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3rd ADVANCED

MATERIALS SCIENCE WORLD CONGRESS

MARCH 21-23
2022

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Adv. Materials Science 2022

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PEERS ALLEY MEDIA

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PROGRAM-AT-A-GLANCE

Adv. Materials Science 2022

DAY 1
MARCH 21, 2022

Scientific Program

GMT-Greenwich Mean Time

Keynote Session

07:30-08:00	**Introduction**
08:00-08:25	**Title: Fibre flow in 3D printing of discontinuous fibre reinforced thermoplastic composites** **Dongmin Yang,** *University of Edinburgh, United Kingdom*
08:25-08:50	**Title: A current investigation into zircon uses in geosciences: Case studies from Southern Italy mountain ranges** **Francesca Micheletti,** *University of Bari Aldo Moro, Italy*
08:50-09:15	**Title: Impact diamonds of Popigai Crater, Siberia: A new advanced natural nanopolycrystalline material** **Nikolay Pokhilenko,** *Russian Academy of Sciences, Russia*

Distinguished Speaker Talks

09:15-09:35	**Title: Supercoiling artificial muscles** **Geoff Spinks,** *University of Wollongong, Australia*
09:35-09:50	**Title: Graphene derivative and metal nanoparticles coated silk fabrics with durable, multifunctional properties for numerous potential applications** **Shovon Bhattacharjee,** *UNSW Sydney, Australia*
09:50-10:10	**Title: Defect induction in crystals by glass crystallization method and its application for photonics** **Kenji Shinozaki,** *National Institute of Advanced Industrial Science and Technology, Japan*
10:10-10:30	**Title: High curie temperature ferroelectrics** **Seiji Kojima,** *University of Tsukuba, Japan*

10:30-10:50	**Title: Compact measurement of the optical power in high-power LED using a light-absorbent thermal sensor** **Jae-Young Joo,** *Korea Photonics Technology Institute, South Korea*

Refreshment Break 10:50-11:05

11:05-11:25	**Title: Advanced graphene aerogel embedded phase change materials (PCMs) for energy harvesting** **Chengbin Yu,** *Seoul National University, South Korea*
11:25-11:45	**Title: Design and preparation of full-spectrum solar light responsive photocatalysts for hydrogen generation** **Junying Zhang,** *Beihang University, China*
11:45-12:05	**Title: Immunomodulating biomaterials** **Weiwei Wang,** *Peking Union Medical College, China*
12:05-12:25	**Title: High-scattering porous polymer structures and their applications** **Shudong Yu,** *South China University of Technology, China*
12:25-12:45	**Title: Oxidizable electrode induced bipolar resistive switching behavior in TE/CdZnTe/Pt structure** **Aoqiu Wang,** *Northwestern Polytechnical University, China*
12:45-13:05	**Title: Advances in gallium nitride metalenses** **Vin-Cent Su,** *National United University, Taiwan*
13:05-13:20	**Title: Failure analysis of DSS 2205 GTA welds and evaluation of the cooling rate effects on localized corrosion with mini-electrochemical cell** **Li Yuan Hu,** *Chang Gung University, Taiwan*

Lunch Break 13:20-13:50

13:50-14:10	**Title: Metalla-ynes and poly(metallayne)s: Synthesis, charaterization and opto-electronic applications** **Rayya A. Al-Balushi,** *A'Sharqiyah University, Oman*

14:10-14:30	**Title: Carbon-based materials for energy storage applications** **Meltem Yanilmaz,** *Istanbul Technical University, Turkey*
14:30-14:50	**Title: Recent advances resistive metallic hydrogen sensors** **Necmettin Kilinc,** *Inonu University, Turkey*
14:50-15:10	**Title: Shape memory phenomena and thermomechanical reactions in reversibility of shape memory alloys** **Osman Adiguzel,** *Firat University, Turkey*
15:10-15:25	**Title: Composite portable shelter system produced by vacuum bagging using recycled reinforcement and matrix materials** **Ayse Genc,** *Calık Denim, Turkey*
15:25-15:45	**Title: Study of radiation shielding materials on microstrip patch antenna for sustainability** **John Nepomuceno Colaco,** *Goa College of Engineering, India*
15:45-16:00	**Title: Analysis of instantaneous poynting vector and application** **Himanshu Kushwah,** *University of Delhi, India*

Refreshment Break 16:00-16:15

16:15-16:35	**Title: A comparison of smear layer removal effects between conventional chemical surface treatment and double-wavelength (Er,Cr: YSGG 2780 nm and diode 940 nm) laser methods on push-out bound strength of three calsium silicate-based materials** **Ezatolah Kazeminejad,** *Golestan University of medical sciences, Iran*
16:35-16:50	**Title: Optimization of deep drawing products by adding effect of texture pattern in draw bead design** **Mohammad Soroush Merkani,** *University of Tehran, Iran*
16:50-17:10	**Title: Technique to avoid membrane punching during triaxial test of crushed aggregate** **Wael Mahmood Albadri,** *Al-Amarah University College, Iraq*

17:10-17:30	**Title: Development and performance evaluation of a pedal operated seed cleaner (POS cleaner)** **Wilber Akatuhurira,** *Makerere University, Uganda*
17:30-17:50	**Title: Sb_2S_3 thin films by ultrasonic spray: Formation and application in solar cells** **Malle Krunks,** *Tallinn University of Technology, Estonia*
17:50-18:10	**Title: Microscale control of ferrofluid toward enabling novel micro-electromechanical systems** **Kenichi Takahata,** *University of British Columbia, Canada*

Panel Discussion

End of Day 1

DAY 2

MARCH 22, 2022

Scientific Program

GMT-Greenwich Mean Time

Keynote Session

07:30-08:00	**Introduction**
08:00-08:25	**Title: Smart coatings: Degradation of priority pollutants on TiO_2 based photocatalytic materials in indoor and outdoor environments-Principles and mechanisms** **Dimitrios Kotzias,** *Institute for Health and Consumer Protection, Italy*
08:25-08:50	**Title: Dental zirconia waste for a sustainable manufacturing of oil-water separation membranes** **Francesca Deganello,** *Italian National Research Council, Italy*
08:50-09:15	**Title: Synthesis, modeling and applications of III-V nanowires and nanowire heterostructures: Opportunities and challenges** **V. G. Dubrovskii,** *St. Petersburg State University, Russia*

Distinguished Speaker Talks

09:15-09:35	**Title: Energy transformation and accumulation in solids, irradiated by charged particles** **Alexander Valyaev,** *Nuclear Safety Institute of the Russian Academy of Sciences, Russia*
09:35-09:55	**Title: Upconversion nanoplatforms as potent agents for cancer theranostics** **Irina V. Balalaeva,** *Lobachevsky University, Russia*
09:55-10:15	**Title: Regularities of acoustic emission under shock loading of glass with a crack** **Sergey Bekher,** *Siberian Transport University, Russia*
10:15-10:35	**Title: Study of corrosion-resistant deposited metal of NPP equipment performed with a strip electrode by arc welding and electroslag welding methods** **Mikhail Timofeev,** *Prometey Central Scientific Research Institute of Structural Materials, Russia*

10:35-10:55	**Title: Role of production procedure on microstructure and chemical composition of $Na_{0.5}Bi_{0.5}TiO_3$ ceramics** **Marija Dunce,** *University of Latvia, Latvia*
10:55-11:15	**Title: Organizing metal atoms and nanoclusters in LC media for novel applications** **Satya Pal Singh,** *Madan Mohan Malaviya University of Technology, India*

Refreshment Break 11:15-11:30

11:30-11:50	**Title: Improving yield and nitrogen use efficiency using polymer coated urea in rice (Oryza sativa L.) under vertisol of Deccan Plateau (Typic Pellustert)** **Gobinath Rajendran,** *ICAR-Indian Institute of Rice Research, India*
11:50-12:10	**Title: Pattern recognition techniques for sand particles** **Jianfeng Wang,** *City University of Hong Kong, China*
12:10-12:30	**Title: Fluorescent single-walled carbon nanotubes for imaging and sensing in the near-infrared** **Gili Bisker,** *Tel-Aviv University, Israel*
12:30-12:50	**Title: A LIME-based explainable machine learning model for predicting the severity level of COVID-19 diagnosed patients** **Freddy Gabbay,** *Ruppin Academic Center, Israel*
12:50-13:10	**Title: Temperature dependent calibration of shape-memory alloy strain sensors** **Thomas Mäder,** *Fraunhofer Institute for Machine Tools and Forming Technology IWU, Germany*
13:10-13:25	**Title: Examining the contribution of factors affecting the electrical behavior of poly(methyl methacrylate)/graphene nanoplatelets composites** **Xiaoling Luo,** *University of Erlangen-Nuremberg, Germany*

Lunch Break 13:25-13:55

13:55-14:15	**Title: Manganese Hexacyanoferrate cathode material for aqueous Zn-ion battery** **Marco Giorgetti,** *University of Bologna, Italy*

14:15-14:30	**Title: Multidisciplinary and statistical approach for the investigation and characterization of archaeological artifacts** **Francesca Falcone,** *D'Annunzio University, Italy*
14:30-14:45	**Title: Employing dicarboxylic acids in the KF-YF_3 system to modulate the crystal phase and optical response of Eu^{3+}-doped materials** **Pablo Serna-Gallen,** *Jaume I University, Spain*
14:45-15:00	**Title: A safe, flexible, and high-performing gel-polymer electrolyte for rechargeable lithium metal batteries** **Julen Castillo,** *Basque Research and Technology Alliance, Spain*
15:00-15:20	**Title: Plasmo-electronic properties of self-organised nanoparticles** **Jeremie Grisolia,** *University of Toulouse, France*
15:20-15:40	**Title: Effect of the chemical composition and dimensionality of halide perovskites for photovoltaic applications on their basic properties: Insights from theory** **Philippe Baranek,** *Edf Lab Paris-Saclay, France*
15:40-16:00	**Title: Effect of adamantane substitutions to improve properties of organic optoelectronic materials** **Jozef Krajcovic,** *Brno University of Technology, Czech Republic*

Refreshment Break 16:00-16:15

16:15-16:35	**Title: Changing the paradigm of pressure injury (PI) prevention: Translating sub epidermal moisture (SEM) assessment technology from bench to bedside** **Ruth Bryant,** *Abbott Northwestern Hospital, USA*
16:35-16:50	**Title: Nanoparticles as cell tracking agents in human ocular cell transplantation therapy** **David C. Mundy,** *Stanford University School of Medicine, USA*
16:50-17:10	**Title: Developing a needle-knife surgical device** **Fabio Ferraz do Amaral Ravaglia,** *University of Campinas, Brazil*

17:10-17:30	**Title: Gas permeameter for polymers and nanocomposites: Improvements and advances** **Gilberto Joao Pavani,** *Federal Institute of Rio Grande do Sul, Brazil*
17:30-17:50	**Title: Development of advanced composite materials by additive manufacturing** **Haniyeh Fayazfar,** *University of Ontario Tech, Canada*
17:50-18:10	**Title: Deposition of biopolymers by cold gas spray** **John Henao,** *National Research Council of Science and Technology (CONACYT), México*

Panel Discussion

End of Day 2

DAY 3
MARCH 23, 2022

Scientific Program

GMT-Greenwich Mean Time

Keynote Session

07:30-08:00	**Introduction**
08:00-08:25	**Title: Foaming epoxy-amine-carbamate: The effect of different neat amines on rheological and cellular morphology** **Du Ngoc Uy Lan,** *Universität Bayreuth, Germany*
08:25-08:50	**Title: Valorization of waste for the materials and energy** **Lucia D'Accolti,** *University of Bari, Italy*
08:50-09:15	**Title: Mechanical properties and thermal stability of fiber reinforced geopolymer composites** **Huirong Le,** *Tsinghua University, China*

Distinguished Speaker Talks

09:15-09:35	**Title: High sodium content P2-type cathode for high-performance sodium-ion batteries** **Ting Jin,** *Northwestern Polytechnical University, China*
09:35-09:55	**Title: Circular polarizing filters based on chiral metasurface** **Xin He,** *Zhejiang University, China*
09:55-10:15	**Title: Fabrication of pore-selectively silver-functionalized honeycomb-patterned film and its application for antibacterial activity** **Do Sung Huh,** *Inje University, South Korea*
10:15-10:30	**Title: Compact dual-band 4-MIMO Antenna elements for 5G mobile applications** **Fayad Ghawbar,** *Universiti Tun Hussein Onn Malaysia, Malaysia*

10:30-10:45	**Title: Hot ECAP implementation in zirconia reinforced aluminium chip matrix (Al6061) composite production** **Sami Abdo Mohammed Al-Alimi,** *Universiti Tun Hussein Onn Malaysia, Malaysia*
10:45-11:05	**Title: Correlation between charge transport- recombination loss kinetics and perovskite solar cell performance investigated by TPV and IMVS measurements** **Rahmat Hidayat,** *Bandung Institute of Technology, Indonesia*

Refreshment Break 11:05-11:20

11:20-11:40	**Title: Structural, optical and electrical characterizations of Cr-doped CuO thin films** **Ilhan CANDAN,** *Dicle University, Turkey*
11:40-11:55	**Title: Pollen morphology and its taxonomic significance of the genus Crucianella L. (Rubiaceae) in Iran** **Soheyla Parsapanah,** *University of Guilan, Iran*
11:55-12:10	**Title: Graphene spin-coated electrode for polyacrylonitrile acoustic nanogenerators** **Sedigheh Aghahyari,** *Sharif University of Technology, Iran*
12:10-12:30	**Title: Energy and CO_2 emission assessments of alkali- activated concrete and ordinary portland cement concrete: A comparative analysis of different grades of concrete** **Ali Alsalman,** *Almaaqal University, Iraq*
12:30-12:50	**Title: Description of the heat capacity of solid phases by a multiparameter family of functions (MPFF)** **Valery P. Vassiliev,** *Lomonosov Moscow State University, Russia*
12:50-13:10	**Title: The evolution of the Zener factor and the isotropy of triple periodic minimal surface structures** **Ramon Miralbes Buil,** *University of Zaragoza, Spain*
13:10-13:25	**Title: Development of GTE turbine air-cooling system to increase its operating parameters** **Ivan Malinovskiy,** *Moscow Aviation Institute, Russia*

Lunch Break 13:25-13:55

Keynote Talk 13:55-14:20	**Title: Advanced biocarbons and their lightweight sustainable green composite materials: A path forward to circular bioeconomy** **Manju Misra,** *University of Guelph, Canada*
14:20-14:40	**Title: Refractory carbides at the temperatures up to 5000K** **Alexander Ivanovich Savvatimskiy,** *Russian Academy of Sciences, Russia*
14:40-15:00	**Title: Virus resonance inactivation using non-ionizing radiation in the microwave regime** **Refael Minnes,** *Ariel University, Israel*
15:00-15:20	**Title: Electromagnetic methods for improved production of additive manufacturing materials** **Imants Kaldre,** *University of Latvia, Latvia*
15:20-15:40	**Title: SERS combined with chemometric analysis for detection and identification of microorganisms: Viruses and bacteria** **Agnieszka Michota-Kamińska,** *Polish Academy of Sciences, Poland*
15:40-16:00	**Title: Optimisation for ultralight and high-stiffness hierarchical structures with tailored lattice metamaterials** **Nan Li,** *Imperial College London, United Kingdom*
16:00-16:20	**Title: *In-situ* formation of Al-Cu based alloy foams** **Ignacio A. Figueroa,** *National Autonomous University of Mexico, Mexico*
16:20-16:40	**Title: Impact of urbanization and development activities on carbon sink and CO_2 mitigating capacity of rubber plantation in Kerala, India** **K. K Ambily,** *Rubber Research Institute of India, India*
16:40-17:00	**Title: Optimum stimulation period for pulse thermography** **Antonio Ramos Silva,** *Porto University, Portugal*

Panel Discussion

End of Day 3

KEYNOTE PRESENTATIONS

DAY 1

PEERS ALLEY MEDIA

Virtual Event

3rd Advanced Materials Science World Congress

March 21-23, 2022

BIOGRAPHY

Dongmin Yang is a Senior Lecturer in Composite Materials at the University of Edinburgh. His current research interests focus on Composites Engineering (materials, manufacturing and structures) and Computational Engineering (multiscale, multiphysics, multiphase coupling). With a background in manufacturing and later experience in structural and materials engineering, his cross-disciplinary research is at the interfaces of underpinning material science, emerging manufacturing technologies and advanced structural analysis and design. He also develops computational techniques and deterministic models to address multiscale, multiphysics and multiphase coupling challenges across engineering disciplines.

Dongmin Yang

University of Edinburgh, United Kingdom

Fibre flow in 3D printing of discontinuous fibre reinforced thermoplastic composites

X-ray micro-tomography (μCT) scans and a coupled multiphase model based on computational fluid dynamics (CFD) and discrete element method (DEM) are used to investigate the fibre flow inside the printer nozzle during 3D printing of short fibre reinforced thermoplastic composites by fused filament fabrication (FFF). Short carbon fibre T300 reinforced nylon-6 composite is selected as the printing material. X-ray CT is performed on the raw filament, in-nozzle melted filament, extruded printing bead and on-bed printing bead to trace the through-process evolution of fibres and voids for the specific nozzle used therein. Qualitative visualisation of voids fraction and fibre orientation, length and fraction, as well as quantitative analysis are carried out using image processing techniques. The results show that the orientation and volume fraction of fibres vary with different internal geometry of the nozzle and fibre misalignment occurs in the on-bed printing bead because of the relative motion between the nozzle and the print bed disturbs the flow field. Also, the fibre length decreases slightly during the printing process due to the collision between fibre and nozzle wall when the melted materials pass the nozzle. Most voids are generated when the melted filament is extruded from the nozzle, and porosity decreases in the on-bed printing bead. In addition, a coupled CFD-DEM is developed, in which the collisions between fibres are considered naturally in DEM by using the Hertz-Mindlin contact law. Once validated against X-ray microtomography (uCT) experimental results, a parametric study is performed using the CFD-DEM model to investigate various fibre lengths, fibre volume fraction and resin viscosity. It shows that the nozzle clogging tends to occur when the fibre length and/or the fibre volume fraction are increased. The use of a polymer matrix with lower viscosity can be effective to eliminate the clogging issue when printing composites with relatively short fibres. The fibre length is dominating when long fibres are used and the clogging is largely independent of the viscosity of the polymer matrix. Finally, a potential solution of using a cone sleeve insert located above the shrinking region to address the nozzle clogging issue is proposed and numerically assessed.

BIOGRAPHY

Francesca Micheletti is a Geologist, PhD Researcher in Petrology and Petrography. Since 2001 she is working at the Earth Sciences and Geo-environmental Department of the "Aldo Moro" University in Bari (Southern Italy). Her research activity focus on: Petrological evolution of the Variscan continental crust, modelling of the chemical composition of the continental crust, geochemical behavior of chemical elements in increasing metamorphic grade in metapelites , study of distribution and behavior of trace and REE elements in zircon, garnet, pyroxene, feldspar and apatite by LA-ICP-MS, neoproterozoic-Cambrian acidic and mafic magmatism, U-Pb geochronology on zircon crystals: a) separation of heavy minerals using high density liquids, b) image analysis (BSE, CL and VPSE detectors) and c) spot dating by SIMS and LA-ICP-MS, detrital zircons dating and paleogeographic reconstructions, evaluation of quartz sandstones for industrial applications, petro-archaeometry. Teaching activity at Bari University in Geological and Natural Sciences courses for past fifteen years.

F. Micheletti
University of Bari Aldo Moro, Italy

A current investigation into zircon uses in geosciences: Case studies from Southern Italy mountain ranges

The study of the zircon involves materials scientists and geoscientists from sub-disciplines including stable and radiogenic isotope geochemistry, sedimentology, igneous and metamorphic petrology, trace element geochemistry and experimental mineralogy.

Over the past thirty years, the more instrumental techniques and analytical procedures have advanced, the more zircon has increased its central role in Earth and Planetary Sciences. First ID-TIMS and then other micro-beam techniques such as SIMS, LA-ICP-MS and SHRIMP have made it possible to resolve the chronology of Earth's geological events from the oldest to the most recent. Besides, highly detailed image analysis of zircon zoning first obtained through SEM (CL and VPSE detectors) is essential to identify specific geological events (magmatic and metamorphic growth) by discerning significant clusters of isotopic age data.

In geosciences, the power of zircon isotopic dating finds its greatest application in reconstructing the evolution of mountain ranges and, in the last fifteen years, issues pertaining to the evolution of the major ranges in Southern Italy (Apennine Chain and the Calabria-Peloritani Orogen), have begun to be clarified thanks to zircon geochronology and its geochemistry.

Accordingly, U-Pb spot ages on detrital zircons from turbiditic successions have helped to tighten the timing of tectono-sedimentary stages during Apennine orogeny and constrain the detrital sources (Fornelli et al., 2021 and references therein). In light of these recently acquired geochronological data, new paleogeographic scenarios can be envisaged for the setting of sedimentary basins during Apennine tectonics.

On the other hand, U–Pb data on zircon from metaigneous and metasedimentary rocks have contributed to understand the peri-Gondwanan evolution from Late-Proterozoic to Paleozoic of the Calabria-Peloritani Orogen, a key sector of the Southern Variscan Belt (Fornelli et al. 2020 and references therein), thanks to the ability of zircon to preserve memory of former detrital, igneous and metamorphic events thought amphibolite-granulite facies Paleozoic metamorphism.

BIOGRAPHY

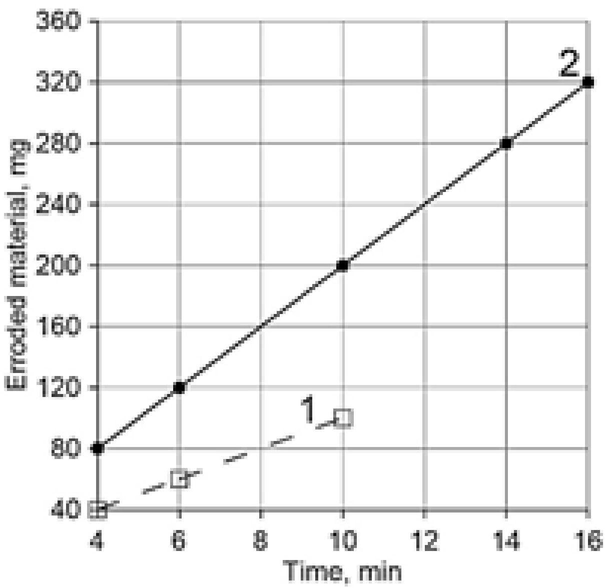
Nikolay Pokhilenko born October 7, 1946 in Siberia, Russia. Graduated in 1970 from Novosibirsk State University (MSc in Geology) and began working at the Institute of Geology and Geophysics of the Siberian Branch (SB) of the USSR Academy of Sciences: Research Engineer; 1973 – Junior Researcher; 1977 – Senior Researcher; 1985 – Head of Diamond Laboratory. In 2006 – Deputy Director and 2007 – 2017 – Director of the Sobolev Institute of Geology and Mineralogy of the SB of the RAS; 2013 - till now – Vice-Chairman (Earth Sciences) of the SB of the RAS; 2017 – till now Scientific Director of the Sobolev Institute of Geology and Mineralogy, SB of the RUS. N.P. Pokilenko worked ~1.5 years at Geophysical Laboratory, Carnegie Institution of Washington, DC; and being an experienced field geologist he also worked during 41 field seasons in Arctic areas of Siberia (28 - in 1969-2012) and Northern Canada (13 in 1994-2006).

Nikolay Pokhilenko

[1]Russian Academy of Sciences, Russia [2]Novosibirsk State University, Russia

Impact diamonds of Popigai Crater, Siberia: A new advanced natural nanopolycrystalline material

The Popigai Crater about 100 km in size was formed ~36 my ago as a result of impact of asteroid ~4-6 km in size with the Earth in Northern Siberia. The target was Archean crystalline rocks of the North-Eastern part of the Anabar Shield enriched in graphite. Graphite at the edge of the crater was transformed during the impact event (P ~ 120-150 GPa and T ~ 3000-4000°C at the epicenter) into nanopolycrystalline material composed by variable amounts of the cubic diamond and hexagonal diamond (lonsdaleite)



with the crystallite sizes ~ 30-70 nm. Potential resources of impact diamonds in the Popigai Crater are huge and are measured by trillions of carats. The technological characteristics of impact diamond are very impressive and significantly better those for synthetic diamonds: 1) 2-2.5 times higher processing speed of superhard materials (abrasive ability); 2) 2-3 times higher wear resistance; 3) 200-250°C higher heat resistance (thermal stability); 4) their specific surface is 0.7-0.8 m2/g, which is 8-9 times higher than that for synthetic diamonds, which contributes to good retention of impact diamonds when compacted with various binders. These characteristics determine high efficiency of use of the impact diamonds in wide range of modern technologies where existing characteristics of synthetic and convectional natural diamonds are insufficient. So, the basic principle of use of impact diamonds is replacement of synthetic and conventional natural diamonds in appropriate technologies with maximum technological and economic benefits.

SCIENTIFIC ABSTRACTS

DAY 1

PEERS ALLEY MEDIA

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Supercoiling artificial muscles

G.M. Spinks
University of Wollongong, Australia

This talk describes a new mechanism for generating large contraction strains caused by swelling of pre-twisted fibres and yarns and is based on our recently published article. The swelling generates torsional strain energy that is released by converting twist to writhe and leading to the formation of loops or 'supercoils' along the fibre length. The same process occurs naturally in double stranded DNA and is partially responsible for the packing of the long DNA molecules into chromosomes. Supercoiling is a common everyday experience that occurs by adding twist to fibres, ropes, cables etc. and produces irritating tangles. However, our study is the first to demonstrate supercoiling without any addition of twist.

The supercoiling muscles utilised helically oriented filaments embedded in a swellable matrix. Best results were obtained by using polyester sewing thread and crosslinked poly(acrylic acid) (PAA). Two sewing threads were embedded with PAA solution, plied together and heat treated to dry and crosslink the PAA using a diamine crosslinker. Immersion of the samples in acid and base solutions caused increasing swelling of the PAA matrix, which was resisted by the polyester filaments. The helical arrangement of the polyester filaments directed the swelling towards a partial untwist. However, if the sample ends were held to prevent rotation but still allow translation, then the swelling caused supercoiling with concomitant reduction in the end-to-end sample length. The amount of contraction strain was strongly influenced by the applied tension because the number of supercoil loops and their diameter depends on the applied stress. Samples that were over-twisted to form coils before crosslinking the PAA were able to generate 'coiled coils' on swelling. These samples showed an unusual combination of both high stroke (70%) and high work capacity (1 J/g) which exceeds the performance of natural muscle by more than 35 times.

Biography

Geoff Spinks received his PhD from the University of Melbourne in 1990 for his work on the mechanical behaviour of polymers and he has maintained a research interest in this area specialising in mechanical actuator materials (artificial muscles). He is currently Senior Professor in the Australian Institute for Innovative Materials and Director of UOW Makerspace. He has worked closely with industry including sabbatical leave with BHP Research and Allied Signal Inc. (USA). His current research includes new product development (such as medical devices and prosthetics) and new manufacturing methods (such as 3D printing) that utilise his artificial muscle materials.

Graphene derivative and metal nanoparticles coated silk fabrics with durable, multifunctional properties for numerous potential applications

Shovon Bhattacharjee, C Raina Macintyre, Prateek Bahl, Uttam Kumar, Xinyue Wen, Abrar Ahmad Chughtai and **Rakesh Joshi**

UNSW Sydney, Australia

In recent times graphene-coated natural fabrics have drawn massive attention due to their unique multifunctional activities. The incorporation of metal nanoparticles (NPs) on top of graphene could boost its properties further because of the synergistic impact of graphene and NPs. Herein, we fabricated reduced graphene oxide (RGO) and Ag/Cu-NPs coated silk (s) fabrics using a simple 'dip and dry, technique and 3-glycidyloxypropyl trimethoxy silane crosslinking agent (CA). Graphene oxide (GO) and NPs were coated onto the silane treated natural silk fabrics, followed by chemical reduction and vacuum heat treatment. The fabricated fabrics showed electrical conductivity, UV-radiation protectivity, self-cleaning activity, electrothermal property, and thermal stability. RGO and Cu-NPs coated samples (S-CA-RGO-Cu) showed better performance than RGO and Ag-NPs coated samples (S-CA-RGO-Ag). Due to the low surface resistance (3.15 kΩ sq−1) S-CA-RGO-Cu, showed excellent Joule heating capacity. Both S-CA-RGO-Ag and S-CA-RGO-Cu showed ~99% inhibition of the E. coli and P. aeruginosa (Gram-negative bacteria) and ~78–99% inhibition of S. aureus (Gram-positive bacteria). HEK293 cell viability >70% indicated good biocompatibility of the fabricated samples. Moreover, the fabrics showed high washing durability by retaining their low surface resistance and good antimicrobial activity even after washing 20 times. The washing durability proves high bonding strength among silk, graphene derivatives, and NPs. The diverse durable functionalities of the fabricated fabrics have made them suitable for numerous potential applications, including personal protective equipment (PPE), protective clothing, wearable smart textiles, motion sensing, sports clothing, and the Internet of Things.

