desirable for removal of heavy metals and other contaminants from waste water because of their important features such as small particle size, high surface area, saturated magnetism, definite pore size and pore volume. This study tends to evaluate the effect of synthetic conditions such as temperature, volume and concentration of precursors on the textural properties of gluconic acid coated magnetic iron oxide nanoparticles. Iron III salt and glucose were used as precursors to prepare the nanomaterials and were characterized using Fourier transform infrared spectroscopy (FTIR), scanning electron microscopy (SEM), energy-dispersive X-ray spectroscopy (EDX), X-ray powder diffractometry (XRD) and thermal gravimetric analysis (TGA). The magnetic properties of the as-synthesized materials were measured using the SQUID magnetometer. Textural properties including surface areas, average pore size and pore size distribution of the studied samples were determined by the Brunauer–Emmett–Teller (BET) method. Results showed that the synthesized samples are paramagnetic and superparamagnetic in behaviour. In addition, the mean pore size of the synthesized samples varies between 3.33 and 7.59 nm. This shows that the nanomaterials are mesoporous in nature and contain large plate-like particles with slit-shaped pores which favour adsorption of waste materials from contaminated water. Surface area of the nanomaterials ranged between 158 and 353.80 m²/g which are far higher than values of the standard magnetic iron oxides reported in literature. The as-synthesized magnetic iron oxide nanomaterials in this study are considered as good candidates for applications such as adsorbents for removal of heavy metals and other organic pollutants from waste waters, photo-electrochemical cells, catalysts and sensors.

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PHOTODEGRADATION OF HUMIC ACID IN AQUEOUS SOLUTION USING A TiO₂ / CARBONACEOUS HYPER-CROSS-LINKED POLYSTYRENE POLYMER NANOCOMPOSITE

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The development of alternative methods to degrade natural organic matter or its components to harmless products is an area that has been attracting significant research interest lately. This paper reports the photodegradation of humic acid using a composite photocatalyst made up of TiO₂ nanoparticles and a carbonaceous hyper-cross-linked polystyrene-type precursor derived from post-consumer waste polystyrene. The physicochemical properties of the TiO₂-carbonaceous hyper-cross-linked polystyrene nanocomposites were determined using Fourier transform infrared spectroscopy, UV-visible spectroscopy, scanning electron microscopy and X-ray diffraction spectroscopy. Batch experiments were used to evaluate the capacity of the materials to photodegrade humic acid in synthetic wastewater samples using a solar simulator. Despite showing marginal band-gap narrowing, the introduction of carbonaceous hyper-cross-linked polystyrene into TiO₂ was accompanied by a 100% increase in the degradation rate of humic acid at a contact time of 90 min. Overall, the photodegradation capacity of the composites increased with an increase in the carbonaceous hyper-cross-linked polystyrene content. The use of post-consumer waste polystyrene in preparing high-value materials is novel and a cost-effective way of water treatment that simultaneously makes a contribution towards alleviating the environmental burden of waste polystyrene.

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