Biography

Shovon Bhattacharjee is a Scientia Ph.D. scholar in the Biosecurity Program, The Kirby Institute, UNSW Sydney, Australia. His Ph.D. research focuses on developing multifunctional next-generation fabrics for PPE development (especially face masks). He is a faculty member in the Department of Applied Chemistry and Chemical Engineering, Noakhali Science and Technology University, Bangladesh. His research interest is exploiting nanomaterials (graphene, nanoparticles, polymers) for public health safety.

Defect induction in crystals by glass crystallization method and its application for photonics

K. Shinozaki[1,2]

[1]National Institute of Advanced Industrial Science and Technology, Japan

[2]JST Presto, Japan

Numerous studies have addressed the excellent properties of Ce-doped YAG crystals for utilization in lighting applications. However, the differences in the photoluminescence and defect formation of YAG crystals obtained by different methods have not been elucidated. In this study, the effects of the crystallization path of YAG: Ce on the local structure of its emission site and defect formation were investigated. Ce-doped YAG crystal were prepared in three ways: (1) solid-state reaction, (2) heat-treatment of YAG glass, and (3) crystallization from a supercooled YAG melt by a controlled cooling process with deep supercooling state. A shift in the photoluminescence peak of 3 nm and a significant enhancement in the thermoluminescence was observed in the sample obtained by the crystallization of a supercooled melt. As the intensity of thermoluminescence has been associated with the defects formed, positron annihilation lifetime spectroscopy was performed to investigate the defects. All crystallized samples exhibited two components of positron lifetime, and both these components increased in the sample.

Biography

Kenji Shinozaki received a Ph.D. in Engineering at Nagaoka University of Technology in 2013. He was a Research Fellowships for Young Scientists of Japan Society for the Promotion of Science (JSPS) in 2013, and he worked as an Assistant Professor at Nagaoka University of Technology from 2013 to 2016. Since 2016, he has worked at National Institute of Advanced Science and Technology (AIST) as a senior researcher. His current research interest includes materials science and fabrication processing of glasses and glass-ceramics for optical and photonic applications.

High curie temperature ferroelectrics

S. Kojima
University of Tsukuba, Japan

High Curie temperatures of ferroic materials such as ferroelectrics, ferromagnetics, and ferroelastics have attracted much attention, while their physical origins are not yet clarified. The year 2020 marks hundred years since the discovery of the phenomenon of ferroelectricity. Ferroelectrics have a rich of functionality such as piezoelectric, electro-optic, nonlinear optic, electrocaloric, energy storage, pyroelectric properties. Ferroelectric materials with high Curie temperatures, TC, and tuning of the TC over a large temperature range are very important for the fundamental sciences and engineering. This paper reviews the various types of high-temperature ferroelectrics with perovskite, bismuth layered, tungsten bronze, and perovskite slab structures, especially $Sr_2Nb_2O_7$ with TC = 1342°C and its family. The superior tunability of the TC is achieved by the substitution of cations in the A- and B-sites of perovskite-like structures. The origin of ferroelectricity with high TC is discussed.

Biography

S. Kojima studied at Department of Physics, Faculty of Science, University of Tokyo, Japan, receiving Bachelor of Science in 1974 and Doctor of Science in 1979. He was promoted to the position of full professor at University of Tsukuba, Japan, and worked as the chair of Institute of Materials Science, University of Tsukuba from 2011 to 2015. He continues his research and teaching as professor emeritus of University Tsukuba. Throughout his carrier, he has been a member of editorial boards for these professional magazins, Ferroelectrics, Materials, Current Applied Physics, Japanese Journal of Applied Physics. He was the chairman of the organizing committee of the 8th Russia/CIS/Baltic/Japan Symposium on Ferroelectrics, Tsukuba, 2006 and the 53th Ultrasonic Electronics Symposium, Tokyo, 2014.

Compact measurement of the optical power in high-power LED using a light-absorbent thermal sensor

Jae-Young Joo[1], **Youyoung Kim**[2] and **Sun-Kyu Lee**[2]
[1]*Korea Photonics Technology Institute, South Korea*
[2]*Gwangju Institute of Science and Technology, South Korea*

LED (Light-Emitting Diode) presents advantages such as luminescence, reliability, durability compared with conventional lighting. It has been widely applied for life, healthcare, smart farm, industry, and lighting from indoor to the automotive headlamp. However, the LED is vulnerable to thermal damage originated from the high junction temperature, especially in high power applications. Hence, it requires precise qualification on the optical power and the junction temperature from the pilot line to secure reliability. In this study, the photo-thermal sensor is pro-posed by employing a sheet-type thermocouple composed of photo-absorbent metal film and thermocouple. This sensor aims low-cost qualification in pilot line for high-power luminous devices and optical monitoring of costly luminaire such as automobile LED headlamp. The sensor is designed to detect the increased temperature response of LED hot spots from the transferred thermal power and absorbed optical power. The temperature response of each sheet-type thermocouple is utilized as a signal output of the absorbed optical

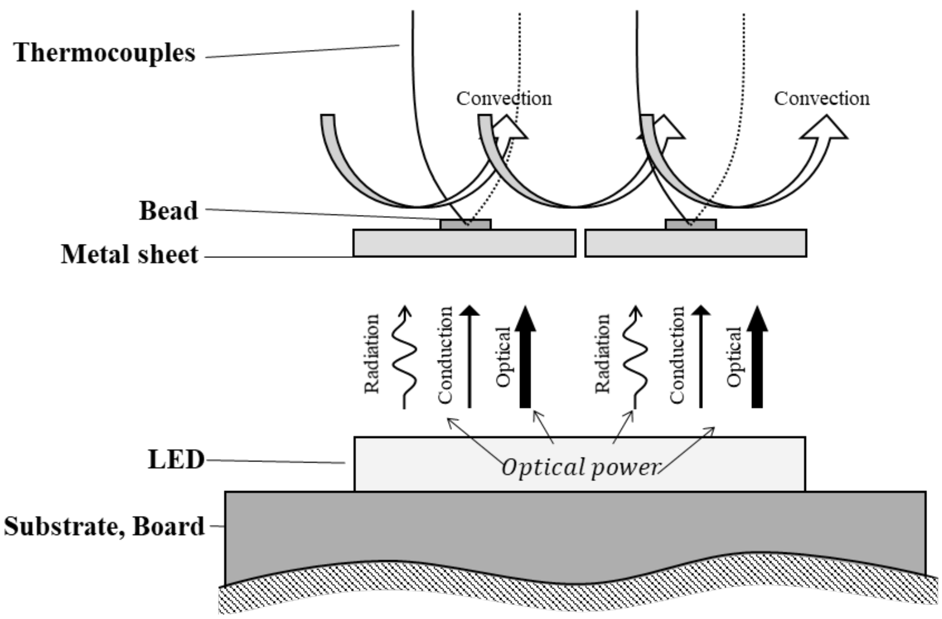

Figure 1. Schematics of photo-thermal sensor

power and hot spot temperature based on the introduced sensor equation. The proposed thermal sensor is evaluated by comparing the experiment with the measured reference value from the integrating sphere and the attached thermocouple at a junction. The experiment result reveals 3% of the maximum error for the optical power of 645 mW.

Biography

Jaeyoung Joo received B.S degree mechanical engineering from the Yeungnam University, Daegu, South Korea, the M.S. and Ph.D. degree in Mechanical Engineering from the Gwangju Institute of Science and Technology, Gwangju, South Korea. He is a senior research engineering with the Korea Photonics Technology Institute in Gwangju, South Korea, where he is engaged in advanced LED lighting technology and integrated optical system for monitoring and sensing applications in industrial fields. His research interests include the micro LED light source and display technology, developing integrated system for lighting control with optical sensor linked to automatic shade, curing technology for silicone encapsulant for LED.

Advanced graphene aerogel embedded phase change materials (PCMs) for energy harvesting

Chengbin Yu[1] and **Young Seok Song**[2]
[1]*Seoul National University, South Korea*
[2]*Dankook University, South Korea*

Phase change material (PCM) has been attracted to the thermal energy storage (TES) application due to the high latent heat, chemical stability, and high thermal density. Pure PCM is never utilized directly when occurs leakage problem during phase transition process. Supporting materials such as shell material, and porous aerogels can restrict the mobility of PCM upon melting and cooling. Thus, form-stable PCM composite is fabricated and still sustain the intrinsic solid state under the change of external temperature. These supporting materials stop PCM from occurring the leakage problem that the PCM composite can absorb or release a large amount of heat effectively. Comparing with shell material, aerogels can hold plenty of pure PCM because of high porosity. High weight percentage of pure PCM has an excellent TES ability during the phase transition process and even increases the efficiency of thermo-electric energy harvesting. However, the capillary force brings to the volume shrinkage of supporting material while infiltrating pure PCM into the porous internal structure. This volume shrinkage causes some weight loss of pure PCM and even decrease the efficiency of thermo-electric energy harvesting. Hence, the supporting material with high mechanical property and flexibility is vital to reduce the volume shrinkage. In this work, graphene aerogel is selected as a supporting material, and polydimenthylsiloxane (PDMS) is embedded to the graphene aerogel by solution spray treatment. The PDMS/n-Hexane solution is sprayed into the graphene aerogel and after n-Hexane is evaporated, the PDMS- embedded graphene aerogel is fabricated completely. Consider the mechanical requirement of PCM composite, cross-linked graphene aerogel is synthesized by using cysteamine vapor method, and graphene/cysteamine aerogel (GCA) is utilized as an advanced supporting material. These modified graphene aerogel can reduce the volume shrinkage, and PCM composites show high efficiency of thermo-electric energy harvesting.

Biography

Chengbin Yu completed his Bachelor's Degree in Polymer Science and Engineering from Beijing University of Chemical Technology (BUCT). He done PhD in Material Science and Engineering from Seoul National University (SNU). Currently he is working as a Researcher at Seoul National University.

Design and preparation of full-spectrum solar light responsive photocatalysts for hydrogen generation

Junying Zhang
Beihang University, China

Solar-light photocatalytic water-splitting for hydrogen generation is an ideal way to generate clean energy. Because most photocatalysts can only work under ultraviolet (UV) and short-wavelength visible (Vis) lights irradiation, preparation of photocatalysts that can absorb long-wavelength Vis and near-infrared (NIR) lights are of vital importance. Elements doping and morphologies tuning were used to improve the photocatalytic hydrogen generation of some typical semiconductors, taking g-C_3N_4, $La_2Ti_2O_7$ and $ZnIn_2S_4$ as examples. Photo-sensitizers including black phosphorous (BP) nanosheets and quantum dots, Au nanoparticles and nanorods, and oxygen-deficient WO_3 were composed with photocatalytic semiconductors to obtain binary or ternary photocatalysts. A serial of photocatalysts such as WO_{3-x}/CdS, Au-$La_2Ti_2O_7$, BP-Au-CdS and BP-CdS-$La_2Ti_2O_7$ that can work efficiently under UV-Vis-NIR light for hydrogen generation have been prepared. First-principles calculation and experimental characterization have been jointly employed to investigate the interface structure, clarify the photo-generated electron and holes transfer procedure, and confirm the key influence factors to the photocatalytic activity.

Biography

Junying Zhang is a full professor in school of Physics, Beihang University, China. Her research interests focus on first-principles calculations and structure-properties relationship of materials for clean energy conversion and storage. Her publications have been cited over 5,900 times with h-index of 41 according to Web of Science. He has been awarded the honours of Excellent Graduate of Tsinghua University, Beijing Nova of Science and technology, New Century Excellent Talents in University of the Ministry of Education of China, Beihang Blue Sky Scholar, and the second prize for Natural Sciences Awards of the Ministry of Education of China.

Immunomodulating biomaterials

Weiwei Wang, Zujian Feng, Pingsheng Huang and **Chuangnian Zhang**
Peking Union Medical College, China

The immune system is quite related to various major diseases including cancer, cardiovascular diseases, and tissue defect. Here we propose that immunomodulating biomaterials can improve the treatment of major diseases by activating immune cells such as dendritic cells (DCs) and macrophages directly *in vivo*. Specially, self-assembled peptide hydrogels were prepared to deliver tumor antigens and TLR agonists. It was demonstrated that the use of hydrogels could significantly increase the uptake of antigens by DCs, thereby facilitating the maturation of DCs and antigen presentation to naive T cells, which elicited antitumor T-cell responses. In combination with immune checkpoint blockade, the immunotherapy efficiency against melanoma could be further augmented. Besides, we found that immunogenic chemotherapy by nanomedicine could induce the immunogenic death of cancer cells and the release of endogenous tumor antigens, which enhanced the recognition of cancer cells by effector T-cells, amplifying the antitumor T-cell immunity. On the other hand, bioinspired glycopeptide hydrogels were fabricated to serve as artificial extracellular matrix (ECM) for tissue repair and regeneration. It was found that in salt solution, glucomannan-Q11 peptide could self-assemble into nanofiber hydrogels with 3D network structure. Significantly, this glycopeptide hydrogel notably polarized bone marrow derived macrophage (BMDM) into M2-type through mannose receptor (MR)-induced ERK/STAT6 signaling pathway. In mice with full-thickness cutaneous defects, the injection of glycopeptide hydrogel tremendously modulated the macrophages recruited in the wound microenvironment into anti-inflammatory M2 macrophages, which greatly accelerated the wound healing. Moreover, the development of antibacterial hydrogel enabled the complete eradication of methicillin-resistant staphylococcus aureus at the wound, thus, further reducing the inflammatory level. Our works clearly demonstrated that the development of immunomodulating biomaterials plays significant role in controlling the immune response for cancer treatment and tissue regeneration. Immunomodulation represents an advanced approach for the treatment of major diseases.

Biography

Weiwei Wang is a professor at the Institute of Biomedical Engineering, Chinese Academy of Medical Science & Peking Union Medical College (CAMS&PUMC). Wang is also the PI of team for "Immunomodulating biomaterials and tissue regeneration". He received his bachelor's degree at Northeastern University in chemistry, his Ph.D. at Tianjin University in chemical engineering and conducted his postdoctoral research at PUMC. He focuses on polymeric biomaterials for immunomodulation and tissue repair and regeneration. He received several awards from IAAM, Tianjin government, Tianjin Association of Science and Technology and PUMC. He is also a membership in Chinese Society for Biomaterials, China Association for Science and Technology, Chinese Society of Biomedical Engineering and Tianjin Society of Biomedical Engineering.

High-scattering porous polymer structures and their applications

Shudong Yu[1,2]
[1]South China University of Technology, China
[2]The Hong Kong Polytechnic University, China

High-scattering media have been widely used in numerous scenarios, including optoelectronic devices, daytime passive radiative cooling, wall paintings and so on. It is well noted that TiO_2-nanoparticles-based nanocomposite is the most common recipe for high scattering media by virtue of the high refractive index of TiO_2 (~2.6). Recent development has shown that porous polymer structures have the potential to serve as excellent alternatives to conventional TiO_2 nanoparticles. However, the intrinsic low refractive index of polymers (~1.5) leads to the insignificant scattering efficiency of porous polymer structures, thereby hindering their further applications. To solve this challenging issue, our group has conducted several works to fabricate high-scattering porous polymer structures by taking inspiration from nature (e.g., Cyphochilus). In this talk, I am going to present the recent progress of our group on the fabrication of high-scattering porous polymer structures and their applications. In detail, several facile and industrially available techniques including supercritical CO_2 microcellular foaming and polymerization-induced phase separation are adopted to enable the ultimate fabrication. By well tailoring the fabrication parameters, porous polymer structures with brilliant whiteness can be achieved, which have been successfully applied onto light-emitting diodes and quantum dots films for light enhancement and daytime passive radiative cooling. In addition, we also fabricate optical diffusers with combined high-transmittance and high-haze by utilizing post encapsulation techniques. Overall, porous polymer structures are strong candidates as efficient scatterers due to their abundance and facile and cost-effective fabrication.

Biography

Shudong Yu received his Ph.D. degree from the South China University of Technology, China in 2019 (supervisor: Prof. Yong Tang). He has spent 1.5 years at the Karlsruhe Institute of Technology, Germany as a visiting scholar from 2017 to 2019 (supervisor: Prof. Uli Lemmer). Currently, he is a postdoctoral fellow at both South China University of Technology and Hong Kong Polytechnic University (supervisors: Prof. Yong Tang and Dr. Dahua Shou). He has received several prestigious awards including Hiwin award for outstanding doctoral dissertation and the 1st prize of science and technology award in Guandong. His current research interests include light management, biomimetics and energy harvesting.

Oxidizable electrode induced bipolar resistive switching behavior in TE/CdZnTe/Pt structure

A. Wang, J. Zhang, G. Zha, L. Xu and **W. Jie**
Northwestern Polytechnical University, China

The resistive switching behavior of CdZnTe film was reported by our group, but the reason for resistive switching behavior is still obscured. The top electrode (TE) has a great effect on resistive switching behaviors, especially on the generation of the resistive switching, the ON/OFF ratio, the retention time and the voltage parameter distribution. This could be explained by different conduction mechanisms in RRAM including phase change effect (PCM), electrochemical metallization effect (ECM), valence change effect (VCM) and polarization-induced charge transfer. TE/CdZnTe/Pt/Ti/SiO_2/Si structures (top electrode TE = Au, Pt, Al, Ti and Cu) were fabricated by magnetron sputtering and thermal evaporation. Bipolar resistive switching behavior was observed in TE/CdZnTe/Pt/Ti/SiO2/Si structure when TE is Al, Ti or Cu, but Pt or Au as TE in TE/CdZnTe/Pt device showed no resistive switching. The interfacial layer (AlOx, TiOx, CuOx)-dominated model was proposed to explain the presence of resistive switching behavior in TE/CdZnTe/Pt device due to oxidizable electrodes. The role of the CdZnTe film is a series resistor after the forming process. Space charge-limited current (SCLC) model was used to analyze the conduction mechanism and ~1019 cm^{-3} trap density in the interfacial layer was calculated by fitting the current-voltage curve. The device properties including voltage parameter distribution, retention property and endurance property were tested, respectively. The Al/CdZnTe/Pt/Ti/SiO_2/Si structure has a good potential as resistive switching random access memory with over 103 ON/OFF ratio and at least 103s retention time. The comparison including switching type, switching mechanism, cycling numbers, retention time and ON/OFF ratio for different chalcogenide materials as resistive switching layer.

Biography

Aoqiu Wang received bachelor degree in the major of material science and engineering from Northwestern Polytechnical University in 2014. She started to the research on CdZnTe film from year 2015 as a master. In year 2016, she became a doctor and her research interest extends to chalcogenides film, especially, the potential of chalcogenides material in RRAM fields. Now, she has investigated the resistive switching mechanism of CdZnTe, ZnSe, ZnTe and ZnS materials. The related publications are under arrangement.

Advances in gallium nitride metalenses

Vin-Cent Su[1] and **Meng-Hsin Chen**[2]
[1]National United University, Taiwan
[2]Atomic Energy Council, Taiwan

The rapid development of optical metasurfaces has been driven by the desire for the miniaturization of optical devices. Also, the metasurfaces realize the novel optical phenomena that are unattainable from conventional bulky and heavy optics. However, the first proposed and studied metasurfaces made of metal nano-antennas severely limit their applications because of low transmission efficiency and weak-cross polarization conversion. Thus, the all- dielectric metasurfaces have rapidly received much attraction, propelled by innovation from many groups around the world.

As one of the most tremendous applications of the metasurfaces, metalenses have rapidly attracted much attention. However, highly efficient metalenses at visible wavelengths require the development of high-aspect-ratio dielectric nanostructures. Various dielectric nano- resonators have been proposed as sub-wavelength constituents for the construction of the visible metalenses. These dielectric nano-resonators can be classified according to different shapes and materials. This talk will present various dielectric materials and different kinds of nano-resonators. Then we will focus on a third-generation semiconductor named as Gallium nitride (GaN) combined with a newly developed hexagon-resonated element (HRE) to achieve metalenses of high performance in the visible. Also, well-developed fabrication techniques have been employed to realize the high-aspect-ratio metalenses working at three distinct visible wavelengths with diffraction-limited focusing efficiencies as high as 93%. The 1951 United States Air Force (USAF) test chart has been chosen to characterize the imaging capability. All of the images formed by the polarization-insensitive metalens show exceptional clear line features, and the smallest resolvable features are lines with widths of 870 nm.

Biography

Vin-Cent Su received his Ph.D. degree from the Graduate Institute of Electrical Engineering, National Taiwan University in 2013. He is currently an Associate Professor of Electrical Engineering Department, National United University. His current research interests include metasurfaces and their applications, light-emitting diodes (LEDs), optoelectronics, high-electron-mobility transistors(HEMTs) and biomedicine.

Failure analysis of DSS 2205 GTA welds and evaluation of the cooling rate effects on localized corrosion with mini-electrochemical cell

Li Yuan Hu, Kuang Hua Hou and **Yi Ching Shih**
Chang Gung University, Taiwan

Duplex stainless steel 2205 is widely used in various applications, especially in petrochemical industry, owing to its resistance to chloride stress corrosion cracking. However, during manufacturing processes, the 50:50 ratio of austenite and ferrite phase is often disturbed by welding, which often leads to the deterioration of corrosion resistance in the heat affected zone (HAZ). In this study, a real world localized corrosion failure of DSS 2205 welds is illustrated, and welding experiments were conducted in the attempt to prevent such failure. The results of failure analysis indicate that the localized corrosion took place in the HAZ immediately adjacent to the fusion boundary and was caused by the welding of two components with different thickness. The higher cooling rate of the thicker component leads to the formation of austenite-depleted-zone, thus lowering the corrosion resistance of the HAZ. Hence, a multipass GTA welding experiment of DSS 2205 was carried out with different cooling conditions to evaluate the effects of cooling rate on localized corrosion resistance and resultant mechanical properties. Slower and faster cooling rates were achieved by a 300°C preheating and water cooling of the base metal, respectively. A mini-electrochemical cell and potentiodynamic polarization were used to evaluate the corrosion resistance of the HAZ. Results show that the water-cooled HAZ demonstrates a more noticeable austenite-depleted-zone, which results in higher passive current and lower Ecorr value. On the other hand, preheating significantly enhances the formation of grain boundary austenite, Widmanstätten austenite, intragranular austenite and partially transformed austenite, thus increases the corrosion resistance. Although preheating is beneficial to the resistance to localized corrosion, DSS 2205 is also sensitive to 475°C embrittlement. Considering that only the inner surface of the weld is exposed to corrosive environment in real world applications, preheating is recommended only for the first welding pass.

Biography

Li Yuan Hu is a Ph.D. student, currently studying in the mechanical engineering department in Chang Gung University, Taiwan. His major involves welding metallurgy, failure analysis and corrosion prevention of metallic materials. For the first few years of his Ph.D. study, he followed his advisor and played important roles in many industrial collaborations. Recently he starts to focus on various electrochemical testing techniques. By comparing or combining electrochemical testing with some existing corrosion testing methods, and applying them on several metallic materials, he is hoping to gather some interesting results and might be able to expand the industrial applications of electrochemical testing.

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Metalla-ynes and poly(metallayne)s: Synthesis, charaterization and opto-electronic applications

R. A. Al Balushi[1], **A. Haque**[2] and **M. S. Khan**[3]
[1]*A'Sharqiyah University, Oman*
[2]*University of Hail, Saudi Arabia*
[3]*Sultan Qaboos University, Oman*

Metalla-ynes and Poly(metallayne)s have emerged as a new class of materials for opto-electronic (O-E) applications. These metal-based complexes and polymers have potential applications in photovoltaics, light-emitting diodes (LEDs), photo-switch and sensors. These materials are of particular interest due to their extended π-electron conjugation along the complex backbone. Besides, these materials can be produced over flexible substrates covering large areas and their photo-physical properties can be tuned by smart variation of the spacer groups. It was found that the luminescence in the pure organic complexes is restricted to fluorescent emissions as the electronic transitions only occur between singlet states in the molecules while the incorporation of a heavy metal allows accessing the triplet states. The inclusion of a heavy metal like Pt(II) along the polymer backbone imparted large spin-orbit coupling to the poly(metallayne) materials to allow light emission from the triplet excited state. The triplet emission is extremely efficient, approaching 100% efficiency at low temperatures, making the Pt(II) poly-ynes good model systems to study the triplet excited state. The introduction of a second d- or f-block metal fragment in the main chain or side chain of Pt(II) polymers has been found to further modulate the underlying properties of the mixed metalla-ynes and poly-ynes.

Here in, I will focus on the synthesis, spectroscopic characterization and photo-physical properties of metal-based complexes and poly-ynes. The opto-electronic (O-E) applications of these type of materials will be also highlighted and discussed.

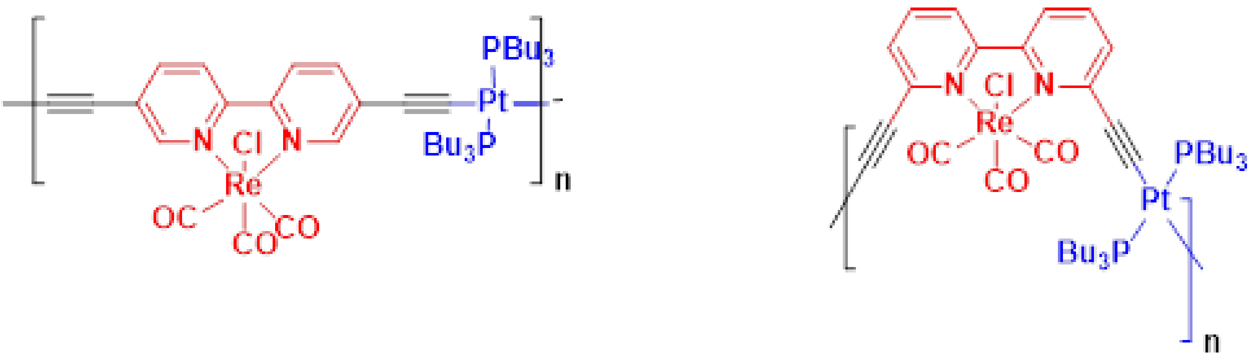

Figure 1 Chemical structures of studied Pt(II) heterobimetallic poly-ynes bearing Cl(CO)3Re(I) as Pendant Sidechain

Without Re(I) pendant		With Re(I) pendant	
Pt(II) complex	**Wavelength (nm)**	**Pt(II) complex**	**Wavelength (nm)**
P1	282, 314, 375, 405	**P3**	346, 450
P2	222, 273, 318, 355, 368	**P4**	390, 405

Table 1 Absorption maxima of meta- (P1 & P3) & para- (P2 & P4) Pt(II) poly-ynes with and without pendant Re(I) moieties measured at room temperature.

Biography

Rayya A. Al-Balushi was born and brought up in A'Sharqiyah, Oman. She received her M.Sc. degree in Chemistry from Sultan Qaboos University (SQU), Oman (2006). She received Ph.D. from the same University in 2016 under the supervision of Professor Muhammad S. Khan and received the Best Ph.D. Thesis award in 2017. She joined ASU as an academic staff in February 2018. She is currently acting as a Head of Department of Basic Science and an Assistant Professor of Chemistry in A'Sharqiyah University (ASU), Oman. Her research interests include designing conjugated polymers for photo-switch, photovoltaic, and LED applications.

Carbon-based materials for energy storage applications

M. Yanilmaz and **E. Abdolrazzaghian**
Istanbul Technical University, Turkey

Considering the serious impacts of climate change caused by greenhouse gases, it is vital to eliminate fossil fuel consumption immediately. Rechargeable batteries have been presented as clean energy storage devices for several applications including but not limited to electric vehicles. It is essential to design high performance electrode materials to reach high energy density and long cycle life in batteries. Carbon nanofibers have been widely studied as energy storage materials in high performance batteries and supercapacitors owing to their high conductivity and good mechanical properties along with tunable morphology. Electrospinning has been commonly employed to fabricate carbon nanofibers. In this study, novel carbon nanofiber-based structures for high performance sodium ion batteries were fabricated via novel, fast and cost-effective technique without applying high voltage. Moreover, several techniques were introduced to modify the morphology and thus improve the performance of carbon nanofiber-based electrode materials. Using sacrificial, low cost polymers; adding highly conductive additives with high surface area; nitrogen doping is some of the techniques used to enhance the electrochemical properties of electrode materials. Besides traditional techniques, binder-free electrodes were also studied. As a result, high specific capacity was observed from carbon nanofiber-based electrodes.

Biography

Meltem Yanilmaz is Associate Professor in Textile Engineering Department in Istanbul Technical University. She got her B.Sc. and M.Sc. degrees in Textile Engineering from Istanbul Technical University. She received her Ph.D degree in Fiber and Polymer Science from North Carolina State University in 2015. Her research interest is on nanofiber production and applications, nanocomposite materials, conductive polymers, electronic applications of nanofibers.

Recent advances resistive metallic hydrogen sensors

N. Kilinc
Inonu University, Turkey

Hydrogen (H_2), as a renewable energy source, has numerous applications such as chemical production, fuel cell technology, rocket engines, fuel for cars etc. The detection of H_2 is so important in safety issue due to the flammable and explosive properties of H_2 gas, in a H_2 source for leak detection, in H_2 production process because of real-time quantitative analysis of production and in determining the human digestive system diseases due to its biomarker properties. H_2 sensors can be divided into seven categories depending on physicochemical detection mechanism and these are catalytic, electrochemical, resistor-based, work function-based, mechanical, optical, and acoustic. We focused on the metallic resistive type H_2 sensor that is a part of a resistor-based H_2 sensor and has many advantages sensor parameters. Palladium (Pd), platinum (Pt), and their alloy are used as sensitive materials for the metallic resistive type H_2 sensor.

Pd, Pt and their alloy in the nanostructure form of nanofilm, nanoporous and nanowire are fabricated by using sputtering, electrochemical deposition and thermal evaporation. The H_2 sensing properties of nanostructured Pd, Pt and their alloy have been investigated depending on temperature and concentration. The sensing mechanism of the nanostructured Pd and Pt resistive H_2 sensors will be discussed in details. In addition, the sensor parameters of the nanostructured Pd and Pt resistive H_2 sensors will be compared. The sensor response of Pd and Pt thin film and the schematic illustration of electrical transport under different conditions at room temperature. Pt thin film shows higher sensitivity and a lower limit of detection than Pd film. However, the advantages of Pd thin film sensor are lower response time and unresponsive to the presence of oxygen compared to Pt thin film.

Biography

Necmettin Kilinc works as an associate professor at Department of Physics, Inonu University, Malatya, Turkey. He received the B.Sc. degree from Marmara University, Istanbul, in 2003, and M.Sc. and Ph.D. degrees from Gebze Technical University in 2006 and in 2012, all in Physics. After his Ph.D., he started to post doc at Optical Microsystems Laboratory Koc University to research cantilever-based biosensors. His research interests are nanotechnology, thin films, metal oxides, metals, organic materials, microfabrication, electrical characterization and bio-chemical sensors.

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Shape memory phenomena and thermomechanical reactions in reversibility of shape memory alloys

O. Adiguzel
Firat University, Turkey

Shape memory effect is a peculiar property exhibited by certain alloy system in the β-phase fields. This phenomenon is initiated by thermal and mechanical treatments, cooling and deformation, and operated by heating and cooling. These alloys have dual characteristics called thermoelasticity and superelasticity, governed by successive thermal and stress induced martensitic transformations, and performed thermally and mechanically, respectively. Thermal induced transformation occurs along with lattice twinning on cooling and ordered parent phase structures turn into twinned martensite structures. Twinned martensite structures turn into detwinned martensite structures by means of stress induced transformation by deforming plastically in martensitic condition. Strain energy is stored in the material with deformation and released upon heating, by recovering the original shape in bulk level, and cycles between original and deformed shapes on heating and cooling, respectively. Superelasticity is also a result of stress induced martensitic transformation and performed in only mechanical manner in the parent austenite phase region. The materials are deformed just over Austenite finish temperature, and shape recovery is performed simultaneously upon releasing the applied stress. The ordered parent phase structures turn into the detwinned structures by means of stress induced martensitic transformation, like the deformation step in shape memory. Superelasticity is performed in non-linear way, unlike normal elastic materials, loading and unloading paths in stress-strain diagram are different, and hysteresis loop reveals energy dissipation. Shape memory effect is performed thermally in a temperature interval depending on the forward and reverse transformation, on cooling and heating, respectively, and this behaviour is called thermoelasticity. Deformation at different temperatures in intermediate region between Martensite start and Austenite finish temperatures exhibits different behaviour beyond shape memory effect and superelasticity, and the materials partially recover original shape. Thermal induced martensitic transformation occurs with the cooperative movement of atoms on {110}-type planes of austenite matrix, by means of shear-like mechanism.

Copper based alloys exhibit this property in metastable β-phase region, which has bcc-based structures. Lattice invariant shears are not uniform in copper-based shape memory alloys, and the ordered parent phase structures martensitically undergo the non-conventional complex layered structures on further cooling. The long-period layered structures can be described by different unit cells as 3R, 9R or 18R depending on the stacking sequences on the close-packed planes of the ordered lattice.

In the present contribution, x-ray diffraction and transmission electron microscopy 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. X-ray diffractograms taken in a long-time interval show that diffraction angles and intensities of diffraction peaks change with the aging time at room temperature. This result refers to a new transformation in diffusive manner.

Biography

Osman Adiguzel graduated from Department of Physics, Ankara University, Turkey in 1974 and received PhD- degree from Dicle University, Diyarbakir-Turkey. He has studied at Surrey University, Guildford, UK, as a post-doctoral research scientist in 1986-1987, and studied on shape memory alloys. He worked as research assistant, 1975-80, at Dicle University and shifted to Firat University, Elazig, Turkey in 1980. He became professor in 1996, and he has already been working as professor. He supervised 5 PhD- theses and 3 M.Sc- theses. He served his directorate of Graduate School of Natural and Applied Sciences, Firat University, in 1999-2004. He received a certificate awarded to him and his experimental group in recognition of significant contribution of 2 patterns to the Powder Diffraction File – Release 2000. The ICDD (International Centre for Diffraction Data) also appreciates cooperation of his group and interest in Powder Diffraction File.

Composite portable shelter system produced by vacuum bagging using recycled reinforcement and matrix materials

A. Genç[1] and **O. Altay**[2]
[1]Calık Denim, Turkey
[2]Tila Composite Representation Domestic and Foreign Trade. Ltd, Turkey

Composite materials, which are increasingly used in many sectors, are one of the developing branches of materials science. Composite materials, which are preferred due to their properties such as light weight, high strength, resistance to outdoor conditions and long life, offer opportunities to meet the need for shelter, especially in the construction sector, thanks to their good heat and moisture resistance. In recent years, the development of production processes sensitive to the use of waste has been supported for a sustainable world. To realize sustainable composite material production, alternative raw materials are needed. In this project proposal, it was thought that instead of glass, carbon, aramid fibers that constitute the reinforcement elements of composite materials, denim fabric wastes, and recycled polyester could be used as resin. It is aimed to produce composite materials resistant to outdoor conditions for the portable shelter system, suitable for emergency installation, by using waste jeans fabrics formed in the denim factory and unsaturated polyester resins recycled from PET (Polyethylene terephthalate) wastes, to be used in natural disasters or in cases of forced migration. Waste denim fabrics and recycled polyester resin; will both meet the need for sustainable raw materials and reduce raw material costs in composite production. Optimum processes and ideal composite material designs will be created so that the composites produced with new sustainable materials that will replace the currently used materials can reach the required strength values. As a production method, in the light of literature review and industry experience; Vacuum bagging method will be used due to its high strength, low cost and ease of production. The mechanical and thermal properties of composite materials produced with different waste denim fabrics and different fiber sequences will be compared with the currently used composite materials (for example: glass fiber + unsaturated polyester) and composite materials with sufficient properties will be determined. In addition, environmental gains will be examined with the life cycle assessment to be made at the end of the study.

Biography

AYŞE GENÇ was borned in 1971 in KARS TURKEY. She is a textile-chemical engineer graduated from METU, Chemical Engineering Department in the year 1994. She has Msc. Degree in Chemical Engineering Department at İnönü University. She is continuing PHD in Textile Engineering Department at Gaziantep University since 2019. She is working now at Çalık Denim Textile as Sustainability, Chemical Compliance and Laboratory Manager and Senior R&D Expert since 2019. She is working since 2003 at Calık Denim. Her special interests are ‘Environmental and Social Sustainability in Denim Fabric Production, Circular Design, R&D Studies in Denim Dyeing and Finishing, Denim Fabric, Woven fabric and Knitted Fabric Production and Dyeing Processes, Technical Textiles and textile-based composites.

Study of radiation shielding materials on microstrip patch antenna for sustainability

J. Colaco and **R. Lohani**
Goa College of Engineering, India

The development of high-frequency wireless communication like 3G or 4G via microstrip patch antennas made of copper subject material has driven the emanation of harmful ionizing electromagnetic radiations as copper is a particularly extremely high electromagnetic conducting material. This radiation has a high effect on the environment which will motive life-threatening to humans, and the natural world. Moreover, the mentioned radiation due to upcoming ultra-high frequency 5G wireless communication will decline the life of humankind and the surroundings causing more rise in Global warming because of heating of earth's atmosphere through combos of ultraviolet (UV) waves, X-rays, Gamma Rays and RF waves as these waves in assortments will generate electromagnetic heat waves at super-high frequencies. In this research study, using FEKO software, the authors have designed, examined and compared microstrip patch antennas made of radiation shielding materials with that of commonly used copper material patch resonating at 2.4 GHz and 26 GHz placed on the frequently used fabrication ease and low-cost substrate such as FR-4, and Rogers RT Duroid 5880. The findings show that the radiation power level diminishes after the usage of microstrip patches made up of radiation shielding materials thus indicating electromagnetic radiation emitted by radiation shielding materials are eco-friendly and will also be sustainable for the environment and living beings. The efficiency of the proposed microstrip antenna with regards to return loss and bandwidth is showing improvements with each radiation shielding material as microstrip patches with that of copper material.

Biography

John Nepomuceno Colaco was born in Goa, India, in 1985. He received the B.E. degree in electronics and telecommunication engineering and M.E. degree in electronics communication and instrumentation from the Goa College of Engineering, Farmagudi, Ponda, Goa affiliated to Goa University, Goa in 2008, and 2016, respectively. In 2008, he joined Zenith Computers Limited, Goa as Trainee Engineer. In 2019, he joined the Department of Electronics and Telecommunication, Goa College of Engineering as Assistant Professor. He is currently pursuing Ph.D. degree in electronics and communication at Goa College of Engineering, Farmagudi, Ponda, Goa. He is the alumni of Goa College of Engineering. He is the member IEEE Bombay section, India. His current research includes Microstrip patch antennas, Metamaterials antennas, Bio-medical and IoT applications, and Image processing.

Analysis of instantaneous poynting vector and application

Himanshu Kushwah and **Jagneet Kaur Anand**
University of Delhi, India

We derive analytical expressions for the spatial evolution of the instantaneous Poynting vector (PV) for optical waveguides and propose new formulae for the propagation length and the penetration depth of the 'instantaneous' PV. These are different from their conventional formulae defined for 'average' PV [1]. Starting from Maxwell's equations [2], we obtain following equations for the electric and magnetic fields of symmetric bound TM modes of a planar symmetric Dielectric-metal-dielectric (DMD) waveguide of core thickness d along the x- axis, infinite in extent in y-axis, and direction of propagation along the z-axis, at an instant t=0 :

$$H_y(x,z) = \begin{cases} \cos(\kappa x)\cos(\beta_r z)e^{-\beta_i z} & ; |x| \le \frac{d}{2} \\ \cos\left(\frac{\kappa d}{2}\right) e^{\gamma d/2}\, e^{-\gamma|x|}\cos(\beta_r z)e^{-\beta_i z} & ; |x| \ge \frac{d}{2} \end{cases} \tag{1}$$

$$E_x(x,z) = \begin{cases} \frac{\beta}{\omega\varepsilon_o {n_m}^2}\cos(\kappa x)\cos(\beta_r z)e^{-\beta_i z} & ; |x| \le \frac{d}{2} \\ \frac{\beta}{\omega\varepsilon_o {n_d}^2}\cos\left(\frac{\kappa d}{2}\right) e^{\gamma d/2}\, e^{-\gamma|x|}\cos(\beta_r z)e^{-\beta_i z} & ; |x| \ge \frac{d}{2} \end{cases} \tag{2}$$

$$E_z(x,z) = \begin{cases} \frac{\kappa}{\omega\varepsilon_o {n_m}^2}\sin(\kappa x)\sin(\beta_r z)\, e^{-\beta_i z} & ; |x| \le \frac{d}{2} \\ \frac{\gamma}{\omega\varepsilon_o {n_d}^2}\frac{x}{|x|}\cos\left(\frac{\kappa d}{2}\right) e^{\gamma d/2}\, e^{-\gamma|x|}\sin(\beta_r z)\, e^{-\beta_i z} & ; |x| \ge \frac{d}{2} \end{cases} \tag{3}$$

Where the symbols have their usual meanings.

The **PV** associated with an electromagnetic wave is given by:

$$\boldsymbol{S} = \mathbf{E} \times \mathbf{H} \tag{4}$$

Substituting Eqns. (1)-(3) in Eqn. (4), we get the expressions for x- (transverse) and z- (longitudinal) components of the PV:

$$S_x(x,z) = \begin{cases} \frac{-\kappa}{\omega\varepsilon_o {n_m}^2}\cos(\kappa x)\sin(\kappa x)\sin(\beta_r z)\cos(\beta_r z)\, e^{-2\beta_i z} & ; |x| \le \frac{d}{2} \\ \frac{-\gamma}{\omega\varepsilon_o {n_d}^2}\frac{x}{|x|}\, cos^2\left(\frac{\kappa d}{2}\right) e^{\gamma d}\, e^{-2\gamma|x|}\sin(\beta_r z)\cos(\beta_r z)\, e^{-2\beta_i z} & ; |x| \ge \frac{d}{2} \end{cases} \tag{5}$$

$$S_z(x,z) = \begin{cases} \frac{\beta}{\omega\varepsilon_o {n_m}^2} cos^2(\kappa x)\, cos^2(\beta_r z)e^{-2\beta_i z} & ; |x| \le \frac{d}{2} \\ \frac{\beta}{\omega\varepsilon_o {n_d}^2} cos^2\left(\frac{\kappa d}{2}\right) e^{\gamma d}\, e^{-2\gamma|x|} cos^2(\beta_r z)e^{-2\beta_i z} & ; |x| \ge \frac{d}{2} \end{cases} \tag{6}$$

Combining Eqns. (5) and (6) we obtain the equations for instantaneous PV due to S_x and S_z [3].

$$\begin{cases} \sin\kappa x\,(\sec\beta_r z)^{(\kappa^2/\beta.\beta_r)} = C_1 & ; |x| \le \frac{d}{2} \\ \frac{x}{|x|}\, e^{(-\beta.\beta_r.|x|/\gamma)}\cos\beta_r z = C_2 & ; |x| \ge \frac{d}{2} \end{cases} \tag{7}$$

C_1 and C_2 are the constants whose absolute values determine the strength of the flux lines.

The penetration depth for instantaneous PV is $\left|\frac{\gamma}{\beta^2}\right|$ due to the presence of the term e^(((-β.β_r.|x|)/γ)) and the propagation length is $\frac{1}{\left(\frac{{\beta_r}^2}{\beta}\right)_i} \backsimeq \frac{1}{\beta_i}$ (obtained by simplifying Eqn. (7)). The corresponding expressions for the 'average' PV are $\left|\frac{1}{2\gamma}\right|$ and $\frac{1}{2\beta_i}$ respectively. We plot the spatial evolution of the instantaneous PV for silica-gold-silica waveguide and show that inside the metal core, it consists of broken flux lines signifying the optical absorption of electromagnetic waves propagating through the metal in order to excite the surface plasmons in a resonant manner in the metal film at the interface [2].

We use the proposed formula for the penetration depth of instantaneous PV to calculate the optimum thickness of the high index dielectric layer to be used as affinity layer or for the enhancement of sensitivity of a surface plasmon resonance-based sensor. Our results match very well with the already reported experimental results [4].

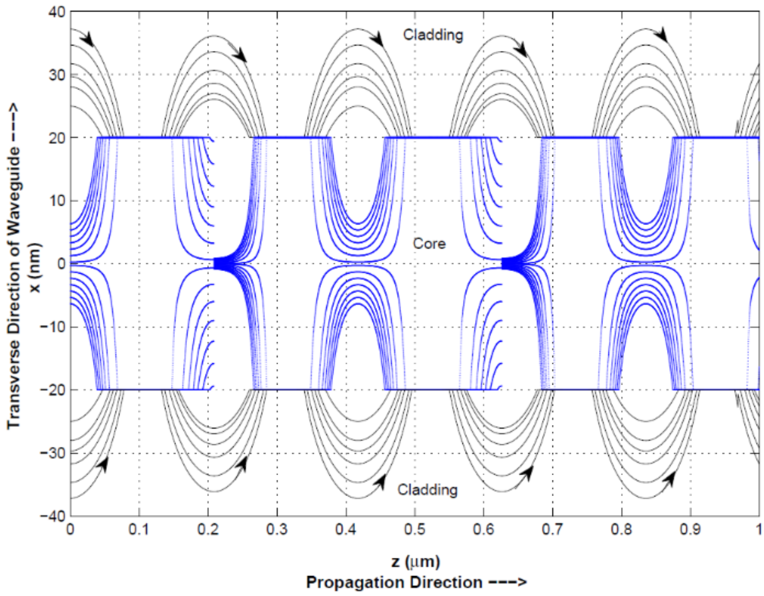


Figure: Spatial Evolution of instantaneous PV in the plane (side view), for the SiO_2-Au-SiO_2 waveguide inside the metal core of thickness , and in the dielectric cladding regions along the direction of propagation for TM_0 mode

Biography

Himanshu Kushwah received the B.Sc. (Hons.) degree in Electronics from the Hansraj College University of Delhi, Delhi in 2008 and the M.Sc. degree in Electronics Science from the University of Delhi South Campus Delhi in 2010. Since 2011, he is teaching Electronics Science to undergraduate students at the Department of Electronics, Keshav Mahavidyalaya, University of Delhi. He is also pursuing Ph.D degree in Electronics at the University of Delhi, South Campus, Delhi India. In addition, he has worked as Design Engineer at STMicroelectronics Inc. from June 2010 to Dec. 2010. His research interest includes the design and development of SPR based optical sensors and their characterization.

A comparison of smear layer removal effects between conventional chemical surface treatment and double-wavelength (Er,Cr: YSGG 2780 nm and diode 940 nm) laser methods on push-out bound strength of three calsium silicate-based materials

E. Kazeminejad
Golestan University of medical sciences, Iran

Objectives and scope: The aim of this invitro study was to evaluate and compare the effect of smear layer removal modification on push out bond strength of MTA, Biodentine and Cem cement as a dental biomaterial. This modification was done by comparing two methods using chemical surface treatment and double-wavelength laser irradiation in endodontics.

Method: One hundred ten human anterior extracted teeth were decoronated, cleaned and shaped to the same size apically and randomly divided into 3 major groups: (1) smear layer preserved, (2) smear layer removed using irrigation with 17% EDTA, and (3) smear layer was removed by double-wavelength (940 nm + 2780 nm) lasers. Three slices of 1±0.1mm in thickness was obtained from each root, so divided into 3 subgroups according to the obturation material used: (A) ProRoot MTA, (B) Cem cement, (C) Biodentine.

The specimens were stored in synthetic tissue fluid for 7 days to allow maximum setting of the root filling materials.

Push-out bond strength test was carried out using a universal testing machine. The bond failure mode was assessed under an optical microscope at 40×.

Results: The mean push-out bond strength in subgroups 1A, 2A and 3A were 5.25± 2.13, 5.36±2.55 and 5.31±2.73 MPa respectively, while those for subgroups 1B, 2B and 3B were 3.35±1.82, 6.33±2.72 and 5.63±3.66 MPa, and for subgroups 1C, 2C and 3C were 5.34±2.70, 5.42±3.04 and 5.42±2.48, respectively.

The push-out strength value was significantly reduced when the smear layer was preserved in the Cem cement groups ($P < 0.05$) while no significant difference was detected in the other groups.

Conclusions: Based on the conditions of this ex vivo study, it can be concluded that smear layer removal is detrimental to the bond strength between Cem cements and dentin.

Biography

Ezatolah Kazeminejad is an Assistant Professor at Endodontic department in dental faculty of Golestan University of Medical Sciences (GUMS) in Iran. His work focuses specifically on the biological impact of the laser in regenerative process in Endodontics through running some projects about its interaction with the biomechanics, biomaterials, stem cells and scaffold which was conducted in his research projects. He is the member of dental research center and stem cell research center at GUMS.

Optimization of deep drawing products by adding effect of texture pattern in draw bead design

Mohammad Soroush Merkani and **Ali Parvizi**
University of Tehran, Iran

Draw beads play an important role in imposing sufficient strain and deformation on blanks in deep drawing process. Using draw beads improve the quality of drawing in terms of creation of details of die on blank and limiting spring back. On the other hand, utilizing draw beads increases die wear and it is inevitable to use lubricant to control the friction and wear rate. In an effort to relegate lubricant from the drawing process and improve the quality of product by controlling the friction between draw beads and blank, the effect of texturing of machining on draw beads were included in design. Three parameters of height, width and length of draw bead as well as the texture pattern created by different machining strategies were considered as input parameters. Three different texture patterns were introduced and the coefficient of friction related to each one was measured using a friction test method. The values of maximum residual stress, maximum plastic strain, maximum punch force, and wrinkling were chosen as output parameters defining the part quality. For case study, the deep drawing process of an industrial die was simulated using ABAQUS/Explicit software. Thereafter, the results of experimental investigation were used for verification of FE model. The effect of each parameter on the quality of drawn parts was investigated using response surface method (RSM). Then, the optimal values of input parameters were obtained by RSM technique. Additionally, the optimization of response surface was carried out using genetic algorithm (GA) contributing to improvement in the output parameters.

Biography

Mohammad Soroush Merkani is a first-year Ph.D. student of mechanical engineering at the University of Tehran, School of Mechanical Engineering. He received his bachelor’s degree in mechanical engineering from Amirkabir University of Technology and a master’s degree in mechanical engineering branch of metal forming in manufacturing and producing from University of Tehran. He has work experience in a renewable energy institute and interested in renewable energies and automotive industries.

Technique to avoid membrane punching during triaxial test of crushed aggregate

Wael Mahmood Albadri[1], Israa Jamal Alhani[2], Mohd Jamaludin Md Noor[3], Soon Yee Wong[4] and **Kim Yuen Wong[5]**

[1]*Al-Amarah University College, Iraq*
[2]*Mazaya University College, Iraq*
[3]*MARA University of Technology UiTM, Malaysia*
[4]*University of Nottingham Malaysia, Malaysia*
[5]*Soilpro Technical Services Sdn Bhd, Malaysia*

Purpose: In triaxial test, a rubber membrane encloses the specimen. The membrane is specifically thin to a thickness of no influence on the test results. However, testing coarse-grained materials in triaxial test might be challenging due to the occurrence of membrane punching. In trial tests, the angular aggregate easily punches the membrane.

Methods: A technique was explored to mitigate membrane punching due to sharp edges of angular materials. One method has filter paper inserted between two membranes and another method has aluminium foil instead of filter paper.

Results: The use of filter paper and aluminium foil as insert materials is successful in preventing the membrane punching. Consequently, the filter paper is not contributing to additional resistance when used as protection between two membranes as compared to aluminium foil.

Conclusion: This paper investigates the performance of the protection materials by experiments. Essentially, the filter paper had no significant effect on test results; this fact was verified through numerical modelling and comparative tests by using rounded particles material.

Biography

Wael M. Albadri obtained his Master of Civil Engineering from Universiti Tun Hussein Onn Malaysia (UTHM). He then pursued a Doctor of Philosophy degree in Civil Engineering at MARA University of Technology (UiTM) and graduated in November 2019 after he received the Excellence Research Award. His research interests include unsaturated soil mechanics and laboratory soil testing.

Development and performance evaluation of a pedal operated seed cleaner (POS cleaner)

Wilber Akatuhurira[1,2], **Peter Tumutegyereize**[1], **Isaac Oluk**[2], **Emmanuel Baidhe**[1,2], **Julia Kigozi**[1], **Ismael Mayanja**[2,3] and **Hussein Balimunsi Kivumbi**[1]

[1]*Makerere University, Uganda*
[2]*Badaye Technologies Limited, Uganda*
[3]*University of California, USA*

Traditional grain cleaning methods such as winnowing are labor-intensive, time-consuming, and inefficient. The commercially available mechanical seed cleaners are associated with high initial, maintenance, and operating costs. This created a need for an intermediate seed cleaning technology bridging between the traditional cleaning methods and mechanical cleaners. Therefore, a Pedal Operated Seed Cleaner (PoS-Cleaner) was developed. POS cleaner powered by a pedaling system, which rotates the cleaning sieves (trommels). This makes it applicable in remote areas without access to fuel or electricity. Seeds to be cleaned are fed into the hopper of POS, which are directed to the inner sieve with mesh sizes larger than seeds to trap large particles such as stones, crushed cobs. The remnants are directed to the two outer interlocking sieves (one sieve fixed and the other adjustable), which emit particles smaller than the seeds such as dust, chaff. The mesh sizes of the outer interlocking sieves can be adjusted, which permits cleaning multiple seeds. POS was tested on maize, beans, and groundnuts, whose cleaning rates were 576.5 kg/h, 375.8 kg/h, and 377.4 kg/h, respectively. Also, the cleaning efficiencies were 95.09% (maize), 87.61% (beans), and 81.67% (groundnuts). Thus, the adaption of POS-cleaner presents a viable cleaning option for smallholder farmers in rural and remote areas with no access to the national grid.

Biography

Wilber Akatuhurira is an industrial designer at Badaye Technologies Limited with 2 years of successful experience in combining art, business and Engineering to make products that simplify work especially for local farmers. He specializes in sketching out ideas, using computer software to develop virtual models and examining production costs to determine manufacturing requirements. He is a fresh graduate from Makerere University with a bachelor's degree in Agricultural Engineering. While in School, he developed a lifting mechanism that was adopted by an Engineering Company and this reduced about 5% of company's operational costs. A strong believer in the power of the developing technology, Wilber is proud to contribute to the satisfaction of the clients through designing high performing and efficient products.

Sb_2S_3 thin films by ultrasonic spray: Formation and application in solar cells

M. Krunks, I. Oja Acik and J.S. Eensalu
Tallinn University of Technology, Estonia

Sb_2S_3 with bandgap of 1,7 eV, absorption coefficient 1.105 cm^{-1} at 450 nm and good stability makes it prime candidate for application as top cell absorber in tandem solar cells or in semitransparent solar cells. In this study rapid, scalable and robust in-air deposition method of ultrasonic spray pyrolysis (USP) has been applied to grow phase pure Sb_2S_3 thin films. $SbCl_3$- thiourea complex and antimony xanthate were used as precursor materials. Thermal analysis study (TG/DTA –EGA-MS) of precursors was performed to study the thermal decomposition reactions and determine the suitable range of temperatures for Sb_2S_3 film deposition.

Two-stage process where continuous amorphous film with uniform thickness is grown by USP at temperatures around 200°C followed by annealing in an inert atmosphere for 5 minutes results in polycrystalline single phase Sb_2S_3 as confirmed by XRD, Raman and EDX study. Using $SbCl_3$-thiourea based precursor the optimal film deposition temperature is 210°C, in case antimony xanthate Sb_2S_3 amorphous film could be grown even at lower temperature (160-180°C) but measures to avoid oxidation during the film growth should be considered. It was shown that an excess of thioamides in spray solution is effective to depress the formation of oxide phase.

Thin film solar cells with structure TCO/TiO_2/Sb_2S_3 /HTM with all component layers prepared by solution methods in air, showed conversion efficiency of 5.5 % at AM1.5G. The effect of Sb_2S_3 absorber layer thickness and type of HTM layer on solar cell output parameters will be discussed.

Biography

Malle Krunks is the Tenured Full Professor at the Department of Materials and Environmental Technology at Tallinn University of Technology, Estonia. She graduated from Tallinn University of Technology as Dipl. engineer in electronics, received PhD degree in 1985 in Physical Chemistry from the Ural Polytechnical Institute, Ekaterinburg, Russia. She has been working on different positions at the Tallinn University of Technology and as visiting researcher in a number of universities in Europe.

Microscale control of ferrofluid toward enabling novel micro-electro-mechanical systems

Kenichi Takahata
University of British Columbia, Canada

Ferrofluids are a type of smart materials that respond to external magnetic fields. They are biphasic suspensions of magnetic nanoparticles that are coated with a surfactant to prevent their agglomeration in a carrier liquid while limiting the attractive van der Waals forces acting among them. A ferrofluid flows toward the location with the highest magnetic flux density in a field gradient that can be externally controlled. This unique feature can be exploited to enable novel micro-electro-mechanical systems (MEMS). One device area that significantly benefits from this feature is micro actuators. Our research team previously revealed that miniaturized magnetic rotors/sliders could be levitated by applied ferrofluid as it was attracted onto their poles, providing an extremely simple and near friction-less bearing, a key element for achieving high-performance rotary/ linear MEMS actuators. We have developed ferrofluid-assisted electromagnetic micro rotary actuators for their application to medical microsystems. One example is the distal optical scanner for endoscopic probes, with which we demonstrated full 360 side-viewing endoscopy via circumferential scanning of laser beam from the probe tip. The ferrofluid-based scanner offers versatile actuation functionality, from arbitrary fine angular stepping to high-speed continuous revolving, allowing for the use of different imaging modalities. Multimodal endoscopic imaging and analysis have been successfully demonstrated using *in-vivo* models by coupling this technology with optical coherence tomography and Raman spectroscopy. Our related studies have also led to other new MEMS devices, including optical switches and variable inductors as well as micromanufacturing processes such as those for implantable sensors and microneedles. This talk will highlight recent progress from these studies focused onto the ferrofluid as a promising route to realizing novel microsystems.

Biography

Kenichi Takahata is Professor in the Department of Electrical and Computer Engineering at University of British Columbia. He received the B.S. degree in physics from Sophia University, Japan, in 1990 and the M.S. and Ph.D. degrees in electrical engineering from University of Michigan, Ann Arbor, in 2004 and 2005, respectively. He had held research positions at Panasonic in Japan from 1990 until 2001. He was Visiting Scientist at University of Wisconsin-Madison from 1999 to 2001 and Senior Research Engineer at 3M, St. Paul, USA from 2005 to 2006. His research interests center around microsystems, medical MEMS, nanomanufacturing, and microplasma control and applications.

KEYNOTE PRESENTATIONS

DAY 2

PEERS ALLEY MEDIA

Virtual Event

3rd Advanced Materials Science World Congress

March 21-23, 2022

BIOGRAPHY

Dimitrios Kotzias (Ph.D in chemistry, University of Bonn/Germany) was Acting Director of the Institute for Health and Consumer Protection (IHCP) and Head (retired) of the Chemical Assessment and Testing Unit at the European Commission's Joint Research Centre (JRC), Ispra/Italy. His research activities focused on trace analysis of organic compounds in complex matrices, photochemical and photocatalytic reactions, photochemical oxidants, indoor air quality and exposure assessment to chemicals and chemical mixtures. Founding member and for many years President of the Mediterranean Scientific Association of Environmental Protection (MESAEP).

Dimitrios Kotzias

Institute for Health and Consumer Protection, Italy

Smart coatings: Degradation of priority pollutants on TiO_2 based photocatalytic materials in indoor and outdoor environments-Principles and mechanisms

The heterogeneous photo-catalysis using semiconductors e.g.TiO_2 is a promising technology for the degradation of environmental pollutants. Preliminary evidence indicates that materials and paints enriched with TiO_2 degrade, upon activation with UV-light, NOx gases and volatile organic compounds (VOCs) e.g. benzene, toluene at concentrations typical for the urban environment. The photocatalytic TiO_2-materials and paints developed are primarily for use outdoors, on facades in high traffic roads.

Due to its band gap of 3.2 eV, TiO_2 is effective only in the UV-region (ca. 5%) of the solar spectrum and with wavelengths <380 nm. Hence, efforts made to increase the area of activity of TiO_2 using visible light, which will expand its application to improve the quality of indoor environments.

The photocatalytic activity of TiO_2 depends on the lifetime of charge carriers - positive holes and electrons - produced on its surface. Recombination of positive holes and electrons occurs in an extremely short time with most charge carriers recombining at the surface of the semiconductor before undergoing redox reactions. In this case no reaction takes place.

One way to reduce or inhibit recombination is to blend/dope TiO_2 with transition metals, which create traps for electrons and /or positive holes and block the charge carriers by reducing the recombination rate. Doping (change/ modification of the crystalline structure of TiO_2) causes a bathochromic (red) shift, which results in a reduction in the energy gap leading to increased absorption in the visible light region. Many transition metals such as V, Cr, Fe, Mn, Ni, Co, Cu, Zn have been explored to reduce the energy gap and facilitate the transfer of electrons to the conduction band and thus extend the spectral range of modified TiO_2 to the area of visible light. In our experiments, 0.1% (w/w) and 1% (w/w) Mn-TiO_2 admixtures were prepared and the ability of the modified photo-catalysts to degrade NO by both solar and indoor illumination was evaluated. Principles and mechanisms of the photocatalytic reaction at the air/catalyst interface and the possible formation of undesired by-products through the photocatalytic reaction of TiO_2 with organic paint matrices are discussed.

BIOGRAPHY

Francesca Deganello is research chemist at CNR-ISMN (Istituto per lo Studio dei Materiali Nanostrutturati) in Palermo (Italy) since 2001. She obtained degree in Chemistry and Ph.D in Chemical Sciences at Università degli Studi di Palermo, Italy. She visited national and international laboratories like Trieste University (Italy), Tokyo University (Japan) and INRS-EMT (Canada). Her current research interests concern the sustainable synthesis of nanomaterials for energy and environmental applications. She is responsible for the ISMN unit of European projects concerning the wastewater pollutants abatement. She is scientific tutor/co-tutor of undergraduate, Ph.D and Post. Doc students. She also deals with the communication and dissemination of Chemistry to schools and public and performs reviewing and editorial activity for materials-related journals.

G. Messina[1], F. Deganello[2] and V. Boffa[1]

[1]Aalborg University, Denmark [2]Italian National Research Council, Italy

Dental zirconia waste for a sustainable manufacturing of oil-water separation membranes

Dental zirconia powder is a common non-hazardous waste from orthodontic laboratories and more than 2000 tons of waste zirconia are treated and disposed yearly. Waste recycling to produce new materials is one of the possible strategies toward sustainable technological development. In this presentation, the sustainable manufacturing of new oil-water separation membranes prepared from dental zirconia waste is discussed. Zirconia-based compounds have outstanding hardness, whiteness, chemical stability, and no toxicity. Our approach combines the advantageous properties of zirconia with reduced production costs, if compared to the commercial zirconia membranes. At the same time, waste is reduced and there is no need to consume materials, time, and energy for producing the nanoparticles usually required for membrane fabrication. Membranes were prepared by spin coating water dispersions of dental zirconia waste on commercial silicon carbide supports. Both the zirconia powders and the obtained membranes were characterized for their chemical physical properties and correlated with the selectivity in olive oil retention and the water permeability.

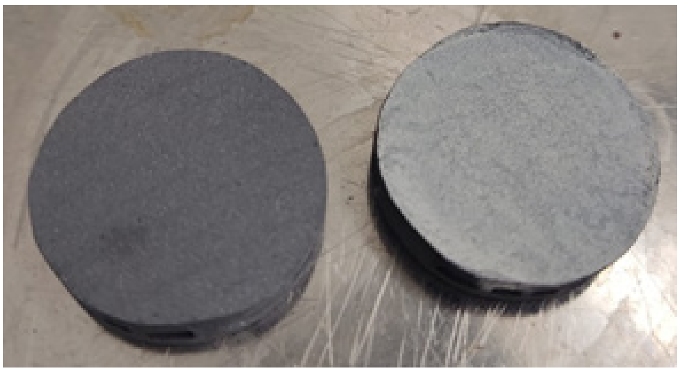


Figure: Silicon carbide support without (left) and with (right) deposited zirconia

BIOGRAPHY

V. G. Dubrovskii is a Professor and Head of the Laboratory of Physics of Nanostructures at Faculty of Physics, St. Petersburg State University. His research interests are in modeling of semiconductor nanowires and design of optoelectronic nanomaterials. He has received a number of awards and honors including Chevalier of Ordre des Palmes académiques, France (2017), Doctor Honoris Causa of Université Clermont Auvergne, France (2020), and Regular high-level visiting scientist in IGAT Base at Beijing University of Posts and Telecommunications, China (2007-2018).

V. G. Dubrovskii
St. Petersburg State University, Russia

Synthesis, modeling and applications of III-V nanowires and nanowire heterostructures: Opportunities and challenges

We will review the state-of-the art research in the field of synthesis and modeling of III-V semiconductor nanowires (NWs) and photonic nano-heterostructures based on such NWs. Some recent advancements will be discussed, including coherent growth in regular arrays on silicon substrates and some growth features of the vapor-liquid-solid growth which enable controllable tuning of the NW morphology, composition, crystal phase and statistical properties of the size distributions within the ensembles of NWs. Opportunities and challenges for optoelectronic applications of III-V NW heterostructures will be discussed, including single photon generation.

SCIENTIFIC ABSTRACTS

DAY 2

PEERS ALLEY MEDIA

Virtual Event

3rd Advanced Materials Science World Congress

March 21-23, 2022

Adv. Materials Science 2022

Energy transformation and accumulation in solids, irradiated by charged particles

Alexander Valyaev
Nuclear Safety Institute of the Russian Academy of Sciences, Russia

All observed phenomenon under irradiation are determined by processes of energy transformation in matter, depended on: (1) initial properties of matter; (2) irradiation parameters (3) characteristics of irradiation medium. Our universal scheme of transformation and accumulation of energy in solids under all types of irradiation, where radiation-stimulated processes and structural and phase damages, that cause the observed modifications of all properties of solids, are analyzed. It is included 33 blocks with its detail explanations shows possible channels of energy redistribution in temporal sequence from beginning of irradiation till formation of stable structures. Blocks are reflected excitation of electron and atomic subsystems, generation of point, linear and volume defects, plasma ablation, generation of acoustic and shock waves, different types of diffusion, mass transfer, thermal and deformation fields, fracture and hardening.

The most interest is the extreme which radiation effects, generate new unique phenomena, unattainable with usual low intense irradiation. They include wide range of plasma, mechanical processes with 1^{st} and 2^{nd} order phase transitions. We consider effects under irradiation with intense pulsed electron (IPEB); and ion (IPIB) beams in dielectrics, metals, alloys and multilayers; brittle fracture of solids by IPEB and long range effects in unirradiated irradiated regions by shock waves with generation of dislocations and hardening at high depth of exposed to IPIB with pulses (10^{-8}–10^{-6}s), intensities (108–1010 W/cm^2) fluences (1–100 J/cm^2/pulse).

These effects were stable, found in different materials using different accelerators in research science centers of Russia, USA and Japan.

These facts testify to the manifestation of some fundamental laws or regularities of radiation interaction with matter.

We used our results in development of new patent protection methods for radiation treatment of solids.

Biography

Valyae Alexander Nikiforovich is a Leading Researcher, Professor and Doctor of Sciences, Division of Ecological Safety and Radiation Risk, Nuclear Safety Institute of Russian Academy of Sciences since 2001. He belongs to Russia. He completed BSc&MSc in electric-mechanical engineering, 1972. He completed Ph.D. – Candidate Degree in Physics and Mathematics Sciences. To be examined on his thesis "Brittle Fracture of Solids Exposed to Intense Pulsed Electron Beams" Polytechnic Institute, Ekaterinburg, Russia, 1978. He completed his Ph.D.-Doctor Degree in Physics and Mathematics Sciences To be examined on my thesis "Radiation Induced and Mechanical Effects in Solids as a Result of High Intensity Electron and Ion Beams Irradiation" Nuclear Physics Institute of Kazakhstan Academy of Sciences, Alma-Ata, 1998.

Upconversion nanoplatforms as potent agents for cancer theranostics

I.V. Balalaeva[1], E.L. Guryev[1], N.Y. Shilyagina[1], V.A. Vodeneev[1], S.M. Deyev[2,3] and **A.V. Zvyagin[1,3,4]**

[1]*Lobachevsky University, Russia*
[2]*Russian Academy of Sciences, Russia*
[3]*First Moscow State Medical University, Russia*
[4]*Macquarie University, Australia*

Theranostic approach is currently among the fastest growing trends in cancer treatment. It implies the creation of multifunctional agents for simultaneous precise diagnosis and targeted impact on tumor cells. Upconversion nanoparticles (UCNP) are inorganic nanomaterial able of photoluminescence in visible and NIR spectral regions when irradiated with longer wavelengths of light. We aimed at creation of theranostic UCNP-based nanoplatforms combining photoluminescence with ability of targeted labeling of cancer cells and treating them with recombinant toxins and radioactive beta-emitting isotope.

We have assembled several types of multifunctional UCNP-based nanoplatforms selective to HER2 receptor overexpressed by cancer cells of many types. The choice of coating polymer and mode of assembly allowed tuning of nanoplatforms charge and colloid stability.

Effective cancer cell labeling with obtained nanoplatforms was confirmed both *in vitro* and *in vivo*. Of importance, combined action of anticancer toxin (recombinant form of pseudomonas exotoxin A) and beta-emitting isotope (yttrium-90) resulted in very strongly expressed synergistic effect, probably, due to protein synthesis arrest and impeded work of antioxidant and DNA-repair system. Embedment of yttrium-90 in the crystalline core of UCNP prevents spreading of its decay products throughout the body, thus, decreasing the risk of undesired side effects.

In an animal study, UCNP-based theranostic nanoplatforms provided visualization of xenograft HER2 expressing tumors and demonstrated their potency in cancer growth inhibition. Moreover, in a model of intraperitoneal metastasis, the treatment with UCNP-nanoplatforms lead to significantly reduced number of the formed metastatic nodes.

We believe that UCNP-based theranostic nanoplatforms can be considered as a promising agent for diagnosis and treatment of cancers. The demonstrated potency of combined targeted and radiopharmaceutical agents in one platform evidences the potential of the approach for further anticancer drug development.

This work was financially supported by the Ministry of Science and Higher Education of the Russian Federation (project No. 075-15-2020-927).

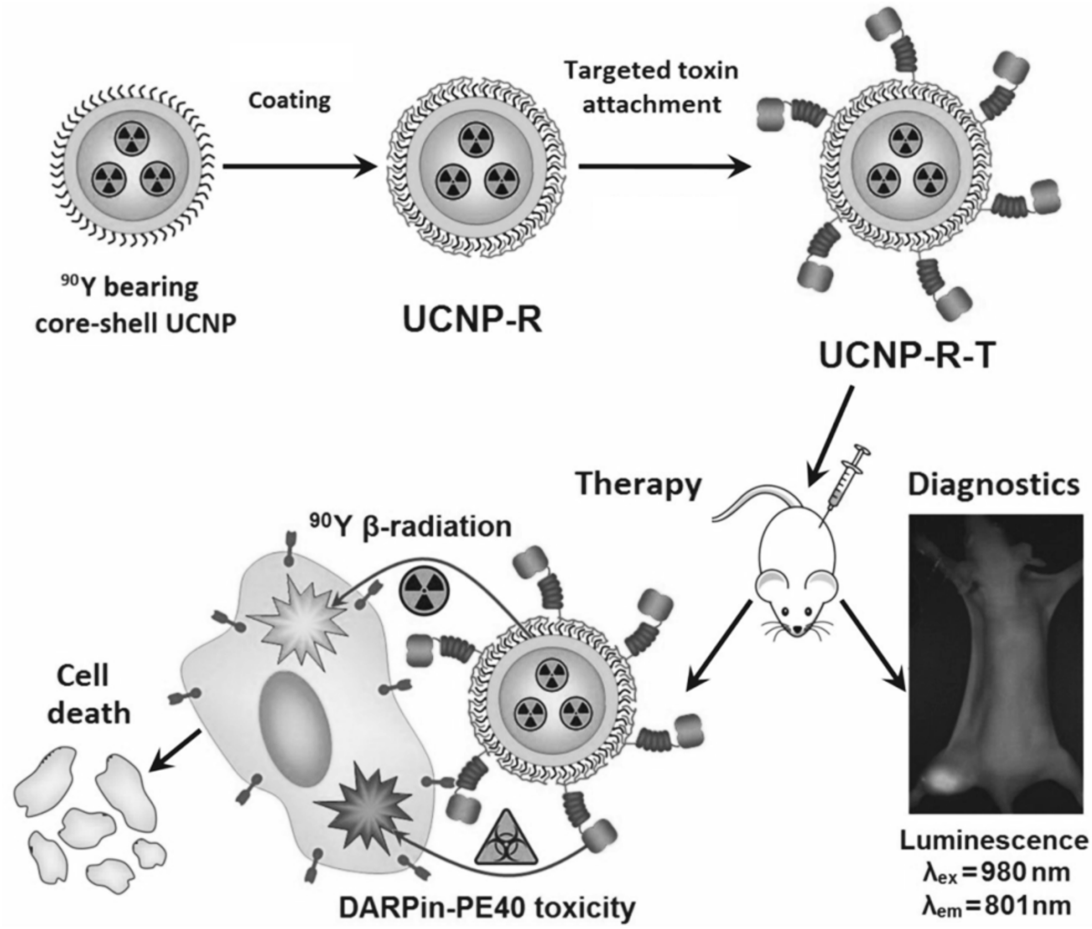


Figure: The scheme of assembly and mode of action of the UCNP-based theranostic nanoplatforms including yttrium-90 isotope and anticancer targeted toxin DARPin-PE40

Biography

Irina V. Balalaeva is an associate professor at Biophysics Department and the principal investigator at Laboratory of Optical Theranostics, Institute of Biology and Biomedicine, Lobachevsky University, Russia. Her fields of interests include application of photoluminescent nanoparticles in optical diagnosis and treatment of cancer; targeted therapy; photodynamic therapy; cancer cell biology; 3D *in vitro* cancer models; role of microenvironment in carcinogenesis and tumor resistance to treatment.

Regularities of acoustic emission under shock loading of glass with a crack

S.Bekher and **A. Popkov**
Siberian Transport University, Russia

The acoustic emission (AE) method is widely used to control pressure vessels, pipelines, units and parts of critical structures, machines and mechanisms. Compared with other methods of non-destructive testing, it allows you to selectively detect the developing defects in the entire test object with fixedly installed sensors. For brittle destructible materials, the loading of which can lead to uncontrolled destruction, AE testing is of limited use.

The aim of this work is a technique for detecting brittle developing defects in glass under impact using the method of AE and strain measurement.

The experiments were carried out on a 2 mm thick sheet glass placed on a damping cardboard backing. An initial crack up to 5 to 15 mm in length was artificially created in glass samples. The impact was carried out by steel balls weighing 9 g. Glass deformations were recorded by a strain gauge system with a sampling rate of 64 kHz and 0.5 ppm relative strain units. AE signals were measured with a sampling frequency of 2 MHz and a detection threshold of 5 μV in the frequency range from 100 to 700 kHz.

It has been experimentally established that in the process of impact action, the transverse shear of the cracks edges can reach 30 μm. Oscillations in the first 30 ms after the impact significantly exceed the level of AE signals. During the time from 100 to 600 s after the impact, relaxation of deformations to an equilibrium state by a logarithmic function of time is observed, associated with delayed fracture of the crack edges. A technique has been developed for detecting cracks in sheet glass under shock loading, based on the registration of AE signals of delayed fracture of the crack edges at the stage of stress relaxation.

Biography

Sergey Bekher was born in 1977 in Tomsk in the Russian Federation. In 2000, he graduated from Novosibirsk State University and received a master's degree in physics. In 2005 he received a Ph.D. degree in technical sciences for his thesis on "Acoustic emission control of wheel pairs of freight cars", in 2018 he received a doctorate in technical sciences for the research work "Integrated control of carriage running gears using strain measurement and acoustic emission ". From 2000 to the present, he worked as a researcher, associate professor, professor and head of a research laboratory at the Siberian Transport University. He participates in and leads research and development work on the creation of methods and equipment for strain measurement, acoustic emission and ultrasonic control of car parts during repair and operation, hazardous production facilities and building structures during manufacture.

Study of corrosion-resistant deposited metal of NPP equipment performed with a strip electrode by arc welding and electroslag welding methods

M. N. Timofeev

Prometey Central Scientific Research Institute of Structural Materials, Russia

To determine the most suitable technological option for the development of equipment for promising NPP, comparative studies of corrosion-resistant cladding were carried out.

Two technological options of corrosion resistant weld deposits on carbon steel were tested:- the first option - automatic submerged arc welding (SAW) with a strip electrode of 20%Cr-10%Ni-1%Nb type with preliminary cladding of 25%Cr-13%Ni type strip electrode;- the second option - automatic electroslag welding (ESW) with a strip electrode of 21%Cr-11%Ni-1%Nb type without preliminary cladding. Investigations of the deposited metal both in the initial state as-welded and after past welding heat treatment at 640 °C for 10 h were carried out.

In both cases, the deposit metal on the surface has a similar chemical composition. The structure is represented by an austenitic matrix with isolated areas of ferrite and finely dispersed carbides. Non-metallic inclusions in the weld metal are typical point oxides. In the case of SAW, the number and sizes of non-metallic inclusions are greater than in the case of ESW.

Due to thermal welding cycles, in multi-pass SAW case, diffusion processes at the fusion boundary with the base metal run more actively than in the case of single-pass ESW. This affects the greater thickness of the decarburized interlayer in the base metal and the carburized interlayer on the side of the deposited metal, as indicated by the results of metallographic tests and microhardness measurements.

The mechanical properties of the deposited metal at static tensile testing of specimens, in the as-welded condicion and after past welding heat treatment for both variants have approximately the same values.

Accelerated corrosion tests for intergranular corrosion resistance showed no difference. In both cases the weld metal was resistant to intergranular corrosion. At testing of deposit metal for pitting corrosion, it was found that the SAW metal has insignificantly higher numerical indicators of corrosion damage than the ESW metal. These differences in resistance to pitting corrosion are explained by the differences in Pitting Resistance Equivalent (PRE): PRESAW = 18.2 and PREESW = 23.

It has been established that SAW and ESW options provide similar characteristics of the deposited metal and can be used for the manufacture of equipment for promising NPP.

Biography

Mikhail Timofeev is a doctor of Central Research Institute of Structural Materials «Prometey», St. Petersburg, Russia. His core interests include the materials science research in the development of welding materials and technologies for welding heat-resistant steels in the nuclear power industry. He is the author of scientific papers aimed at improving the mechanical properties of welded joints in nuclear reactor vessels. His doctoral project is to creation of welding consumables, providing increasing the service characteristics of weld joints of nuclear and petrochemical reactor-body from Cr-Mo-V-steels.

Role of production procedure on microstructure and chemical composition of $Na_{0.5}Bi_{0.5}TiO_3$ ceramics

M. Dunce, E. Birks, L. Bikse, M. Antonova, O. Freimanis, K. Kundzins and M. Livins
University of Latvia, Latvia

$Na_{0.5}Bi_{0.5}TiO_3$ (NBT) and NBT-based solid solutions are known as ones of the most perspective lead-free ferroelectrics. Although they are widely studied concerning improvement of physical properties, research of role of production procedure is left without sufficient attention. In this work, we present a thorough study of influence of processing on microstructure and chemical content of NBT ceramics, as well as intentionally and non-intentinally created deviations from the stoichiometric composition. Scanning electron microscopy, energy-dispersive X-ray spectroscopy, X-ray diffraction, dielectric spectroscopy and polarization measurements are used as the main techniques for characterization. It is shown that grain size increases upon sintering temperature, with appearing of abnormal grain growth at high temperatures, while porosity has minimal values at approximately 1160°C. Energy-dispersive X-ray analysis reveals presence of Bi-deficient inclusions, which appear due to evaporation of Bi on calcination stage. While, during sintering, reducing of Bi content is not detected – composition of the matrix

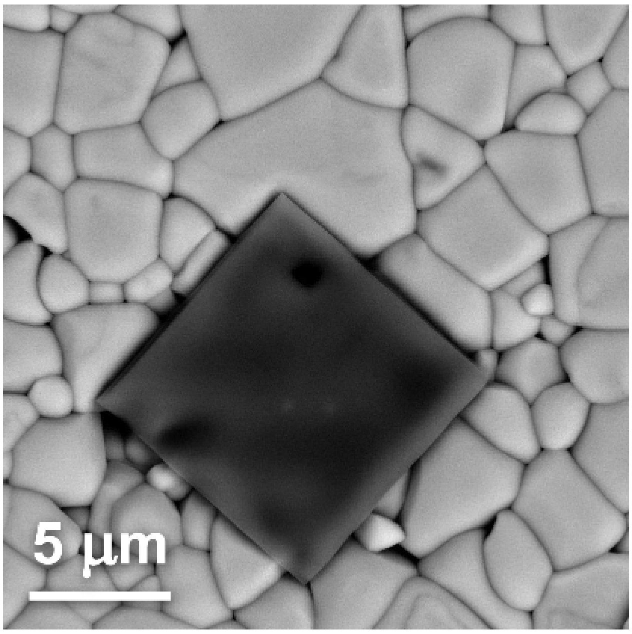


Figure: SEM micrograph of NBT ceramics with TiO_2 inclusion.

grains remains highly stoichiometric and concentration of inclusions does not increase.

Whereas, thermal treatment of the ceramics at temperatures above 1160°C causes intense evaporation of Bi from the surface and appearance of large concentration of TiO_2 inclusions as a consequence. Chemical composition of inclusions appearing in NBT ceramics with excess Bi added during processing contains large concentration of Ti. This rather leads to excess of Na in the NBT matrix grains and not excess of Bi, as it could be expected. Taking into account high stability of NBT regarding deviations from stoichiometry, local chemical composition of NBT-(SrBi) TiO_3 solid solutions is studied. The results are also accompanied with studies of involving hot isostatic pressing in the processing of NBT ceramics, helping to improve its density.

Biography

Marija Dunce is a leading researcher at the Department of Ferroelectric Materials of the Institute of Solid State Physics, University of Latvia (ISSP UL) in Riga, Latvia, where she works since 2005. She has PhD in Solid State Physics from the University of Latvia. Currently she works in the framework of her post-doctorate research project and investigates influence of production procedure and parameters on NBT and NBT-based lead-free ferroelectric ceramics, involving such ceramics characterization techniques as scanning electron microscopy, energy-dispersive x-ray spectroscopy, x-ray diffractometry and dielectric spectroscopy.

Organizing metal atoms and nanoclusters in LC media for novel applications

Satya Pal Singh and **Archana Kumari Singh**
Madan Mohan Malaviya University of Technology, India

Recently we have studied various liquid crystal (LC) molecules by doping them with metal atoms and their nano-clusters. We have investigated different properties such as polarizability, entropy, dipole moment, thermal and electrical energy, specific heat capacity, bandgap etc. as well as the effect of oping on these properties The variations in properties were verified by quantifying physical observables using IR, UV and NMR spectra of these compounds. This has been a least explored area. The chemical reactivities and the stabilities of the LC molecules were first observed using DFT calculations. DFT calculations with B3LYP/6-311G (d, p) and LanL2DZ basis sets were used first to optimize their structures and there their properties were sampled. The observations were focused on formation of nanodots by nucleation process at the chemically active sites of the LC molecules. We further verified the liquid crystalline phase after binding metal atoms and nanodots at room temperature via XRD spectra obtained using VESTA Software. We

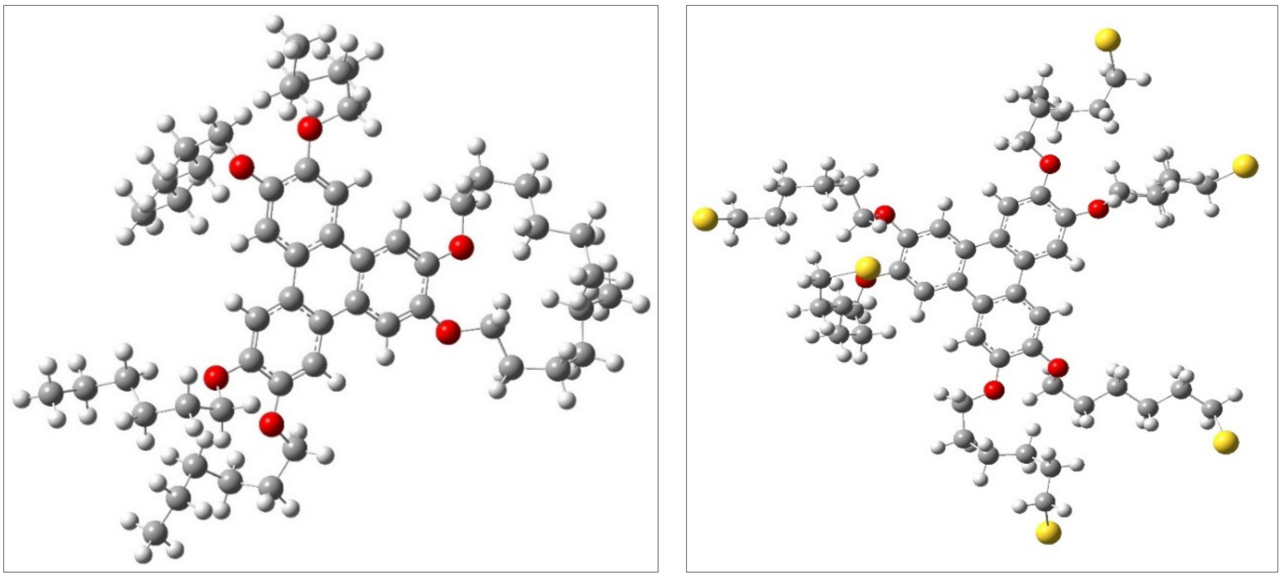


Figure: Optimized structure of 2,3,6,7,10,11-Hexakis [hexyloxy] triphenylene (semi-LC molecule) left and gold atom doped semi-LC molecule (right);

have uniquely defined and used a new method to obtain band-gaps in these LCs using UV-vis spectra by drawing three-tangent-lines. Our observations show very good agreement with band-gap values obtained from HOMO-LUMO concept. We further extend our work with gold and platinum dots by tailoring alkyl groups at different lengths and try to find alkyl specific variations. Remarkable thing is that gold and platinum nanodots and their complexes have been found useful in cancer treatment. Being a relatively more volatile candidate than the dots alone, LCs may offer some relief to the patients under treatment because of its biocompatible nature.

Biography

Satya Pal Singh is working as Assistant Professor at Department of Physics and Material Science since 2009. Before joining the institution, he has worked as Research Scientist at Indian Institute of Technology, Kanpur, India for nearly two years. He has availed Summer Research Fellow (SRF) jointly given by Indian Academy of Science, Indian National Science Academy & National Academy of Science in the year 2012. He has supervised 01 postdoc and currently guiding 02 Ph.D scholars.

Improving yield and nitrogen use efficiency using polymer coated urea in rice (Oryza sativa L.) under vertisol of Deccan Plateau (Typic Pellustert)

Gobinath Rajendran, Surekha Kuchi and **Vakada Manasa**
ICAR-Indian Institute of Rice Research, India

Polymer coated urea (PCU) was evaluated for its efficiency under two rice establishment methods [transplanting method (TP) and direct-seeded rice (DSR)] during two crop seasons (rabi, dry season and kharif, wet season). The results indicated that split application of PCU @ 75 and 100% recommended dose of nitrogen (RDN) were at par and resulted in significantly higher yields (46 and 49%) than normal urea in splits, respectively, during rabi 2015–2016 under transplanting method. During kharif-2016 under transplanting method, grain yield was maximum with 100% RDN from PCU single dose (5.13 t ha^{-1}) which was on par to 100% PCU in 3 splits (4.62 t ha^{-1}) and 75% PCU (4.80 t ha^{-1}) as a basal dose. In DSR, significantly higher grain yield was recorded in 100% RDN supplied through PCU as basal dose (6.16 t ha^{-1}). The maximum nitrogen use efficiency indices were observed in 75% PCU (split) followed by 100% PCU (Split) in rabi-2015–2016 but in the case of kharif-2016, basal application of 100% PCU found to be superior followed by 75% PCU. Thus, PCU proved its efficiency by saving 25% of N in transplanted rice in both wet and dry seasons and by considerable labor saving due to single basal application in case of transplanting as well as DSR in the wet season.

Biography

Gobinath Rajendran is currently working as Scientist (Soil Science) in ICAR-Indian Institute of Rice Research (IIRR), Hyderabad, India; joined in Indian Council of Agricultural Research (ICAR), Ministry of Agriculture and Farmer's Welfare in the year of 2016. He is currently involving in the field of development of smart nutrient delivery fertilizer materials for crops especially, nano technology, modified materials etc., and handling of multiple government and private organization projects in the area.

Pattern recognition techniques for sand particles

Jianfeng Wang
City University of Hong Kong, China

The pressing need to recognize and track individual sand particles in fundamental research on geomechnics has promoted the rapid development of particle tracking techniques in recent years. This talk presents the latest development of a few innovative pattern recognition techniques for identifying and atching intact and crushed sand particles. These techniques include particle volume-based tracking (PV-track), particle radius -based track (PR-track), spherical harmonics-based tracking (SH-track) and point cloud -based tracking (PL-track). Specifically, PV-track and PR-track are suitable for tracking particles within a neighborhood area but the tracking accuracy and reliability decreases with the increasing deformation of the sand specimen. SH-track is a much more powerful and robust technique which makes use of the SH invariant describing the multiscale morphological features of sand particles. However, the common limitation of PV-track, PR-track and SH-track is that they can only be applied to intact particles with solid structures (i.e., non-porous structure). In contrast, PL-track can deal with both intact and crushed sand particles and has been successfully used to match a group of crushed quartz particles. More importantly, PL-track can be integrated with machine learning techniques to achieve intelligent recognition and tracking, and has been successfully used to identify a group of highly porous carbonate sand particles. The implementation of all these particle tracking techniques is based on the X-ray microtomography scanning of a miniature specimen of sands, which provides the source data for the pattern recognition exercise.

Biography

Jianfeng Wang is currently an Associate Professor at City University of Hong Kong. He is internationally well known for his works in the field of micromechanical characterization and modelling of granular soils. He has been awarded the prestigious international prizes of 2011 Geotechnical Research Medal (UK Institution of Civil Engineers) and 2010 Higher Education Institutions Outstanding Research Award - Natural Science Award (the Ministry of Education of China). His research has attracted over 7 million HKD of external grants including the Research Grant Council (RGC) of Hong Kong SAR and National Science Foundation of China (NSFC). He is currently serves as a Scientific Editor of Journal of Rock Mechanics and Geotechnical Engineering (The Chinese Academy of Science), and an Editorial Board Member of Soils and Foundations (The Japanese Geotechnical Society).

Fluorescent single-walled carbon nanotubes for imaging and sensing in the near-infrared

Gili Bisker
Tel-Aviv University, Israel

Single-walled carbon nanotubes (SWCNTs) have unique optical and physical properties, and they benefit from the ease of surface functionalization and biocompatibility. Semiconducting SWCNTs fluoresce in the near-infrared (nIR) part of the spectrum, which overlaps with the transparency window of biological samples where absorption, scattering, and autofluorescence are reduced. Further, they do not photobleach or blink. Upon tailored surface functionalization, adsorption of target analytes onto the nanotube corona can result in spectral modulations manifested as either an intensity change or a shift in the peak emission wavelength. Hence, SWCNTs can be used as nIR optical probes for imaging and sensing in biological samples enabling real-time optical detection with both spatial and temporal resolution.

I will present recent discoveries of protein nanosensors for fibrinogen and insulin using SWCNTs functionalized with variants of poly(ethylene glycol)1–3. The recognition also occurs in serum environment, showing that the SWCNTs sensors work in this complex environment despite the potential nonspecific adsorption. I will show recent demonstrations of real-time feedback on insulin secretion by beta-cells4, real-time monitoring of enzymatic activity5, and recognition of a cellular oncometabolite6. Finally, I will present *in vivo* imaging of fluorescent SWCNT within nematodes7, and super-resolution imaging of SWCNT8. These results open new avenues for synthetic recognition of biological macromolecules with optical signal transduction, and hold great promise for medical and clinical applications.

Biography

Gili Bisker is a Senior Lecturer at the Biomedical Engineering Department at Tel Aviv University and she is a Zuckerman STEM Leadership Program Fellow. Before Joining Tel Aviv University, he worked at the MIT Chemical Engineering Department and at the MIT Physics Department as a postdoc. Gili holds a B.A. in Math and Physics as a graduate of the Technion Excellence Program, an M.Sc. in Physics, and a Ph.D. in Nanoscience and Nanotechnology, all from the Technion – Israel Institute of Technology.

A LIME-based explainable machine learning model for predicting the severity level of COVID-19 diagnosed patients

F. Gabbay, S. Bar-Lev, O. Montano and N. Hadad
Ruppin Academic Center, Israel

The fast and seemingly uncontrollable spread of the novel coronavirus disease (COVID-19) poses great challenges to an already overloaded health system worldwide. It thus exemplifies an urgent need for fast and effective triage. Such triage can help in the implementation of the necessary measures to prevent patient deterioration and conserve strained hospital resources. We examine two types of machine learning models, a multilayer perceptron artificial neural networks and decision trees, to predict the severity level of illness for patients diagnosed with COVID-19, based on their medical history and laboratory test results. In addition, we combine the machine learning models with a LIME-based explainable model to provide explainability of the model prediction. Our experimental results indicate that the model can achieve up to 80% prediction accuracy for the dataset we used. Finally, we integrate the explainable machine learning models into a mobile application to enable the usage of the proposed models by medical staff worldwide.

Biography

Freddy Gabbay received his B.Sc., M.Sc. and Ph.D. in Electrical Engineering from the Technion – Israel Institute of Technology, Haifa, Israel. In 1998, he worked as a researcher at Intel's Microprocessor Research Lab. In 1999, he joined Mellanox Technologies and held various positions in leading switch product line architecture and ASIC design. In 2003, he joined Freescale Semiconductor as a senior design manager and led the design of baseband ASIC products. In 2012 he rejoined Mellanox Technologies where he served as Vice President of Chip Design. Today he is an associate professor and the head of the Computer and Information Sciences Department at the Ruppin Academic Center, Emek Hefer, Israel. His research interests include VLSI design, computer architecture, machine learning and domain-specific accelerators. Prof. Gabbay holds 19 patents and is a senior member of IEEE and IEEE Computer Society.

Temperature dependent calibration of shape-memory alloy strain sensors

T. Mäder, B. Senf, M. Zoch, S. Liebig and **W.-G. Drossel**
Fraunhofer Institute for Machine Tools and Forming Technology IWU, Germany

Regular metallic strain gauges are elastic up to 0.3 percent strain. They can be applied on metallic structures to monitor strain and loading to implement structural health monitoring (SHM). Composite materials comprise a higher elastic strain, e.g. about 0.5 percent strain for glass-fibre reinforced plastics (GFRP). SHM of GFRP therefore demands strain sensors with higher elasticity. Novel shape-memory alloy strain sensors (SMASS) are fatigue resistant up to 1.5 percent strain and are a simple solution for that requirement. These novel sensors show a higher temperature dependence in comparison to regular strain gauges (Mäder et al., 2021). Investigations are made to find an adequate solution for temperature compensation. Hence, different configurations of Wheatstone bridges are tested.

A four-point bending test device, which can be used inside a climate chamber, was developed. Four-point bending tests guarantee a homogenous strain distribution over the strain sensor and are regularly used for calibration. The SMASS were applied on GFRP bars in longitudinal and transverse orientation to the center line. The single SMASS were electrically connected in different Wheatstone bridge configurations. Different temperature levels were approached. Each temperature step included a balancing time to guarantee an equal temperature distribution in the whole setup. Several bending cycles were done on each temperature level. Strain, sensor signals and temperature were monitored.

All tested sensor configurations eliminate the temperature dependent strain signal drift. All configurations retain an almost stable absolute zero value of the sensor bridge signal over all tested temperatures. The different configurations comprise various gauge factors. All gauge factors are non-linear and temperature dependent. The best performance was achieved with the bending configuration with one sensor on the tension and the other on the compression side of the specimen bar. Tension and bending can be reliably monitored. The monitoring of compression is possible at temperatures above 20°C.

Biography

Thomas Mäder received the Dipl.-Ing. degree in mechanical engineering, in 2007 and the Dr.-Ing. degree in mechanical engineering, in 2014, both from the Technische Universität Chemnitz, Chemnitz, Germany. From 2007 to 2013, he was a Research Assistant with the Institute of Materials Science and Engineering, Chemnitz, Germany. His research interest includes strain sensing and structural health monitoring of composite materials, carbon fibres, coating of materials, shape-memory alloy materials and the development of strain sensors for elastic materials.

Examining the contribution of factors affecting the electrical behavior of poly(methyl methacrylate)/graphene nanoplatelets composites

Xiaoling Luo[1] and **Dirk W. Schubert**[1,2]
[1]University of Erlangen-Nuremberg, Germany
[2]Bavarian Polymer Institute, Germany

In this study, poly(methyl methacrylate) (PMMA)/graphene nanoplatelets (GNPs) conductive composite films with different morphologies were fabricated from the same constituent materials using four fabrication techniques, solution casting (SC), SC followed by hot pressing (SCP), melt mixing followed by SC (MSC), and melt mixing followed by hot pressing (MP). Morphologies of dispersed GNPs and electrical properties in both in-plane and perpendicular directions were investigated and compared systematically. The conductivities, which varied up to two orders of magnitude and decreased in the sequence of SC > MSC >SCP >MP, were described as a function of GNPs volume fraction by using a McLachlan equation to reveal the electrical percolation thresholds (Φc). The Φc of the composites varied from 0.42 ± 0.13 vol % (SC, perpendicular) to 3.26 ± 0.48 vol % (MP, in-plane). The difference in the conductivity and Φc between two measuring directions is ascribed to GNPs orientation, while that for different processing methods is explained in terms of GNPs size, GNPs distribution, and dispersion state. The contribution of the above factors in each procedure was discerned individually, the results were discussed and compared with other experimental studies and simulations as well. The comparative study shows that the SC method endows the composite with the optimum electrical properties in both directions due to the large size, good dispersion and exfoliation of GNPs, and bad distribution of segregation structures.

Sample	SC	MSC	SCP	MP
Mean GNPs size (μm^2)	1141-1281	522-868	684-1109	550-613
	GNPs vol. %↑, size↑	←	GNPs vol. %↑, size↓	←
GNPs orientation	GNPs vol. %↑, orientation↑	←	←	←
Macroscopic distribution (in-plane)	+ (GNPs segregation)	←	++++	←
Micro-scale distribution (perpendicular)	+++	+ (layered structure)	+++	←
Nano-scale dispersion (exfoliation)	++++	+++	+++	+

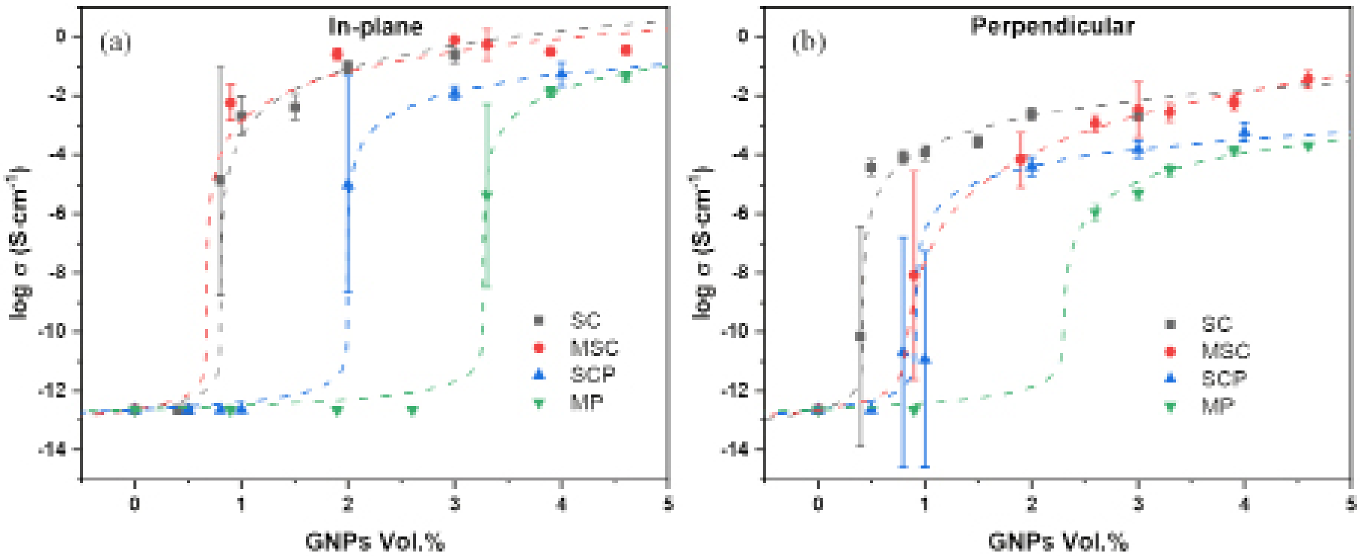


Figure: Logarithm of the conductivity (log σ) in (a) in-plane direction and **(b)** perpendicular direction as a function of GNPs volume fraction. The dashed lines show the best fit utilizing McLachlan equation.

Biography

Xiaoling Luo is a Ph. D student at the Institute of Polymer Materials, Friedrich-Alexander-University Erlangen-Nuremberg, Germany. She received a B.S. (2014, Polymer Science and Engineering) and M.S. (2017, Polymer Science and Engineering) from Sichuan University, China. Her research is focused on the fabrication, characterization, modeling and application of conductive polymer composites containing carbon-based fillers under the supervision of Prof. Dirk W. Schubert.

Manganese Hexacyanoferrate cathode material for aqueous Zn-ion battery

M Giorgetti[1], M Li[1], M Maisuradze[1], R Sciacca[1], M Berrettoni[2], G Aquilanti[3] and **J R Plaisier[3]**

[1]*University of Bologna, Italy*
[2]*University of Camerino, Italy*
[3]*Elettra – Sincrotrone trieste, Italy*

Manganese hexacyanoferrate (MnHCF) has attracted much attention as promising cathode material for Li and Na ion batteries, owning to its low cost, environmental friendliness, high specific capacity and voltage plateau. Here, the electrochemical performance and electronic structure information of MnHCF were studied in aqueous Zn-ion batteries (ZIBs). Based on the cyclic voltammetry and galvanostatic charge/discharge results, an activation of Fe-sites during beginning cycles was observed, and the capacity contribution of Fe-sites increases from 30% to 86% at C/20 during the first 10 cycles. The local geometric and electronic structure information of MnHCF was investigated by X-ray absorption spectroscopy (XAS) in a set of ex-situ electrodes. X-ray absorption spectroscopy is a synchrotron radiation based technique that is able to

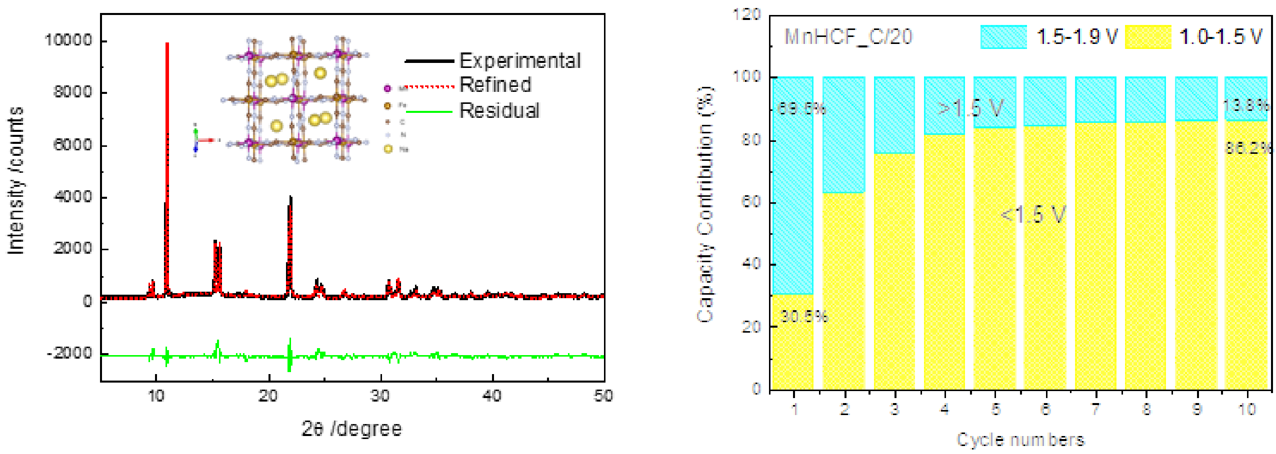


Figure: Refined XRPD structure of manganese hexacyanoferrate (left) and capacity contribution of the Fe and Mn redox couples as a function of cyclability (right) provide information on local structure and electronic properties in a chemically selective mode. From Fe K-edge spectra, it shows a consistent oxidation and reduced state in charged and discharged electrodes. Spectra also indicate that there is no apparent change for the local Fe-sites environment. However, the XAS spectra of Mn K-edge show apparent change after 10 cycles. Compared to the rhombohedral phase of Zinc hexacyanoferrate (ZnHCF), a -Zn-CN-Fe- structural framework was detected in the cycled MnHCF samples, and this suggests that a part of Zn replaced Mn-sites, with concomitant dissolution of the Mn-sites. The gradual activation of Fe-sites at the beginning cycles can be attributed to the alleviation spatial resistance with the dissolution of Mn-sites, and the replacement of Zn for Mn explains the decreasing capacity during cycling.

Biography

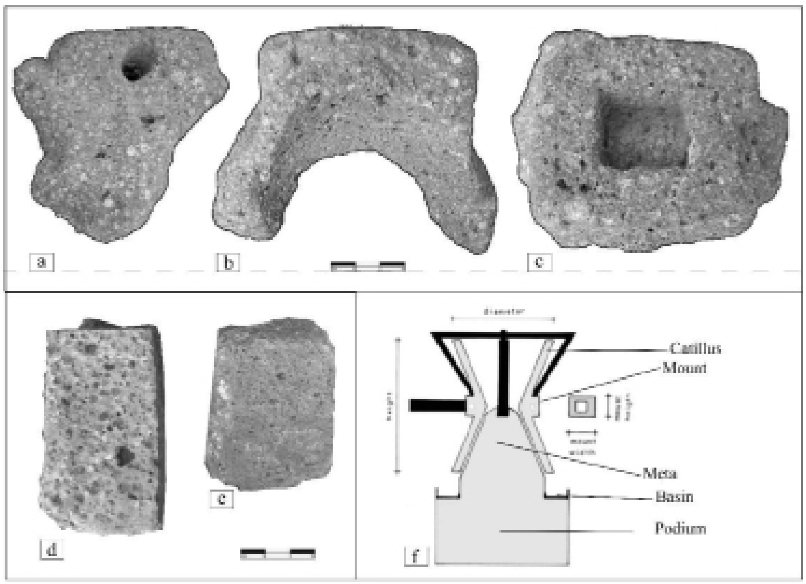
Marco Giorgetti is an Associate Professor at the University of Bologna and local coordinator of the Erasmus Mundus Joint Master Degree in Advanced Spectroscopy in Chemistry (ASC). He has coordinated more than 30 projects in synchrotron radiation facilities. He received Ph.D. in Chemical Sciences (1998) in Italy and held a two-years post-doc position at the University of Minnesota, Minneapolis (1998-2000). The research activity of he covers the field of the structural and electronic characterization of materials and solutions by core level spectroscopies, such as X-Ray Absorption Spectroscopy, the applied electrochemistry, sensors, the synthesis and characterization of materials for batteries, and methodology for data analysis.

Multidisciplinary and statistical approach for the investigation and characterization of archaeological artifacts

F. Falcone[1], **F. Castorina**[2], **R. E. Francis**[3], **A.Dionisio**[4] and **F. Stoppa**[1]

[1]D'Annunzio University, Italy
[2]University of Study of Roma "Sapienza", Iatly
[3]Johnson County Community College, USA
[4]Belle Arti e Paesaggio dell'Abruzzo, Italy

A well-preserved Pompeiian-type millstone fragment was retrieved from the chance discovery of Roman ovens dating to the V-VI century BCE in the area of Santa Arabona Manoppello in Italy. This is the first evidence of an hourglass millstone in Abruzzo. The hourglass grinder is comprised of a lower conical stone called a meta and an upper one shaped like an open hourglass, or catillus. The meta is fixed to a base at the central point of the height of the catillus, that of maximum narrowing. Two holes were drilled to fix the wooden poles to be used for the yoke of the draft animals. This fragment was analyzed through archaeometry, petrography, geochemistry, statistical analyses, and radiogenic isotopes at the University G. d'Annunzio. The source location of the stones was narrowed down to the areas of Etna, Roccamonfina, and Vulsini due to the petrography, geochemistry, and statistical



data elaboration of leuicititic and basaltic rocks from Central Italy and Sicily. The accurate identification of the provenance of the stone used to produce the millstone results in a better understanding of commercial trade routes and Roman entrepreneurship throughout Italy. The correlation between the production site and its stones' dispersion throughout the Roman Empire is of great interest for understanding the vast network of Roman roads, their manageability of commerce, and the organization of their products to the outlying areas of their Empire and in the case of this discovery, specifically to the area of Abruzzo Italy. This paper offers an example of which methodologies may ensure a correct estimation of possible rock sources, overcoming petrographic uncertainty, moreover, is a new multidisciplinary approach to identify Cultural Heritage materials with statistical method applied to history and earth sciences.

Biography

Francesca Falcone has a degree in Technologies and Diagnostics for the Conservation and Restoration of Cultural Heritage from the University of Camerino and a master's degree in Science and Materials for Conservation and Restoration from the chemistry department of the University of the Studies of Florence. She is currently working on a Ph.D. at the University of Chieti with a project for the protection and conservation Cultural Heritage in regional museums of Abruzzo in risk disasters situations through the evaluation of scenarios followed by innovative aspects of mitigation.

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Employing dicarboxylic acids in the KF-YF_3 system to modulate the crystal phase and optical response of Eu^{3+}-doped materials

Pablo Serna-Gallén, **Héctor Beltrán-Mir** and **Eloísa Cordoncillo**
Jaume I University, Spain

Among many inorganic materials, fluorides are the most appealing candidates for optical applications because of their low phonon energy associated with the crystal lattice. The compounds of the KF-YF_3 system (particularly YF_3 and KY_3F_{10}) doped with Ln^{3+} ions have shown outstanding optical response during the last years. Although Ln^{3+}-doped fluorides have been prepared in the literature with different capping agents that allow their surface modification, no attempts have been made to prove whether the use of dicarboxylic ligands in the KF-YF_3 system can be successful or not.

Based on the aforementioned points, Eu^{3+}-doped YF_3 and KY_3F_{10} materials were prepared hydrothermally in a wide range of pH values without the use of surface chelators and adding oxalic or tartaric acid using KBF_4 as the fluoride source. It has been proved for the first time the effective use of dicarboxylic ligands as chelating agents to modulate the surface and thus the crystal phase evolution in the KF-YF_3 system. The morphologies and crystal structures of the materials displayed a critical dependence on the pH and the dicarboxylic acid used. Consequently, the materials exhibited a modulated optical response: orangish-yellow emissions, high quantum efficiencies (65–133 %), and very long lifetimes (7–12 ms). The calculation of the Judd-Ofelt parameters also allowed to establish a relationship between the physicochemical properties of the phosphors and their luminescence.

The above novel strategy could arouse widespread interest since it could also be applied to a vast gamut of compounds from the extended family of yttrium/lanthanide fluorides and find interesting applications in bioanalytics, photonics, or white light-emitting diodes.

Biography

Pablo Serna-Gallén is graduated in Chemistry with honors from the University Jaume I, Spain, and got a Master's Degree in Applied and Pharmacological Chemistry with further specialization in Advanced Materials. Currently developing his Ph.D. degree at the same university, his research focuses on optical materials with fluoride-type structures doped with lanthanide ions. He has obtained numerous important national and local awards for his academic marks and research, such as the "Suschem" National Award for the best academic record of Chemistry Sciences (9.71/10), runner-up award in the National "XVII Archimedes University Contest", or different Literary Prizes of Scientific Divulgation. In addition, he is a member of the governing board of the Official Chemists College and Chemists Association of the Valencian Community and he is also a member of the Spanish Society of Academic Excellence.

A safe, flexible, and high-performing gel-polymer electrolyte for rechargeable lithium metal batteries

Julen Castillo[1,2], **Alexander Santiago**[1], **Xabier Judez**[1], **Iñigo Garbayo**[1], **Maria C. Morant-Miñana**[1], **Heng Zhang**[1], **Michel Armand**[1] and **Chunmei Li**[1]

[1]*Basque Research and Technology Alliance, Spain*
[2]*University of the Basque Country, Spain*

The use of gel polymer electrolytes (GPEs) is of great interest to build high-performing rechargeable lithium metal batteries (LMBs) owing to the combination of the good electrochemical properties coming from the liquid and improved safety of the polymer host. In this work, we report a facile and scalable one-pot preparation method of a GPE based on a highly safe polyethylene glycol dimethyl ether (PEGDME) plasticizer in a poly (vinylidenefluoride-co-hexafluoropropylene) (PVDF-HFP) polymer matrix. The prepared GPE exhibits excellent safety (non-flammability and thermal stability up to 250°C) and outstanding electrochemical properties at room temperature (high ionic conductivity of 3.4×10^{-4} Scm^{-1}). Moreover, GPE delivers good C-rate response and high capacity (ca. 1 mAh cm^{-2} at C/10). Notably, the prototype pouch cell (ca. 19 mAh at C/10) provides remarkable safety, mechanical flexibility, and strong tolerance towards bending and cutting. These results suggest that the prepared GPE is a promising candidate for the development of high-performance, flexible and safe LMBs that operate at room temperature.

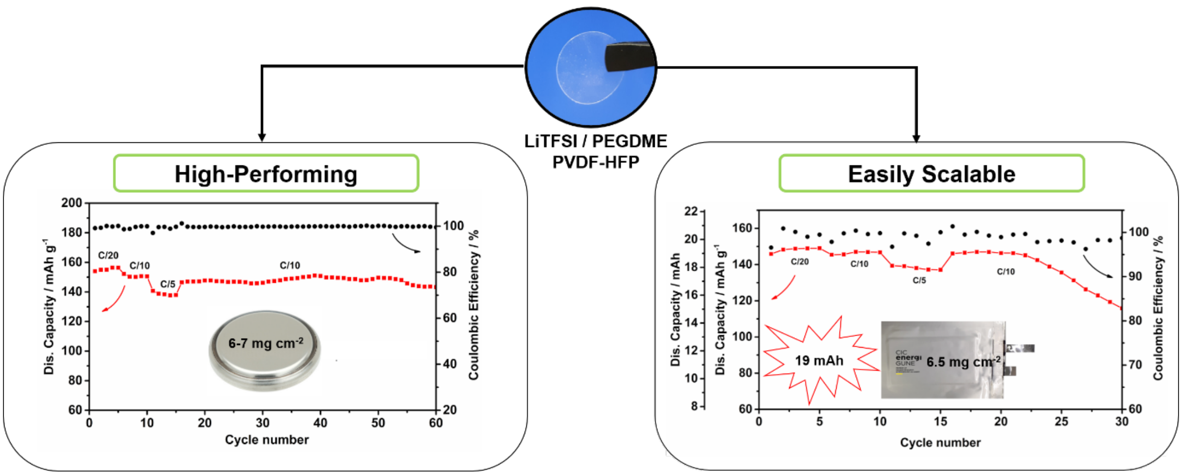

Figure 1. Battery test performance at coin and pouch cell level at different C-rate

Biography

Julen Castillo finished his degree in Chemical Engineering in 2018 at the University of the Basque Country (UPV-EHU). During his last year of studies, he joined the company Petróleos del Norte SA as an internship student where, among other things, was dedicated to the adaptation of the API 751 safety standard to the alkylation unit of that company. He obtained a postgraduate scholarship awarded by the UPV/EHU to complete the interuniversity master´s degree in Chemical Engineering at the UPV/EHU and Universidad de Cantabria. In 2019, he joined CIC energiGUNE focusing on the development of gel polymer electrolytes for its application in lithium-sulfur batteries. Currently, he is doing his doctoral studies at CIC energiGUNE as a member of the Electrochemical Energy Storage group, focalizing on the development and the study of the upscaling process of batteries for ambient temperature operation based on solid and safe electrolytes.

Plasmo-electronic properties of self-organised nanoparticles

Jérémie Grisolia, Louis Merle and **Adnen Mlayah**
University of Toulouse, France

The coupling between charge transport and surface plasmons in metal nanostructures is the driving force of the emerging "plasmo-electronics" field, which may lead to a new class of light responsive nano-devices. Exploiting such a field need the conversion of light into charge carriers flowing through self-assembled NPs that requires the understanding of quite complex phenomena involving several interaction steps (plasmon-photon, electron-electron, electron-phonon). Here, we report on the plasmo-electronic properties of self-assembled monolayers of colloïdal gold nanoparticles (NPs) formed on a polyimide flexible substrate and on freestanding membranes. In these studies, impedance spectroscopy measurements were used to investigate the electrical properties of the NP assemblies in terms of an equivalent macroscopic electrical circuit, describing the overall self-assembled NPs, and composed of a resistance, a capacitance and a photoconductance (Figure 1a). The NP assemblies deposited on a flexible polyamide substrate were submitted to a uniaxial strain which allows to monitor the interparticle distance in the sub 10nm regime and hence to probe their plasmo-electro-mechanical properties. In particular, the dependence of the photo-capacitance on laser irradiation intensity and wavelength is measured, and the role of the surface plasmon resonance was pointed out. In the case of NP assembly deposited on freestanding membranes, we show that the

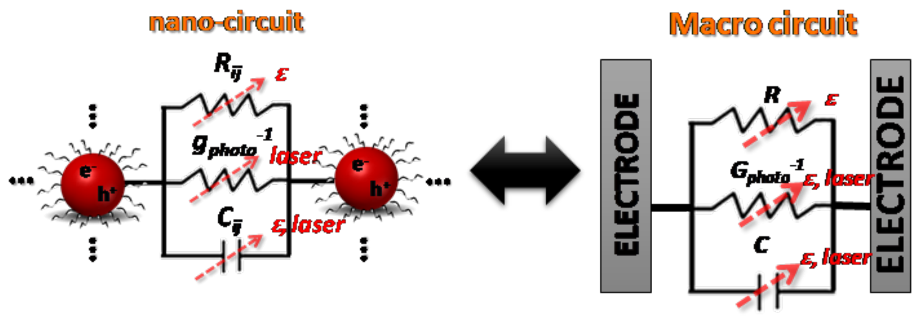

Figure 1: (a) Schematics of the macro-circuit describing the overall NPs assembly and

(b) the nano-circuit consisting by two neighboring nanoparticles.

photo-current generation and charge transport are due to a bolometric phenomenon involving laser induced temperature heating up to 40 degrees combined with trapping/detrapping of the charges at defect sites.

On the basis of these experiments, the electrical equivalent macro-circuit was found to be directly connected to a local nano-circuit composed of a local inter-particles resistance Rij, a capacitance Cij and a photo-conductance gij-1(Figure 1b) which depend on the NP size, nature of the ligands, distance between nanoparticles, and spatial arrangement of both the ligands and the NPs within the assembly. Actually, the mechanisms at the different characteristic scales still need to be understood in terms of relation-ship between the local opto-electronic properties at the nanoparticle scale and the macroscopic characteristics of the photo-conductance (spectral dependence and positive or negative) properties of the NP assembly. We thus report on the development of the nano-circuit junction model to bridge the gap between the nano and the macro-circuit.

Biography

Jeremie GRISOLIA received is PhD in physics from the University of Toulouse III (France) in 2000 at CEMES/CNRS. He started in the MEMS industry at OPSITECH's startup, a spin-off of CEA-LETI producing optical system on a silicon chip. Since 2002, he joined INSA Toulouse and is now full Professor and director of the physics department. His research at the LPCNO laboratory focuses in electrical characterization of nanoparticle assemblies (transport and impedance spectroscopy). Currently, he is developing the field of plasmoelectronic coupling electron transport with plasmonic.

Effect of the chemical composition and dimensionality of halide perovskites for photovoltaic applications on their basic properties: Insights from theory

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[2]Institut Photovoltaïque d'Ile-de-France, France

The chemical compositions and dimensionality (3D (bulk), 2D (surfaces, interfaces, thinfilms) and 0D (nanorod)) of materials for photovoltaic applications strongly influence the performances of solar cells. Their impact concerns mainly the electronic properties and the domains and surfaces stabilities of the different compounds. In the photovoltaic domain, hybrid halides perovskites have displayed dramatic advances; but their instabilities against light, heat, and moisture remains a technological lock for their commercial development. This presentation aims to illustrate the ability of the atomic based on first-principles approaches to describe electronic, structural and dynamical properties of halide perovskites. It mainly focuses on the influence of their dimensionality on their basic properties and on the simulation of the insertion and adsorption of H_2O, CO, CO_2 and O_2 in the bulk materials and on various surfaces of different halides perovskites. These different data were interpreted in terms of electronic charge population analysis, band gap evolution, vibration spectra, and, insertion and adsorption energies.

Biography

Philippe Baranek is researcher in the research and development division of Electricité de France (EDF). He received the PhD degree in 1998 from the University of Sciences and Technologies of Lille, France. His research focus on the atomic modelling of the structural, electronic, dynamic and dielectric bulk and interfaces properties of materials for the production and storage of electricity. Currently, his activities are mainly dedicated to the photovoltaic applications..

Effect of adamantane substitutions to improve properties of organic optoelectronic materials

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[1]Brno University of Technology, Czech Republic
[2]Johannes Kepler University Linz, Austria
[3]Università degli Studi di Bari Aldo Moro, Italy

Nowadays many organic semiconductors have been developed to improve the device performance, where most of the efforts focus on the design and synthesis of new π-conjugated backbones. Alkyl chains (linear, branched) or fluoroalkyl chains are commonly used side chains in organic semiconductors. These side chains generally do not directly contribute to charge transport in organic semiconductors and are usually used as solubilizing groups. Adamantane is the simplest diamondoid and possesses exceptional physical properties. Moreover, adamantane is more stable saturated hydrocarbon isomer of such a small molecular weight.

Here we present a new approach by adamantane substitution of π-conjugated dyes which have significant influence to final optical and electrical properties of studied materials. This allows us to systematically study the effect of adamantane solubilization side groups to induce π–π interactions between the conjugated cores through adamantyl–adamantyl stacking. Careful choice of adamantane substituent may provide a highly ordered crystalline organization of the material with the efficient interconnection of crystalline domains and intermolecular π-orbital overlap, thus providing charge carrier mobilities even higher than that of the parent material.

This approach can be universally applied for many types of semiconducting organic materials containing the imide motive, where solubilization is achieved by side-group substitution.

Biography

Jozef Krajcovic is Associate Professor of Organic Chemistry at Brno University of Technology, Faculty of Chemistry (FCH BUT). Leader of the group of Synthesis of Advanced Materials. He currently coordinates the research activity on the study and synthesis of new conjugated heterocyclic systems, organic dyes and pigments for sustainable energies, and synthesis of Nature-inspired molecules for organic bioelectronic applications. Moreover, he also provides investigation about the synthesis of perovskite single crystals and perovskite nanoparticles.

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Changing the paradigm of pressure injury (PI) prevention: Translating sub epidermal moisture (SEM) assessment technology from bench to bedside

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[1]Abbott Northwestern Hospital, USA
[2]Bruin Biometrics LLC, USA

Background: The current standard of pressure injury (PI) care does not provide anatomically specific prevention to at-risk patients. SEM assessment technology uses clinically proven algorithms to identify increased risk of PIs. Anatomy-specific SEM assessments enable clinicians to provide early and precise interventions that are significantly effective in PI prevention.

Purpose: Formal, controlled clinical studies were conducted to demonstrate the value of SEM assessment technology in identifying increased risk of PIs. Subsequently the technology was implemented as an adjunct to routine clinical assessments in everyday PI care practice in multiple care settings.

Methodology: Two foundational observational studies enrolled 125 participants with confirmed PIs or suspected deep tissue injury and 50 healthy study participants. A third blinded, longitudinal, prospective clinical study enrolled 189 participants. A formal, pragmatic, real-world pressure ulcer reduction program (PURP) evaluated 2,439 patients across 34 care facilities by incorporating SEM technology as the only change to existing daily PI prevention workflows.

Results: Observational studies resulted in:

- Two spatial algorithms indicating sensitivity of 87-82% and specificity of 88-51% at the conservative cutoff of SEM $\Delta \geq 0.6$.
- Receiver operating characteristic (ROC) curves computed areas-under-the-curve (AUC) of 0.7809-0.9181 (95% CI, $p<0.0001$).

The third blinded study resulted in:

- Sensitivity of 87.5% (95% CI) and specificity 32.9% (95% CI).
- AUC was 0.6713 (95% CI, $p<0.001$).

Real-world data analysis showed:

- 90.5% PI incidence reduction in acute care settings.
- 3-fold reduction in incidence risk with SEM assessment technology as a dominant quality strategy over other care pathways.
- Sensitivity of 62.3-75.0% and a specificity of 45.2-61.7% with AUC's ranging from 62.5-66.0% (95% CI, $p<0.001$).

Conclusion: The diagnostic accuracy of SEM assessment technology exceeded that of clinical judgment alone in both controlled clinical study settings and in a variety of care settings with diverse real-world population. SEM assessment technology has advanced from bench to bedside in the real world.

Biography

Ruth Bryant is a Principal Research Scientist/Nursing at a large Midwestern quaternary care center (Abbott Northwestern Hospital, Minneapolis, MN). In her role, she oversees clinical inquiry projects by the nursing staff, mentors doctoral students, and conducts clinical research. Her areas of research include patient safety, pressure injuries, subepidermal moisture, wound healing, patient engagement, and healthcare worker wellbeing and retention. Her career spans over 30 years as a board certified Wound, Ostomy, Continence (WOC) Nurse, the Director of two WOC Nursing Education Programs and the co-creator of the first web-based WOC nursing education program, the webWOC Nursing Education Program. She is also the founding editor and currently co-editor of "Acute and Chronic Wounds: Current Management Techniques", now in its 5th edition. She is well known nationally and internationally as a wound care expert and Past-President of the Association for the Advancement of Wound Care (AAWC).

Nanoparticles as cell tracking agents in human ocular cell transplantation therapy

David C. Mundy and **Jeffrey L. Goldberg**
Stanford University School of Medicine, USA

Cell transplantation is a promising strategy for treating degenerative eye disorders for which no curative therapies exist, including age-related macular degeneration (AMD), diabetic retinopathy, and glaucoma. While past and ongoing clinical trials of ocular cell transplantation have demonstrated encouraging findings, our insight into their successes and failures is limited, in large part due to the difficulty of following the fate of the transplanted cells in the human eye. Here we explore the potential use of nanoparticles (NPs) as cell tracking agents in ocular cell therapy, highlighting their advantages over other labeling methods such as fluorescent reporters and DNA barcoding. Two classes of NP—gold nanoparticles (GNPs) and superparamagnetic iron oxide nanoparticles (SPIONs)—may be particularly well-suited for longitudinal cell tracking in the eye, owing to their safety profile and compatibility with clinical imaging modalities. To establish these NPs as viable cell trackers in human ocular cell therapy, further research should be aimed at elucidating their eye-specific imaging characteristics, safety, and clearance. Our ability to accurately assess the critical processes in ocular cell transplantation—delivery, distribution, immune acceptance, retention, and integration—will help accelerate the progress of regenerative medicine in the eye.

Biography

David Mundy studies Medicine at Stanford University School of Medicine. His research is focused on harnessing regenerative approaches to restore vision in the eye. He received his undergraduate degree from Stanford University, where he was a Bio-X fellow and earned the Dean's Award for Academic Excellence. At Stanford Medicine, he was awarded the Medical Scholars Grant and has authored several papers on natural killer cell biology and tumor immunology. Currently, his main research interests include: (1) developing hydrogels for stromal replacement and stem cell delivery to facilitate tissue regeneration; and (2) developing theranostic nanoparticles for ocular regenerative therapy.

Developing a needle-knife surgical device

Ravaglia, Fabio FA and **Cliquet Jr, Alberto**
University of Campinas, Brazil

Scope: Nowadays, a new era of orthopedic surgery is taking place. Procedures like ultrasound-guided interventions, invasive pain orthopaedics interventions, started to be widely performed.

Objective: The aim of the project is a virtual development of a needle-knife surgical device to be useful for minimally invasive orthopaedic surgical procedures and other surgical procedures.

Method: Three different needle devices were compared. One is a base model

1 and the other two are experimental models 2 and 3. They are based on a metal guide for intravenous catheter 14Gx2''. The base one model 1 is the metal guide for intravenous catheter 14Gx2''; the experimental model 2 is a flat beveled edge, and experimental model

.3 is a board bevel edge they are all graduated, parylene-coated, with a stop handle needle guard.

The devices were developed by 3D Design 3D STEP Standard Format, Catia V5 Format, and 2D Format Design and 3D Model.

They were biomechanically simulated with Virtual Biomechanical Strength Simulation (Software Simulia Abaqus)..

The Strengths were assessed by Needle Strength Analysis (CAE Simulation).

Results: The present study compares three models. A control base model 1 and two experimental models; model 2 and model 3.

Model 3 presented similar features in rigidity to the baseline model 1 (3,6%). They have a similar performance.

The tip of model 3 increased a tension of 15%; but does not mean fracture risk 22. S

Conclusion: These devices seem suitable for eco assisted orthopaedic surgery interventions and other procedures according to virtual analisis. Further *in vivo* procedures must be performed.

Biography

Fabio Ferraz do Amaral Ravaglia is an Brazilian Orthopaedic Surgeon qualified at the Sao Paulo Federal University in 1985. He participated in the Overseas Doctors Training Surgeon program of the Royal College of Surgeons of England from 1991 to 1994. He was qualified for Master Degree of Science 2010 at State University of Campinas (Brazil). Since 2010 Alberto Cliquet Júnior; the Head of Orthopaedic Department of State University of Campinas (Brazil) has been working in developing a Needle Knife Surgical Device. They patented this first prototype after clinical studies. Alberto and Fabio are writing the second generation of the Needle Knife Surgical Device and is the doctoral project at State University of Campinas (Brazil).

Gas permeameter for polymers and nanocomposites: Improvements and advances

Gilberto João Pavani[1], **Sérgio Adalberto Pavani**[2] and **Carlos Arthur Ferreira**[3]

[1]*Federal Institute of Rio Grande do Sul, Brazil*
[2]*Federal University of Santa Maria, Brazil*
[3]*Federal University of Rio Grande, Brazil*

Gas permeability in homogeneous semi permeable materials such as semicrystalline polymers is the object of research in several fields, in particular, in the oil and natural gas prospecting industries. However, information on gas transport coefficients under extreme pressures and temperatures is rarely found in the literature. Therefore, the objective of this work is to showcase a medium pressure gas permeameter suitable for polymeric and polymeric nanocomposite plates, developed by the authors, which was validated with Nitrogen at 1 MPa and 69ºC (342.15 K) using pure high density polyethylene samples (HDPE) and samples with nanoclay, redoing the tests published in a previous work. The obtained results were compared against data gathered in a previous work and data found in literature, validating the new model of this equipment, which is capable of analyzing gas permeability under the described conditions with greater accuracy than the previous model for the values of the transport coefficients of Nitrogen in HDPE, demonstrating that the implemented improvements and advances were adequate, allowing the measurement of the transport properties of gases permeating polymeric and nanocomposite plates, necessary information for the design of risers for the transportation of oil and natural gas, for example.

Biography

Gilberto João Pavani graduated in Mechanical Engineering from Federal University of Rio Grande do Sul - Brazil (1991), postgraduate in Systems Analysis from Pontifical Catholic University of Rio Grande do Sul - Brazil (1994), degree in Informatics from Federal Center for Technological Education of Minas Gerais - Brazil (1996), postgraduate in Occupational Safety Engineering from Unisinos - Brazil (2001), master's degree in Computer Science from Federal University do Rio Grande do Sul - Brazil (2003) and doctorate in Materials Science (student) from Federal University of Rio Grande do Sul. - Brazil. Professor at the Federal Institute of Education, Science and Technology of Rio Grande do Sul - Brazil. Interested in polymeric composites, mechanical manufacturing processes and work safety. Author of several books in the field of Mechanical Engineering.

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Development of advanced composite materials by additive manufacturing

H. Fayazfar
University of Ontario Tech, Canada

Development of novel composite materials compatible with additive manufacturing while satisfying multifunctionality and cost for end-use applications is an urgent need to address limited materials available for AM. In this research, we developed novel nanocomposite materials based on zirconia bioceramic embedded in polymer matrix compatible with a customized material Jetting system. This new generation in-house developed MJ system is one of the scarce 3Dprinters of its kind which enables high-speed 3Dprinting (20 times faster than the current extrusion/jetting AM methods) of high viscous inks (upto 10^7 mPa.s). By inserting additives/surfactants to different amounts of photocurable polymers and Zr nanopowders, tailoring the rheology/feedstock concentration, and optimizing the printing parameters, we innovatively prepared a suitable feedstock for MJ printing and troubleshot arisen printing issues (e.g. nozzle clogging and Zr nanoparticles inhomogeneity in the polymer matrix), which are among the most significant challenges of developing compatible composite materials for extrusion-based 3Dprinting. A two-step sintering was developed to burn out the polymers, shrink the porosities, and obtain densified crack-free Zr components with high mechanical/structural properties to meet the demanding requirements as dental restorations. The exciting results stemming from this work inspired another research on developing a conductive polymeric composite including silicone (matrix) and carbon fiber (filler) for 3Dprinting of flexible wearable sensor for health monitoring applications. Feedstock concentration and printing parameters were optimized to attain printability, curability, and electrical properties of the feedstock. Particularly, carbon fiber loading and aspect ratio were optimized to attain the lowest percolation threshold and good electrical conductivity while prohibiting nozzle clogging issue. A number of potential applications of developed composite sensors including human motion detection such as finger movements and bending at the arm were evaluated. The outcomes showed significant innovative advancements in filling the gaps in current state-of-the-art to develop compatible composite materials for AM for biomedical applications.

Biography

Ramona (Haniyeh) Fayazfar is currently an assistant Professor in Mechanical and Manufacturing Engineering department in University of Ontario Tech, Canada. Her main research concentrates on Nanostructured Composites/Hybrid Materials, Advanced Manufacturing (Nano Fabrication and Additive Manufacturing), Electrochemical Synthesis of Nanostructured Materials, Advanced Coatings and Surface Treatment, Biosensors for Point-of-Care Diagnostics and Health Monitoring. The outcomes of her research have been published in high prestigious journals/conferences and covered by various media outlets. She got the Best Research Award from "Intern. Research Awards on New Science Inventions ", 2021. Prior to joining Ontario Tech, she was a postdoctoral fellow in Multi-Scale Additive Manufacturing group in University of Waterloo. She received her Bachelor’s, Master’s, and PhD degrees in Materials Engineering from Sharif University of Technology, Iran. She has been awarded the University commemorative plaque and medal from the President of SUT for being ranked first among all graduated PhD and Master’s.

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Deposition of biopolymers by cold gas spray

J. Henao[1], **D. Garcia**[2], **A. Giraldo**[3], **P. Forero**[4], **J. Corona**[2] and **C. Poblano-Salas**[2]

[1]*National Research Council of Science and Technology (CONACYT) - CIATEQ A.C., México*
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[3]*National Research Council of Science and Technology (CONACYT) - CINVESTAV, México*
[4]*CINVESTAV, México*

The low-pressure cold spray process is a technique originally developed for the fabrication of industrial metallic coatings. Hence, it is not currently useful for the preparation of polymer coatings unless the introduction of some modifications into the gun is considered. Polymer coatings can have very interesting functional applications in the biomedical field, as they can provide bioactivity and enhance biocompatibility of metallic implants. Given the interest in this type of coatings for biomedical applications, some efforts have been performed by our research team to understand the thermo-kinetic conditions that some biopolymers undergo while they are processed by low pressure cold spray. This knowledge has allowed us to introduce some modifications into the cold spray gun design to enable this technique for the fabrication of polymer coatings. The results of our research suggest that dimensions of the cold spray gun nozzle are crucial to modify the kinetic and thermal history of the in-flight particles in the process; those changes can also be optimized to promote the formation of the coatings. Although, further efforts must be endeavor to understand the mechanisms acting upon the polymer particles during impact to fully understand the bonding mechanisms involved.

Biography

John Henao is a fellow researcher from Mexico´s national council of science and technology (CONACYT). He occupies a full-time research position at the advanced materials department in CIATEQ A.C. His research interest is focused on the development of biocompatible coatings by thermal spray processes for biomedical applications. He has also been working on other topics such as metallic glass coatings for corrosion/wear applications, intermetallic/ceramic coatings for energy applications, and additive manufacturing of metals. In recent years, he has published some book chapters and several peer-reviewed papers on these topics.

KEYNOTE PRESENTATIONS

DAY 3

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BIOGRAPHY

Du Ngoc Uy Lan currently works as a research associate at of Polymer Engineering, University of Bayreuth, Germany. His research focuses on the preparation and characterization of epoxy foams by solid-state physical/chemical foaming and aqueous emulsion technique; and thermal mechanical degradation of thermoplastic composites.

From 2010 – 2019, he served as a Senior Lecturer in Polymer Engineering at the School of Materials Engineering – University Malaysia Perlis, Malaysia. He had worked as a Senior Chemist in Synthomer - Malaysia in 2010 and a Chemist in Adidas, Vietnam 2004 – 2006. He pursued his Master degree in Polymer Engineering at University Science Malaysia from 2001 – 2003. He was a JICA scholar and earned his Ph.D. in Polymer Engineering under AUN/Seed-Net sandwich program between University Science Malaysia and Kyoto University-Japan in 2006 – 2009.

Du Ngoc Uy Lan

Universität Bayreuth, Germany

Foaming epoxy-amine-carbamate: The effect of different neat amines on rheological and cellular morphology

The use of carbamate to foam epoxy depends significantly on the precured modulus to stabilize the cellular structure. The optimum precured modulus is developed from the reaction of epoxy and the neat amine. The selection of neat amine relies on its reaction temperature with epoxy, which is required to be lower than 70°C (the decomposition temperature of carbamate). This study focuses on the foaming rheological behavior of epoxy-carbamate filled three different neat amines. They are bisphenol-A diglycidyl ether epoxy (DGEBA), isophorone diamine carbamate (IDPA.CO_2), N-aminoethylpiperazine (AEP), 2,4-Diamino-1-methyl-cyclohexan (DMC) and isophorone diamine (IDPA). Three mixtures of DGEBA-amine-carbamate are filled in 25% and 75% volume of a close mold. The precuring is carried out by 60°C for 2 hours. The foaming and complete curing are conducted at 180°C for 1 hour. Having H-active at piperazine, AEP reacts with DGEBA faster and develops a higher precured modulus compared to DMC and IDPA. It is importantly noticed that DGEBA-30AEP-70IDPA.CO_2 shows viscoelastic behavior beyond 138°C (Rheological storage modulus is lower than loss modulus; and tan delta is larger than 1). The reaction between DGEBA and the H-active at piperazine of AEP only produce a linear linkage and is unable to further crosslink compared to primary amine (-NH_2). This results in a larger cell size cell size (167μm) and a lower density (285 kg/m^3) as well as a lower glass transition temperature Tg of DGEBA-30.AEP-70IPDA.CO_2 foam. Having quite similar chemical structure, both DMC and IPDA produce the epoxy foams having similar densities of 301 kg/m^3 and 305 kg/m^3 and the average cell sizes of 103 μm and 106 μm, respectively.

BIOGRAPHY

Lucia D'Accolti obtained a tenure track position as Researcher in Chemical Sciences in1994 at the University of Bari (Italy). In 1999, she moved to the University of California–Los Angeles (UCLA, USA) where she worked as visiting researcher with Prof. C.S. Foote. She has been Professor Associate at the University of Bari. Her research interests are in the synthesis and reactivity of dioxirane and inorganic peroxides, synthesis and application of heterogeneous organo-catalysts, and photocatalysts for selective oxidation reactions. In recent years she has carried out several studies, in the field of green chemistry, with attention to bioplastics and biofuels, and more generally to eco-design.

Lucia D'Accolti
University of Bari, Italy

Valorization of waste for the materials and energy

The valorisation of waste represents a new challenge for green chemistry, because it allows to avoid consuming soil and water that is non-renewable resources. Applying non-critical raw materials catalysts and a cradle to cradle approach, it is possible obtain chemicals such as formic acid, hydrogen corrier, levulin acid, and biofuels.

BIOGRAPHY

Huirong Le is currently a principal investigator of The Future Laboratory of Tsinghua University leading the Future Materials Design Research Center. He received a bachelor's degree of engineering in 1989, and received a doctorate in engineering in March 1994 from Tsinghua University. He joined the University of Surrey in 1996, then the University of Cambridge in 1997 as a postdoctoral researcher. He was promoted to Senior Research Associate at Cambridge in 2000. He became a lecturer at the University of Dundee in 2005, then an associate professor at Plymouth University in 2011 and then professor at the University of Derby in 2015. He has led or participated in about twenty research projects funded by EU, EPSRC and Innovate UK. He became a Fellow of the Institution of Materials Minerals and Mining (FIMMM) in July 2018 and Fellow of the Institution of Mechanical Engineers (FIMechE) in October 2018 and Fellow of Royal Society of Arts in January 2022.

Huirong Le

Tsinghua University, China

Mechanical properties and thermal stability of fiber reinforced geopolymer composites

This paper investigated the thermal resistance, mechanical properties and phase evolution of geoploymer ceramics reinforced with mullite fibers. The geopolymer composites were prepared from kaolinite and mullite fibers with phosphoric acid as activator. X-ray diffraction (XRD), thermogravimetry and differential scanning calorimeter (TG-DSC), Fourier transform infrared spectroscope (FTIR) and scanning electron microscope (SEM) were used to determine the phase evolution and strengthening mechanisms. With the addition of mullite fibers, the mechanical properties increased by at least 20%. The optimum flexural strength exceeded 13 MPa. It was found that mullite fibers have desirable interface bonding with this type of geopolymer leading to both crack deflection and fiber pullout strengthening mechanisms. This is correlated with the significant strengthening effect of the fibers. The linear shrinkage after heat treatment at 1150°C ~1550°C was investigated. The addition of mullite fibers reduced the linear shrinkage significantly up to 1350°C. It was found that the large linear shrinkage above 1450°C was due to the decomposition and melting of $AlPO_4$ phase.

SCIENTIFIC ABSTRACTS

DAY 3

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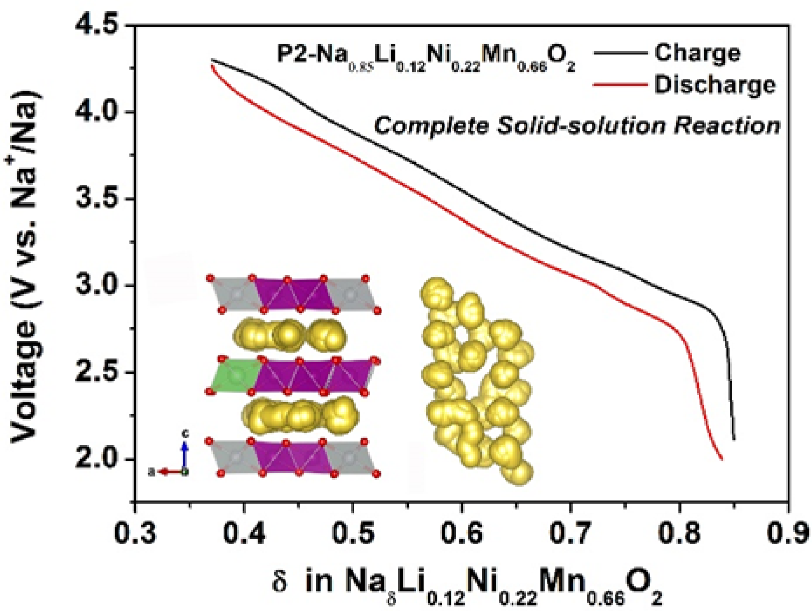
Adv. Materials Science 2022

High sodium content P2-type cathode for high-performance sodium-ion batteries

Ting Jin
Northwestern Polytechnical University, China

P2-type layered oxides suffer from an ordered Na^+/vacancy arrangement and P2→O_2/OP_4 phase transitions, leading them to exhibit multiple voltage plateaus upon Na+ extraction/insertion. The deficient sodium in the P2-type cathode easily induces the bad structural stability at deep desodiation states and limited reversible capacity during Na^+ de/insertion. These drawbacks cause poor rate capability and fast capacity decay in most P2-type layered oxides. To address these challenges, a novel high sodium content (0.85) P2-type cathode-$Na_{0.85}Li_{0.12}Ni_{0.22}Mn_{0.66}O_2$ was developed. *In situ* XRD shows both P2→O_2/OP_4 phase transitions and Na+/vacancy ordering can be successfully converted into a complete solid solution dominated region after Li substitution. The complete solid-solution reaction over a wide voltage range ensures both fast Na+ mobility (10-11 to 10-10 $cm^2\ s^{-1}$) and small volume variation (1.7%). The high sodium content P2-$Na_{0.85}Li_{0.12}Ni_{0.22}Mn_{0.66}O_2$ exhibits a higher reversible capacity of 123.4 mA h g^{-1}, superior rate capability of 79.3 mA h g^{-1} at 20 C, and 85.4% capacity retention after 500 cycles at 5 C. This work highlights the importance of the solid-solution reaction mechanism in a high sodium content P2-type cathode, which ensures higher reversible capacity, superior cycling stability and remarkable rate capability.



Biography

Ting Jin is a professor at the State Key Laboratory of Solidification Processing and the School of Materials Science and Engineering at Northwestern Polytechnic University, China. She received her PhD in 2020 from Nankai University (China) and her B.S. in materials chemistry from Northwest University (China) in 2015. Her research interests focus on the design and fabrication of advanced electrode materials for energy storage and conversion, such as rechargeable lithium-ion and sodium-ion batteries.

Circular polarizing filters based on chiral metasurface

X. He, J. Li, X. Liu and **X. Hao**
Zhejiang University, China

Chirality is a structural feature in which two objects are mirror images of each other, similar to the left and right hands. For example, we can find the chirality in DNA, cholesteric liquid crystals, screws, and circular metal spirals. Meanwhile, the left circular polarization and right circular polarization light tracks are mirror images, like the above chiral structures.

Metal gratings based on the Plasmonics are sensitive to linear polarization light. The 3D helices can be considered as the integral of metal gratings twisted with a constant angle along the propagating direction. By adjusting the twist angle and effective length of the polarization charge oscillation, the anisotropy of a single arc can be successfully transformed into a broadband double anisotropic optical response. Moreover, the chiral metasurface exhibits nearly uniform circular dichroism and asymmetric transmission to circularly polarized light. Therefore, we can use chiral metasurfaces to make circular polarizers.

The application of circular polarization imaging is particularly extensive, covering various fields such as biomedical imaging, material science, space remote sensing, and military target recognition, including such as flying airplanes, living cells and tumor lesion detection, which can greatly improve our lives and promote the development of science and technology. For example, when we conduct medical research, the main disadvantage of polarization gating of light backscattered from tissue is that surface reflections affect the image. The combination of images obtained by using linearly polarized and circularly polarized light can produce polarization-gated images without surface reflection, no need additional optical devices and materials.

In view of these various types of omni-directional applications, we do need chiral metasurface based circular polarizers.

Biography

Xin He is currently working at Zhejiang University as a Postdoctoral researcher. He obtained a PhD and a Master's degree at the University of Melbourne. His PhD research interests include plasmonics, spectral imaging and other metasurface based optical devices (e.g., polarizers, phase shifter, metalens). He obtained advanced skills on COMSOL Multiphysics, FDTD and Micro/Nano fabrications. He also created a prototype of a multispectral image sensor with six bands, the minimum full width half maximum (FWHM) is 17nm in the near IR wavelength.

Fabrication of pore-selectively silver-functionalized honeycomb-patterned film and its application for antibacterial activity

D. S. Huh, S. Falak and **B. K. Shin**
Inje University, South Korea

Pore-selective silver (Ag)-functionalized honeycomb-patterned (HCP) polystyrene (PS) films were fabricated via a modified breath figure method using an interfacial chemical reaction and its application for an antibacterial film using the role of micro-trapping pit was systematically studied. PS polymer solution containing ferrocene which acts as a reducing agent was cast under humid conditions containing silver nitrate ($AgNO_3$) to induce an interfacial chemical reaction between ferrocene and $AgNO_3$ at the water droplet/polymer solution interface. The antibacterial activity of the film against *Escherichia coli* and *Staphylococcus aureus* was assessed by the micro-dilution method and crystal violet assay. The study of BF for a functional HCP film by accompanying an interfacial chemical reaction for the pore-selective Ag functionalization shows that specific metal or inorganic materials could be pore-selectively functionalized by a similar method under various conditions, thus potentially giving the HCP films various applications.

Biography

Do Sung Huh is working as a Professor of Department of Chemistry, Inje University, South Korea. He completed PhD in Korea Advanced Science and Technology (1989).

Compact dual-band 4-MIMO Antenna elements for 5G mobile applications

Fayad Ghawbar, Jumadi A. S, H. A Majid, Aimi S.A Ghafar, Faiz A. Saparudin and **B.A.F Esmail**
Universiti Tun Hussein Onn Malaysia, Malaysia

The Multiple Input Multiple Output (MIMO) system in the 5G wireless communication system is essential to enhance channel capacity and provide a high data rate resulting in a need for dual-polarization in vertical and horizontal. Furthermore, size reduction is critical in a MIMO system to deploy more antenna elements requiring a compact, low-profile design. A compact dual-band 4-MIMO antenna system has been presented in this paper with pattern and polarization diversity. The proposed single antenna structure has been designed using two antenna layers with a C shape in the front layer and a partial slot with a U-shaped cut in the ground to enhance isolation. The 4-MIMO antenna elements were printed orthogonally on an FR4 substrate with a size dimension of 36 × 36 × 1.6 mm^3 with zero edge-to-edge separation distance. The proposed compact 4-MIMO antenna elements resonate at 3.4-3.6 GHz and 4.8-5 GHz. The s-parameters measurement and simulation results agree with a slight frequency shift of the measurement results at the upper band due to fabrication imperfection. The proposed design shows isolation above -15 dB and -22 dB. The MIMO diversity performance has been evaluated in terms of efficiency, envelope correlation coefficient (ECC), diversity gain (DG), total active reflection coefficient (TARC), and channel capacity loss (CCL). The total and radiation efficiency were above 50 % across all parameters at both frequency bands. The ECC values were lower than 0.10, and the DG results were about 9.95 dB in all antenna elements. TARC results exhibited values lower than -25 dB at the dual-bands. Moreover, the channel capacity losses in the MIMO system were depicted using CCL, resulting in values lower than 0.4 Bits/s/Hz. As a result, the proposed design is adequate for 5G applications.

Biography

Fayad Mohammed Ghawbar is an Engineering Technology Ph.D. candidate at Universiti Tun Hussein Onn Malaysia, Batu Pahat, Malaysia. He has received the Master of electrical engineering in 2015 from Universiti Tun Hussein Onn Malaysia. Previously, he has obtained his first degree from Universiti Malaysia Pahang, Malaysia, with honors, in electrical & electronics engineering in 2013. His current Ph.D. research is under RF Microwave MIMO technology for 5G applications, especially smartphones. Besides, he is doing recent research about metamaterials to be deployed in high order MIMO antennas for 5G smartphones to reduce the mutual coupling effect.

3rd Advanced
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Hot ECAP implementation in zirconia reinforced aluminium chip matrix (Al6061) composite production

Sami. Al-Alimi[1], M.A. Lajis[1], S.Shamsudin[1], Ahmed Wahib[1], Wenbin Zhou[2] and **Abdulkareem A. Hezam[2]**
[1]Universiti Tun Hussein Onn Malaysia, Malaysia
[2]Imperial College London, UK

The demand of aluminium in transportation sector is growing rapidly due to the high strength to weight ratio requirement for fuel saving and performance purpose. There is a need to develop a sustainable recycling process without melting phase for the secondary aluminium production that can further save the energy, reduce the greenhouse gas emission level and global warming. Therefore, a meltless equal channel angular pressing (ECAP) method was introduced to process the aluminium wastes in the form of chips to achieve the forementioned agenda. In this study, the composites made of aluminium AA6061 chips reinforced with 5%, 10%, and 15% volume fraction of ZrO_2 powder were produced under the different processing temperatures of 450°C, 500°C, 550°C. The experimental results were analysed using the design and analysis of experiments (DOE) principle and assisted by the Minitab 18 software. It was reported that the maximum yield strength and hardness increased to 119.26 MPa and 65.25 VH compared to 100.26 MPa and 50 VH (as-received AA6061) respectively.

Biography

Sami Abdo Mohammed Al-Alimi received the B.Eng. degree in the faculty of mechanical and manufacturing Engineering, Universiti Tun Hussein Onn Malaysia (UTHM), Malaysia 2014, and Master in 2016 form the same university. Passed Ph.D viva on 9/62021. He worked on metal forming of light metals by plastic deformation techniques. He is a researcher in solid-state recycling of light metals, and plastic deformation forming techniques, he worked as a research assistant with an internal grant university. His research interest is in enhancing mechanical and physical of light metals properties, such as aluminium in the composite or pure form as long as developing and combined forming techniques which are superior ways to reproduce metals as same or close to the pure properties.

Correlation between charge transport-recombination loss kinetics and perovskite solar cell performance investigated by TPV and IMVS measurements

Rahmat Hidayat and **Adhita Asma Nurunnizar**
Bandung Institute of Technology, Indonesia

Metal halide perovskite has attracted much attention because of its prospect as high-efficiency solar cell material. In terms of power conversion efficiency (PCE), the perovskite solar cells (PSC) are now competing with silicon solar cells. PSC contains a polycrystalline perovskite layer with random grain sizes and shapes, which may cause various kinds of defect sites on its grain surface and liberated unpaired ions at the intergrain region. Such conditions may cause perovskite layer degradation and parasitic electronic process, leading to poor cell performance and a short operating lifetime. We have performed a study by employing transient photovoltage (TPV) spectroscopy and Intensity Modulated Photo-Voltage Spectroscopy (IMVS). The measured TPV decays exhibit different characteristics on the rise part, in a short interval after photoexcitation, depending on the perovskite mesoscopic morphology. The rise part can be fit by a decay function derived by employing the convolution theorem, as the result of the electron transport process in the perovskite layer, with trapping-detrapping processes and back-transfer process at the perovskite/TiO_2 interface. There is a correlation that the cell with a poorer performance exhibit a longer rise part. The decay part may exhibit a multi-exponential decay characteristic. For a cell with a good performance, a simple multi-exponential decay characteristic can be observed, which can be associated with electron back-transfer via defect states formed at the perovskite grain surface. In a poorer cell, the fast decay component exhibits a stretched exponential decay characteristic, which is a typical non-simple first-order trapping and recombination process by involving electron transport through surface defects. We may also suggest that such decay characteristics are related to a localized lattice relaxation around defect sites. We can also see the correlation of those TPV characteristics with Nyquist plot characteristics obtained from the IMVS measurements, including at the low-frequency arc that is associated with unpaired/mobile ion migration in the slow time scale (hundreds of milliseconds).

Biography

Rachmat Hidayat graduated from the Department of Physics, Institut Teknologi Bandung, in 1993, Master and Doctoral Program of Electronic Engineering of Osaka University in 2001. He is presently a senior lecturer and researcher at Physics of Magnetism and Photonics Research Division, Faculty of Mathematics and Natural Sciences, Bandung Institute of Technology, Indonesia. His research fields are related to optical-photonics material and devices with a major interest in solar cells, light-emitting devices, and plasmonics. He is also currently involved in rechargeable battery and CO_2 recycling research.

Structural, optical and electrical characterizations of Cr-doped CuO thin films

Ilhan CANDAN[1], Silan BATURAY[1] and **Cihat OZAYDIN[2]**
[1]*Dicle University, Turkey*
[2]*University of Batman, Turkey*

The polycrystalline copper oxide (CuO) thin films have been produced using method of spin coating onto the soda lime glass (SLG) as well as substrate of p-type Si (1 0 0) wafers at 500 ºC in furnace. The obtained undoped and Cr doped thin films of CuO have been comprehensively characterized via X-ray diffraction (XRD), ultraviolet–vis (UV–Vis) spectroscopy, the current–voltage (I–V) and capacitance–voltage (C–V) characteristics for providing information on quality of the crystalline nature, change in energy band gap and electrical properties, respectively. Structural analysis results which obtained from XRD data demonstrate that CuO films conjunction with Cr doping indicated that all thin films have monoclinic polycrystalline nature, with two main peaks of (-111) and (111) with dhkl about 2.52 and 2.32 Å, respectively. The transmittance and energy band gap value of undoped and Cr doped thin films of CuO ranging in varying concentration ratio have been determined in the wavelength region of 300 to 1100 nm. The highest value has been found to be around 33 % related to 3% Cr doping in the visible range. UV–Vis spectrum analysis results indicate that both transmittance value and energy band gap of the CuO films are changed with increasing Cr doping ratio in CuO solution at room temperature. The band gap energy was determined to be between 1.67 and 2.03 eV with increasing Cr concentration. The I–V and C–V characteristic of Cr:CuO/p-Si diodes were associated with the CuO/p-Si diodes. It is seen that doping of Cr had a significant change on the obtained devices' performance. Thus, the Cr:CuO/p-Si diodes generated by 1% Cr doping using spin coating method had the highest light sensitivity compared with those of the other diodes.

The electrical parameters of Cr:CuO/p-Si diodes with different doping ratios (0%, 1%, 2% and 3%) at 300 K and dark conditions.

Sample	n	ϕ_b (I-V) (eV)	I_0 (A)	RR (for ±1V)	$\phi_{b\,(Norde)}$ (eV)	R_s (kΩ) (Norde)
0%Cr:CuO/p-Si	2.28	0.73	1.16×10^{-8}	170.7	0.791	4.173
1%Cr:CuO/p-Si	2.17	0.81	4.55×10^{-10}	2335.4	0.734	0.312
2%Cr:CuO/p-Si	2.47	0.75	5.26×10^{-9}	30.4	0.803	36.74
3%Cr:CuO/p-Si	2.14	0.77	2.22×10^{-9}	557.2	0.859	1.064

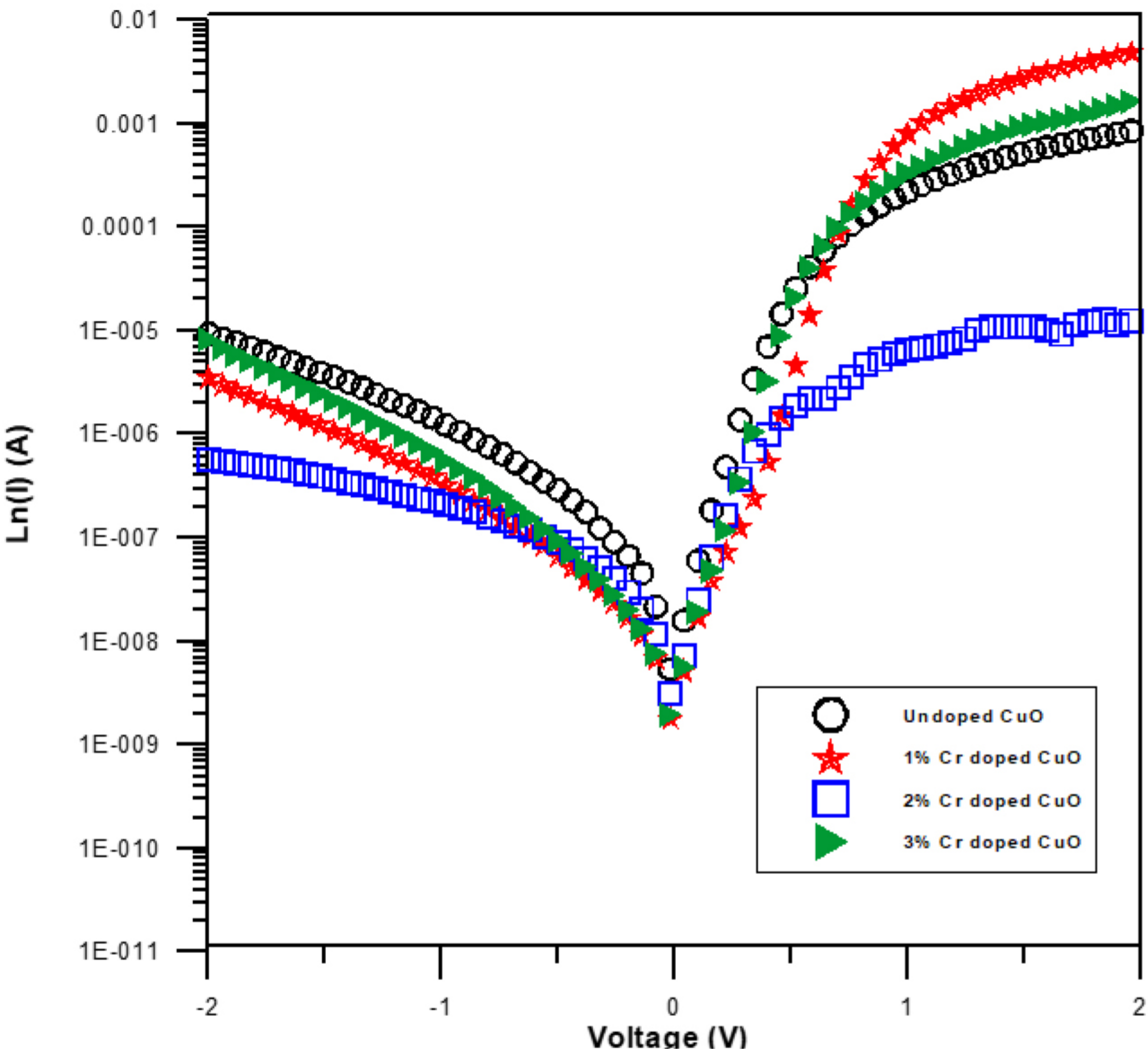

Figure: Semi-logarithmic I-V plots of the Cr:CuO diodes in dark.

Biography

Ilhan CANDAN completed undergraduate education at Selcuk University, Physics Teaching Department. Then, he went to England (UK) for graduate education. He completed master's degree (MPhil) in Atom, Molecule and Laser Physics at University College London (UCL) in London under supervision of Prof. Dr. Peter Barker and Dr. Jonathan Underwood. He completed PhD in Physics working plasmonic Au and Ag nanoparticles at Dept. of Physics, Dicle University. Currently he is working as a research assistant at Dicle University, Physics Department. Areas of expertise and research interests; lasers, Atomic and molecular physics, plasmonic nanoparticles, sensors and thin films..

Pollen morphology and its taxonomic significance of the genus Crucianella L. (Rubiaceae) in Iran

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University of Guilan, Iran

The genus Crucianella L. (Rubiaceae) is an old world member of the tribe Rubieae, supertribe Rubiidinae and subfamily Rubioideae. The genus consist of ca, 35 species, distributed mostly in southwest Asia. Morphologically, Crucianella is an autogamus genus comprising species with more or less quadrangular stems; leaf with leaf like stipules in whorls of 4-10; simple or branched spike inflorescence; flowers subtended by a bract and two prophylls, without calyx, corolla salver-shaped, 4-5 merous with appendiculate lobes; heterostylous, capitate stigma and fruit schizocarp with two mericarps.

The Pollen morphology of nine species of Crucianella L. and ten subspecies of C. gilanica representing two sections: Roseae and Crucianella, was investigated using light microscope (LM) and scanning electron microscope (SEM). All the studied species (except for C. angustifolia) are palynologically described here for the first time. The pollen grains were monad, isopolar, radial symmetrical and relatively small. The largest pollen grains were observed in C. angustifolia (P=24.12 μm, E=26.04 μm), while the smallest pollen was found in C. gilanica subsp. carduchorum (P=16.32 μm, E=12.57 μm). The shape of pollen changed from spheroidal to oblate-spheroidal, prolate-spheroidal, suboblate, subprolate and prolate. The pollen grains were zonocolpate and their number of colpi ranged from 6 to 10. The result showed five different types of sexine ornamentation: perforate, reticulate, microreticulate, microfoveolate and psilate. The sexine of all examined specimens was covered with microspines.

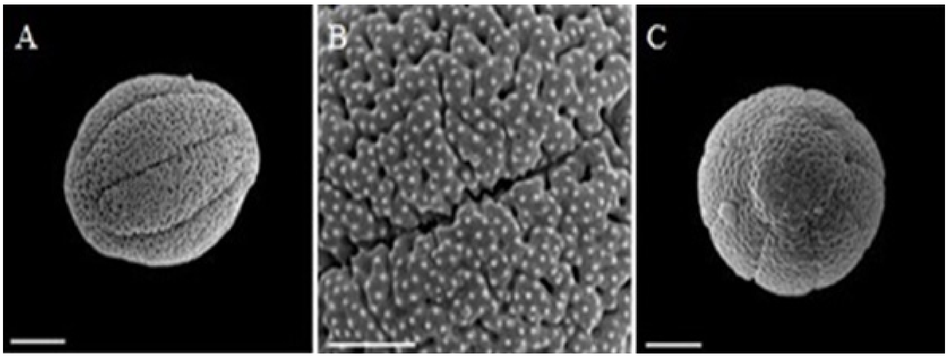

Figure 1: SEM micrographs of pollen grains in Crucianella platyphyla; - A: equatorial view; B: exine sculpturing; C: polar view; - Scale bars: polar and equatorial view = 5 μm; exine sculpturing = 2 μm.

Table. Some characteristic features of the investigated pollen in Iranian species of Crucianella.

Taxon	P (μm) Min (M±SD) Max	E (μm) Min (M±SD) Max	Aperturs no.*	Size perf. (μm)	SO**	Shape
C. angustifolia	21.08(24.12±2.68)28.49	21.91(26.04±2.68) 31.27	9-10	0.47(0.8±0.21) 1.11	Reticulate	S-OS
C. ciliata	17.92(22.75±2.45)28.79	19.14(21.9±2.59)28.95	8-9-10	0.12(0.18±0.04)0.24	Microfoveolate	S-PS
C. filifolia	18.07(20.05±1.57)23.13	10.36(13.55±2.12) 17.66	7-8-(9)	0.11(0.14±0.03)0.17	Perforate	P
C. chlorostachys	17.06(18.67±1.26)21.14	12.43(16.45±2.31) 20.03	(8)-9-(10)	0.09(0.14±0.04)0.23	Microfoveolate	S-PS
C. exasperata	17.56(22.09±2.27)25.89	12.19(16.37±2.53) 21.98	(6)-7-8	0.08(0.11±0.02)0.16	Perforate	P
C. platyphyla	19.84(22.27±1.58)25.26	14.62(19.82±2.9)27.12	8-9	0.22(0.34±0.08)0.52	Microreticulate	S-PS
C. sintenisii	17.13(18.45±0.9)19.87	11.21(14.82±1.74) 19.25	6-7	0.12(0.2±0.04)0.27	Microfoveolate	SP
C. suaveolens	17.46(20.1±1.49)22.44	19.21(23.45±2.5)28.92	7-8	0.11(0.19±0.05)0.25	Microfoveolate	SO
C. gilanica:						
subsp.*gilanica*	19.75(21.4±1.04)22.85	17.02(19.7±1.98)23.17	7-8	0.18(0.24±0.06)0.39	Microreticulate	S-PS
subsp. *suleimanica*	18.66(20.35±1.49)23.11	14.11(18.83±2.95) 22.98	7	0.15(0.22±0.04)0.29	Microfoveolate	S-PS
subsp. *nezvensis*	16.62(19.72±1.67)22.36	13.26(16.3±1.69)19.35	6-7	0.14(0.27±0.06)0.41	Microreticulate	SP
subsp. *elbursensis*	15.02(16.68±1.3)19.56	15.18(16.83±1.26) 19.3	7-8-(9)	0.11(0.15±0.03)0.19	Microfoveolate	S-OS
subsp. *damghanensis*	17.29(19.09±1.27)21.98	12.67(16.16±2.43) 21.86	6-7-8	0.12(0.21±0.04)0.26	Microreticulate	SP
subsp. *kotschyi*	15.45(17.72±1.34)19.63	10.38(14.97±2.04) 18.65	6-7	0.22(0.29±0.05)0.36	Microreticulate	SP
subsp. *carduchorum*	14.82(16.32±0.92)18.81	10.58(12.57±1.02) 15.38	7-8	_	Psilate	SP
subsp. *glauca*	18.75(19.87±0.99)21.45	13.04(19.65±2.49) 23.25	7-8	0.26(0.36±0.1)0.57	Microreticulate	S-PS
subsp. *transcaucasica*	15.41(18.84±1.79)21.23	11.87(15.74±2.22) 19.04	6-7-8	0.18(0.28±0.09)0.48	Microreticulate	SP
subsp. *transcaspica*	17.6(22.15±4.53)30.61	16.87(23.71±3.61) 28.56	6-7	0.23(0.29±0.07)0.49	Microreticulate	S-OS

The current survey shows that the pollen morphological characters of the studies species are taxonomically informative and may provide good help in identification purposes. We used multivariate analysis to determine the potential contribution of palynological data to the species relationships. The result of cluster analysis and principal component analysis showed pollen morphological affinities between the two studied sections.

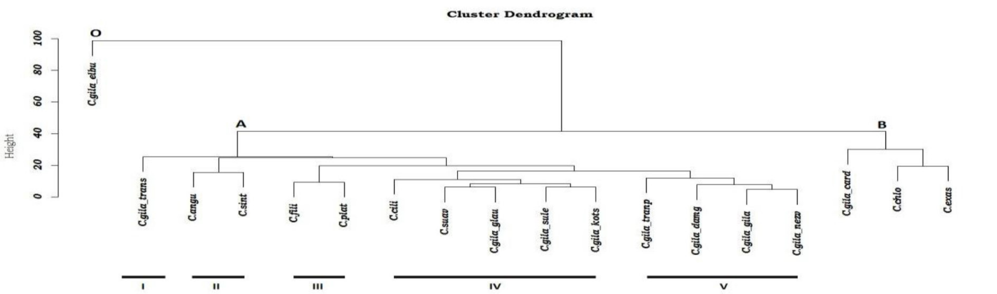

Figure 2: UPGMA dendrogram based on qualitative and quantitative pollen morphological characters of eight species of Crucianella and ten subspecies of C. gilanica : The species and abbreviation used are as follows: Crucianella angustifolia (C.angu), C. ciliata (C.cili), C. filifolia (C.fili), C. chlorostachys (C.chlo), C. exasperata (C.exas), C. platyphyla (C.plat), C. sintenisii (C.sint), C. suaveolens (C.suav), C. gilanica subsp. gilanica (C.gila_gila), C. gilanica subsp. suleimanica (C. gila_sule), C. gilanica subsp. nezvensis (C.gila_nezv), C. gilanica subsp. elbursensis (C.gila_elbu), C. gilanica subsp. damghanensis (C.gila_damg), C. gilanica subsp. kotschyi (C.gila_kots), C. gilanica subsp. carduchorum (C.gila_card), C. gilanica subsp. glauca (C.gila_glau), C. gilanica subsp. transcaucasica (C.gila_trans) and C. gilanica subsp. transcaspica (C.gila_tranp).

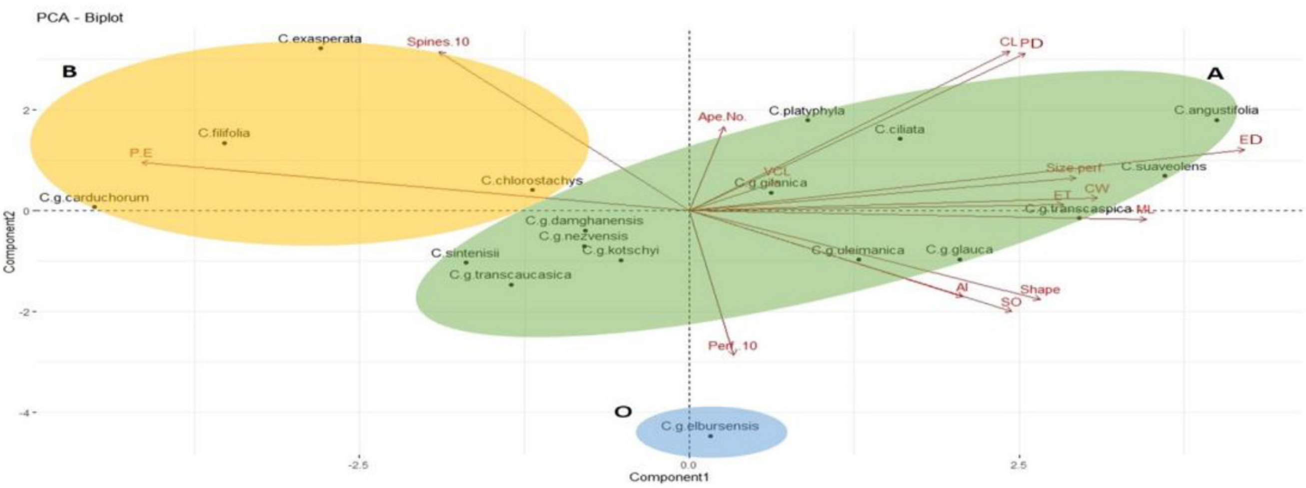

Figure 3: Principal component analysis (PCA) of the qualitative and quantitative pollen morphological characters of eight species of Crucianella and ten subspecies of C. gilanica : The abbreviations used: PD- polar diameter, ED- equatorial diameter, P.E- polar/equatorial diameter, CL- colpus length, CW- colpus width, AI- apocolpium index, ML- mesocolpium length, ET- exine thickness, SO- sexine ornamentation, Aper.no- Apertures number, Perf.10- perforations number per 10 µm2, Spines.10- spines number per 10 µm2, Size.perf.- size of perforations, VCL- variation in colpi length.

Biography

Soheyla Parsapanah is a PhD student in plant systematic of Guilan University. She loves her major and work a lot. Her thesis is about "Biosystematic study of the genus Crucianella L. (Rubiaceae) in Iran". Her expertise in her lab is pollen of plants. Pollen grains world is very interesting for her and she found some correlation between our world and its. She believe if we could study pollen grains accurately, we can be inspired by it to take models and build new stuffs for living, and make life easier for human beings.

Graphene spin-coated electrode for polyacrylonitrile acoustic nanogenerators

Sedigheh Aghahyari
Sharif University of Technology, Iran

In this work, two-electrode application methods were compared, and the best electrode for new copolymer of PAN acoustic nanogenerators was found, which is simple and inexpensive compared to other methods, and it had the advantage of producing sound that was good enough compared to other works. For further work, using an ILS surfactant as a doping agent is the best because studies based on sources have shown that the best way to improve the output of acoustic nanogenerators is to choose the best dopant. If the dopant is not good enough, it results in only a slight change in the output. ILS was suggested because it could increase the output of piezo tests perfectly and now there is a time to test it for acoustic tests. The electrodes of nanogenerators are not very important for increasing the output of nanogenerators, but their cost makes researchers find the cheapest and easiest way. Among the different electrode application methods, printing and using nanomaterials have received much attention in recent years, so the two above methods are investigated in this work. In the first work in this area, finding the best nanofiber web parameters included nanofiber diameter, thickness of the nanofiber web, area of the nanoweb, presence of holes on the electrode and the area of the hole and its position, and the kind of chosen polymer found to be important. They found that the output is higher in extraordinary sound pressure, sound frequency, and way of applying sound on the layer, which should be optimized. In further studies, this group found that increasing the number of holes and making them smaller can help higher outputs. In the last work of this group, the PAN nanofiber web found better outputs than the PVDF copolymer, so another subject for writing an article is to do the best of this article for the PAN nanofiber web, which was done here. Additionally, *in situ* synthesis of Ni on the nanofibers was a way to reduce the piezoelectric output.

Also, these nanofibers can change into carbon fiber which may detect or produce the sound and they are the promising subjects for next works.

Biography

Sedigheh Aghahyari studied a Master's in Amirkabir University of Technology in fibrous nanostructures and currently she is studying Ph.D. in Sharif University of Technology in nanoscience.

Energy and CO_2 emission assessments of alkali- activated concrete and ordinary portland cement concrete: A comparative analysis of different grades of concrete

A. Alsalman[1, 2], **L. Assi**[3], **R. Kareem**[4], **K. Carter**[3] and **P. Ziehl**[3]

[1]Almaaqal University, Iraq
[2]Tatum Smith Welcher Engineers, USA
[3]University of South Carolina, USA
[4]Shatrah Technical Institute, Iraq

Studies have indicated that alkali-activated concrete (AAC) is comparable to ordinary Portland cement concrete (OPCC) in terms of mechanical properties (eg. compressive strength, tensile strength, flexural strength, and modulus of elasticity) and can deliver environmental advantages compared to OPCC. This research assesses the energy and CO_2 emissions associated with OPCC and AAC. Three grades of concrete were selected; 40, 60, and 100 MPa to cover a wide range of concrete that can be used for several purposes. The 40 MPa is considered standard strength concrete, and it is common for most structural uses where exceptional compressive is not required. On the other hand, the 60 MPa is high strength concrete with compressive strength > 55 MPa. Finally, the 100 MPa is ultra-high- strength concrete with compressive strength ≥ 100 MPa.

Analysis shows that the selection of constituent materials can considerably influence the energy and emission of AAC and OPCC. Ordinary Portland cement (OPC) is the primary contributor to the energy and emission of OPCC, accounting for 80% of energy and 91% of emissions of OPCC. The activating solution of AAC, meanwhile, is the main contributor to the energy and CO_2 emission of AAC. Normal strength AAC (40 MPa) shows 46% less energy and 73% less CO_2 emission than OPCC. However, high-strength AAC (60 MPa), using metakaolin as a base material, experiences higher energy (8%) than OPCC yet the emission is 40% less than OPCC. A substitution of fly ash for metakaolin results in superior efficiency of AAC compared to OPCC. Two mixtures of ultra-high-strength AAC (100 MPa) result in contradictory findings. One mixture with sodium hydroxide and silica fume activating solution shows 5% and 30% less energy and emission, whereas the other mixture with a sodium hydroxide and sodium silicate activating mixture is less efficient than OPCC.

Biography

Ali Alsalman is a faculty member at the Civil Engineering Department at Almaaqal University and a structural engineer at Tatum Smith Welcher Engineers, Inc. He earned his Ph.D. in civil engineering with a structural engineering focus from the University of Arkansas in Fayetteville AR, United States of America. His area of interest is civil engineering materials and structures. Besides, Ultra-High Performance Concrete (UHPC), geopolymer concrete, and CO_2 emission are his major concerns.

Description of the heat capacity of solid phases by a multiparameter family of functions (MPFF)

V.P. Vassiliev
Lomonosov Moscow State University, Russia

The standard thermodynamic constants are very important for all branches of science. The correct description of the heat capacities in a wide temperature range is especially difficult to find a solution. The nontrivial concept permitted us the possibility to find a fairly simple solution to this issue. This solution helped to describe the specific heat in a wide temperature range of a large class of isostructural sphalerite phases as a single system unambiguously. A fragmental description of some phase is like a vision of one part of a large mosaic picture. A single description of such a phase does not allow one to see the integrity of the entire ensemble. The 4th group of pure elements in addition to diamond, silicon, germanium, alpha tin, and diamond-like lead was taken as the base. Flerovium (^{114}Fl) closes this group. There should be no other elements in this group according to the fine structure

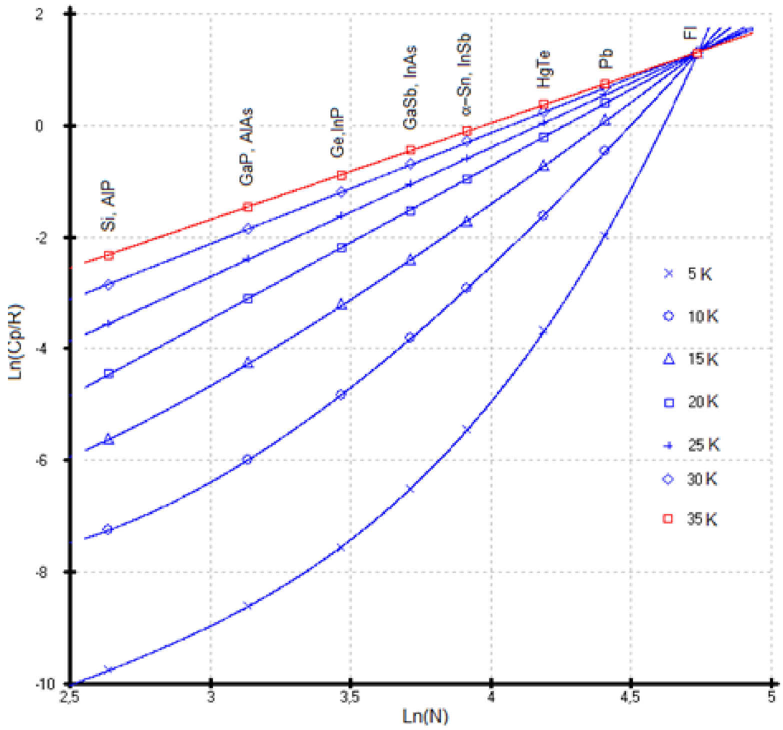

Figure: Low temperature isotherms Ln (Cp/R) vs Ln(N) of sphalerite structure.

constant or the Sommerfeld constant α. As a consequence, the limiting value of the heat capacities of phases with a sphalerite structure falls on the 114th element (114Fl) and has a value of C_p = 30.5 J • mol-at^{-1} • K^{-1}. This value arises when plotting the isotherms Ln (Cp / R) versus Ln (N), where N is an atomic number of an element of the IV group or the sum of atomic numbers of $A^{III}B^{V}$ or $A^{II}B^{VI}$ compounds per mole-atom. This method can be applied to the other isostructural phases.

Biography

Valery Vassiliev is a lieder researcher in the laboratory of chemical thermodynamics of the Chemical Department in Lomonosov University (Moscow). He has more 100 scientific publications, concerning thermodynamic properties and phase of diagrams of semiconductor system systems A^{II} - B^{IV}, A^{II} - B^{VI}, A^{III} - B^{V}, A^{III} - B^{VI} and metallic systems on the basis of rare earth metals. He is the author of review papers for the Handbook "Thermic constants of compounds", edited by academician V. P. Glushko, Edition VINITI (All-Union Institute of Scientific and Technical Information). He is a recognized specialist in the method of electromotive forces. Last years he established a strict relationship between the thermodynamic constants of binary compounds and the Periodic Law. Between 1989 and 2012 he worked as a visiting professor at universities in France, Italy and China.

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The evolution of the Zener factor and the isotropy of triple periodic minimal surface structures

R. Miralbes, D. Ranz and **B. Jiménez**
University of Zaragoza, Spain

Triple periodic minimal surface structures (TPMSs) are lightweight scaffolds that are composed of some repetitive cells. This paper is centered on gyroid, diamond, and Schwarz primitive TPMSs.

The internal structures of the cells of TPMSs are generated to thicken a surface that is defined by a mathematical equation; the thickness of these walls establish the volume fraction (ρ*) that is the relationship between the filled volume of the TPMS and the total one. These surfaces have a minimum relationship between the area and volume, and, consequently, their specific mechanical properties and capability to absorb energy per unit of mass are maximum.

However, the mechanical properties of TPMSs can vary in each direction; therefore, in certain directions, TPMSs have lower mechanical properties that can imply a higher probability that the structure fails in this direction; this would generate a weak point. Thus, this article centers on the analysis of the anisotropy of the mentioned TPMSs.

Analysis of the anisotropy is made using N-topology software, and different ρ* are analyzed. Additionally, the Zener factor is studied, and the anisotropy is graphically plotted. The

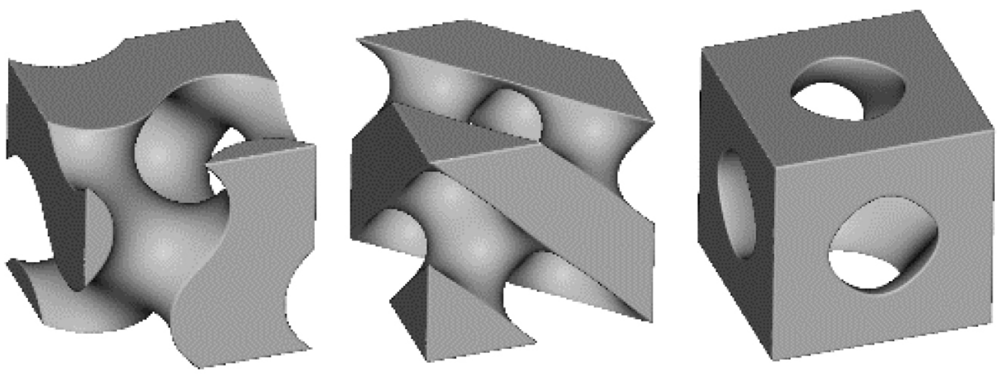


Figure: Different unit studied cell TPMS; from left to right: gyroid, diamond and Schwarz primitive graphic representational shape of the anisotropy indicates how the TPMSs' mechanical properties vary depending on the direction.

Results show that, whilst gyroid structure present a low anisotropy and a closed to 1 Zener factor, that indicate a lower anisotropy too, for any ρ*, in the case of diamond and Schwarz-P structures there is a high anisotropy for low ρ*. Additionally, in these cases, diamond structure presents a Zener fraction lower than 1 that indicate higher mechanical properties in longitudinal directions (X, Y, Z) than in others but in the case of Schwartz-P, this factor is high that indicate higher stiffness in the lateral directions than in the longitudinal ones.

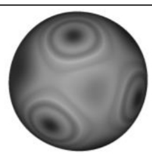
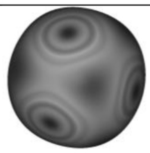
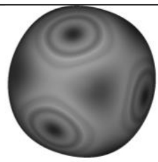
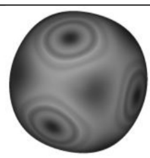
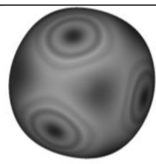
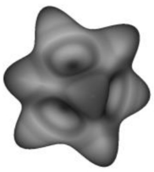
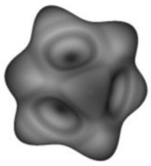
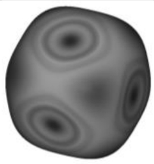
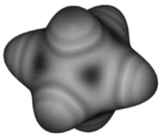
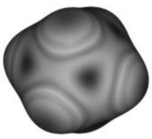
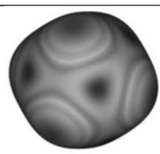
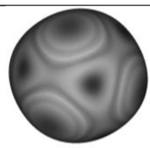
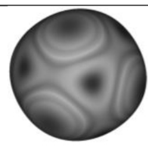
ρ*	10%	20%	30%	40%	50%
Gyroid					
	1.0387	1.1085	1.1341	1.451	1.14
Schwarz-P					
	3.2101	2.4979	1.8305	1.6082	1.3588
Diamond					
	0.5594	0.7454	0.838	0.9209	0.9829

Table: 3D plot of the anisotropy for the TPMS and Zener ratio

Biography

Ramon Miralbes Buil is professor of technical drawing in the University of Zaragoza (Spain) since 2008. He obtained his bachelor in Industrial Engineering in 2005 and his PhD in 2008 in this university. His main research fields are the mechanical characterization of complex structures generated by additive manufacturing and in the characterization of eco-materials such as cork agglomerates, luffa, micellar materials, etc. He has published more than 34 JCR paper and 5 other types of papers, 10 chapters in books, 3 books and more than 40 contributions in different congress. He is also the president of the INGEGRAF association and reviewer of projects for the Spanish government and for the CEE. He was also the main researcher in the GEDiX research group during 6 years.

Development of GTE turbine air-cooling system to increase its operating parameters

Ivan Malinovskiy[1,2], **Valery Nesterenko**[1], **Andrey Starodumov**[1,2] and **Evgeniy Marchukov**[1,2]
[1]*Moscow Aviation Institute, Russia*
[2]*Experimental Design Office named after A. Lyulka, Russia*

The results of investigations for the structural schemes of cooling systems of the aircraft bypass gas turbine engine (GTE) turbines are presented. A new scheme of the cooling air supply to the working blades of high-pressure turbine is proposed. The front cavity of the nozzle and rotor blades is cooled continuously, regardless of the engine operating mode. The air for cooling the working blade of the turbine is supplied by the transit tube through the vane from the cavity located in front of the place where the supply is cut off, which ensures the constant boost of the front cavity of the HPT blade. In order to eliminate heating from the turbine disk and centrifugal pumping, the swirling device is installed directly under the blade lock, where the supply of cooling air to the cavity is arranged. The turbine disk is cooled by a separate stream of air, taken from the secondary zone of the combustion chamber, which is generated by the second row of swirling devices. The brush seal and labyrinth are installed under the swirling device, that supplies cooling air to the blades of turbine, and the device of air swirling, that cools the turbine disk, is located in the upper part of the disk, immediately below the labyrinth. The higher efficiency of brushes, the location of swirling device, that cools the disk, under the labyrinth in the upper part of the disk, as well as decrease in the number of labyrinth teeth and, as a result, the reduction of pressure drop across the labyrinth between the disk cooling cavity and the dummy cavity enable to direct the main part of air down the disk to its sleeve and further along the shaft of the rotor into the dummy cavity.

Biography

Ivan Malinovskiy was born in Transnistria. Graduated from the Moscow Aviation Institute. He specialize in aircraft engines and power plants. Now he is a graduate student at the Moscow Aviation Institute and an engineer at the Experimental Design Office named after A. Lyulka.

BIOGRAPHY

Manju Misra is a professor and Tier 1 Canada Research Chair (CRC) in Sustainable Biocomposites in the School of Engineering and holds a joint appointment in the Department of Plant Agriculture at the University of Guelph. Additionally, she is the Research Program Director of the Bioeconomy Panel for the Ontario Agri-Food Innovation Alliance, a program between the Ontario Ministry of Agriculture and Rural Affairs (OMAFRA) and the University of Guelph. She completed her Bachelors, Master's, M.Phil and PhD from Ravenshaw College at Utkal University in India focusing on Chemistry with a specialization in Polymer Chemistry and Natural Fibers during her graduate program. She has authored more than 750 publications, including 437 peer-reviewed journal papers, 21 book chapters, and 53 patents. She was also the editor or co-editor of 4 books in the area of biocomposites and nanocomposites. She has received many awards including the Lifetime Achievement Award from the BioEnvironmental Polymer Society (BEPS). In 2020, she was selected as one of Canada's Most Powerful Women: Top 100 Award Winner in the Manulife Science and Technology category from the Women Executive Network.

Manju Misra
University of Guelph, Canada

Advanced biocarbons and their lightweight sustainable green composite materials: A path forward to circular bioeconomy

Lightweight green composites from renewable resources are attracting increased attention from advanced manufacturing sectors. A strong momentum for weight reduction in auto parts is motivated by a need for a better fuel economy. To increase renewable content in materials, we use thermo-chemical conversion (pyrolysis) of biomass/agri-food residues to overcome the key challenges associated with the use of traditional natural fibres in melt processed biocomposites. Biocarbons obtained from inexpensive biomass, including farm wastes/ residues and food processing wastes show tremendous potential for affordable biocomposite materials. In addition, biocarbons have been also used effectively in composites with waste plastics. Overall, biocarbon composites can be very effective as one of the enabling strategies towards sustainable materials and a circular bioeconomy.

Refractory carbides at the temperatures up to 5000K

A. Savvatimskiy and **S. Onufriev**
Russian Academy of Sciences, Russia

A high-speed method for measuring the thermophysical properties of the most refractory carbides in the liquid phase at high temperatures has been developed. Owing to short duration of current heating (microseconds), the significant financial costs are not required to provide long-term high temperature maintenance. In addition, refractory crucibles are not needed to preserve the liquid phase of the substance. The sample in the liquid state does not change its shape and retains its position in space for a dozen microseconds. This allows recording the properties in the liquid state using high-speed oscillography.

Experimental results of the physical properties for refractory carbides (ZrC+C; ZrC; TaC+HfC; HfC; TaC) at high temperatures are presented. The samples were in the form of thin plates with a thickness of about 150 microns, which were heated by a current pulse of about 20-30 kA during 5-10 microseconds. The properties were measured: the input Joule heating energy or enthalpy H (including melting heat), specific heat Cp, electrical resistance R. The measurement uncertainties for the properties H; Cp; R, are – 7%; 15%; 5%, accordingly.

The temperature was measured by an optical method with a pyrometer based on a high-speed photodetector PDA-10A (Thorlabs) using a known emissivity. To study ZrC+C, samples were used in the form of a wedge-shaped model of a black body (developed in the USA by Mendenhall back in 1911). Therefore, knowledge of the emissivity was not required.

A steep increase in the specific heat Cp is observed just before the start of melting. The reason is the occurrence of non-equilibrium paired Frenkel defects (vacancy + interstitial atom). These defects arise due to insufficient time for normal diffusion and the appearance of equilibrium vacancies under such a short time of the experiment. The appearance of non-equilibrium defects is accompanied by the occurrence of abnormally high electron emission. The latter arises, perhaps, due to a decrease in the Fermi energy for a solid state under conditions of rapid heating. Energy costs in obtaining abnormal specific heat are insignificant and do not exceed 7% from measurement enthalpy H.

The results obtained for the physical properties of the refractory carbides are necessary for the creation of thermal protection in the nuclear power industry and in the aerospace field. In addition, they shed light on the appearance of new physical effects during rapid shock loading of a solid substance under high temperature.

Biography

Alexander Ivanovich Savvatimskiy is a Chief researcher of JIHT (Joint Institute for High Temperatures RAS) since 2010. From 1997 to 2010 he was a scientific secretary of National Committee on Thermophysical Properties of RAS and a Head of the Laboratory. From 1994 to 2010 he worked as Head of electro-exploding scientific Laboratory, Institute of High Energy Density and Joint Institute for High Temperatures Russian Academy of Sciences (RAS). 1982 - 1994 Senior scientist (Institute for High Temperatures Russian Academy of Sciences). 1967 - 1982 Junior scientist (Institute for High Temperatures Russian Academy of Sciences). 1966 - 1967 Engineer (Institute for High Temperatures Russian Academy of Sciences). In 1999 he earned Highest Degree in Thermophysics and molecular Physics. His doctoral thesis is "Experimental investigations of physical properties (metals, alloys and graphite) under microsecond electrical pulse heating", Institution of degree: Institute for High Temperatures RAS. In 1975 he completed Ph.D. in experimental thermophysics. Thesis: “Measurements of melting heat and resistance of liquid refractory metals at the melting region under fast electrical heating”. Institution of degree: Institute for High Temperatures RAS. 1959-1966 - Undergraduate, Moscow Power Engineering Institute, speciality: Thermophysics. 1957-1959 - Laboratory assistance in All-Union heat-engineering Institute. 1957 - Finished secondary school in Moscow.

Virus resonance inactivation using non-ionizing radiation in the microwave regime

R. Minnes and **A. Barbora**
Ariel University, Israel

The COVID-19 pandemic, which has been with us for the past two years, has brought to mind the inherent danger in the spread of viral epidemics. A new strain of virus or a variant of an existing virus can sometimes spread very quickly and lead to the death of many before drugs or vaccines are developed. Rapid and effective treatment of the virus that inhibits the spread of the virus can turn a viral outbreak with the potential of a global epidemic, into a local outbreak that is limited in scope. However, the process of developing biochemical drugs or vaccines for viruses is a long process, followed by an equally long process of regulatory approval (FDA). To develop a biochemical drug, one must characterize the virus and identify unique markers for it. Such drugs or vaccines may prove ineffective against variants of the virus that have been able to develop resistance to the drug / vaccine. So, such drugs do not necessarily prevent recurrent waves of viral outbreak. In previous work we analyzed one of the natural oscillation modes of the COVID-19 virus membrane. We calculated that electromagnetic radiation at a frequency in the GHz range will bring the membrane to a resonant state and allow the membrane to rupture, thus causing an inactivation of the virus. Patients will not be harmed if they are exposed to radiation in this range, and the damage will be limited to the virus. In this research we are developing a system that will allow us to perform measurements on virus samples and determine the natural frequencies of the oscillation modes. We will calculate and measure the threshold of power densities required to inactivate different viruses by exposing them to radiation at the measured resonant frequency. The findings of this study might be used in the future to develop a physical-based method for a quick and effective treatment of viral outbreaks.

Biography

Refael Minnes has completed a B.Sc. in Biophysics and a PhD in Physics from Bar Ilan University and postdoctoral studies from University of Pennsylvania School of Medicine. He is a faculty at Ariel University Department of Physics and the head of the Bio-electromagnetism Laboratory. In his research he explores the interactions of electromagnetic waves, specifically in the UV-Vis-IR range, with biological tissues and cells.

Electromagnetic methods for improved production of additive manufacturing materials

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University of Latvia, Latvia

Additive manufacturing is one of the rapidly growing industries today. There are various types of metal additive manufacturing allowing to create complicated custom parts quickly and effective. Limiting factors of this technology are slow printing process and high cost of the initial material. Raw material for metal 3D printing is special powder or wire. Metal powder for additive manufacturing needs to have spherical shape, amorphous structure and narrow size distribution. Metal powder is produced by gas atomization process where metal is melted, and droplets are dispersed by inert gas jet. This process still has some shortages and that is why additive manufacturing quality metal powder is still expensive, thus limiting faster adaption of the technology. Wire is produced by controlled oriented solidification.

In this work we investigate the application of electromagnetic processing to improve material production process for metal additive manufacturing. Stationary magnetic field and injected electric current is one of the methods how to induce force in the liquid metal and affect its solidification. Pulsed magnetic fields can be a good tool for grain refinement and how to control equiaxed to columnar transition. This may solve several issues and affect the production process leading to better outcome and possibility to control various aspects of the metal solidification process. Institute of Physics University of Latvia has great experience and experimental basis to carry out this research. Various experimental research results well be presented.

Biography

Imants Kaldre research interests in applied magnetohydrodynamics, solidification of metallic alloys, metal matrix nano-coposite production, electromagnetic processing of materials and applied physics related to process metallurgy. He finished Ph.D from Grenoble University in France in 2014. Dissertation: Thermoelectric current and magnetic field interaction influence on the structure of binary metallic alloys. Recently he is working in projects related to electromagnetic production of particle strengthened Metal Matrix Composites. He is also working on the innovative production of Titanium from Ti-tetrachloride by electroslag process. He is deputy director of the Institute of Physics University of Latvia since 2017 and member of the scientific board of Institute of Physics University of Latvia since 2015. Member of the Latvian young scientist's society.

SERS combined with chemometric analysis for detection and identification of microorganisms: Viruses and bacteria

A. Kamińska[1], **E. Witkowska**[1], **K. Niciński**[1], **D. Korsak**[2], **T. Szymborski**[1] and **S. Berus**[1]
[1]Polish Academy of Sciences, Poland
[2]University of Warsaw, Poland

The present work demonstrates that surface-enhanced Raman scattering (SERS) coupled with biochemical methods and principal component analysis (PCA) is a reliable and fast method for detection and identification of pathogenic bacteria and virses.

The proposed SERS-based method for bacteria identification challenges the standard biochemical methods in terms of simplicity, specificity and rapidity (maximum 60 s for single SERS measurement). The direct SERS analysis of bacteria (even single bacteria cell) is performed directly from SERS-active nanostructures incorporated into a microfluidic module. The recorded SERS data of bacteria will be categorized (assigned to particular bacterial species) using data analysis software based on a database SERS created for bacteria. The longtime of incubation of bacteria will be eliminated and the total analysis including numerical analysis of recorded SERS data will not exceed 15 minutes. Additionally, the proposed FORMI device can be introduced to International Organization for Standardization (ISO) standards for bacteria identification, to avoid or skip the time-consuming methods routinely used in laboratories and as a result the time of analysis will be dramatically reduced. Presented approach opens a new path in microbiological diagnostics for sensitive, simple, quick, and on-site detection of pathogenic bacteria including environmental and clinical microbiology (hospitals, health center), food industry and environmental protection.

Biography

Agnieszka Michota-Kamińska is a leader of the "Plasmonic nanostructures for bio-spectroscopic analysis" group in the Institute of Physical Chemistry, Polish Academy of Sciences, Poland. Her research interest is focusing on the Raman vibrational and the surface-enhanced Raman spectroscopy, as well as the surface plasmon resonance for the detection and identification of biomolecules (e.g. peptide, protein, DNA, viruses, antigens, antibodies, bacteria, fungi) for analytical and medical applications.

Optimisation for ultralight and high-stiffness hierarchical structures with tailored lattice metamaterials

N. Li and **L. Zhu**
Imperial College London, United Kingdom

Lattice structures, composed of periodically distributed lattice cells, are bioinspired hierarchical lightweight structures with high stiffness-to-weight and strength-to-weight ratios. We have developed three novel optimisation frameworks for the optimal design of ultralight and high-stiffness hierarchical structures with tailored lattice metamaterials, considering manufacturing effects (additive manufacturing building direction effects) and structural safety (yield criterion). Our first optimisation framework enables simultaneous optimisation of the distributions of relative densities, effective elastic moduli, and anisotropy of metamaterials in lattice structures. A numerical homogenisation method is adopted to characterise the anisotropic effective elasticity tensors of lattice metamaterials. Neural-network-based surrogate models are developed to bridge the geometric information (lattice strut radii) and the effective material properties of lattice metamaterials. Thus, tailoring of relative properties of lattice metamaterial is enabled by optimising lattice strut radii. In the first framework, conformal lattice structural optimisation is also enabled by optimising the orientations of lattice cells, allowing them to be conformal to the curved boundaries of higher-hierarchical-level structural features to achieve a better approximation of the boundary curvatures, and align with the paths of major principal stresses to further improve structural efficiency. Our second optimisation framework experimentally (quasi-static uniaxial compression tests, room temperature) calibrates the effects of building direction (BD) of selective laser melting on the effective elastic Young's moduli of lattice metamaterials. The calibration of the BD effects has been integrated into our optimisation framework to enable the BD effects to be considered during optimising cell orientations for conformal lattice structures. Our third optimisation framework has introduced fillets to the strut joint regions of lattice cells to improve the yield strength of the lattice metamaterials. A yield constraint, based on von Mises yield criterion, using experimentally characterised effective properties of filleted lattice metamaterials, has been developed for this framework to ensure the structural safety of the optimised lattice structures.

Biography

Nan Li is a Senior Lecturer and the Research Leader of the Advanced Manufacturing Group, at the Dyson School of Design Engineering, Imperial College London. Her team on Lightweight Design for Manufacturing addresses a major challenge facing the transport industry world-wide: developing technological breakthroughs in the manufacturing and design of high-performance lightweight vehicles for a more environmentally friendly footprint. She has more than sixty publications and ten patents, and extensive experience in applied research projects with industry, funded by multiple research councils and companies. She was awarded the 'Rowbotham Medal' 2017 by the Institute of Materials, Minerals and Mining (IOM3) for her outstanding contribution to the innovative use of materials for automotive applications.

In-situ formation of Al-Cu based alloy foams

I. A. Figueroa and **J. M. Hernández-Soto**
National Autonomous University of Mexico, Mexico

Al- base metallic foams were produced without the need of space holders or blowing agents ("*In-Situ*" route). The porosity formation mechanism and the effect of the icosahedral phase in some Al -Cu- Fe alloy compositions are presented. These alloys were produced in an induction furnace under an argon atmosphere. Next, the alloys were slowly solidified inside the furnace crucible. Several heat treatments were carried out to obtain the highest percentage of porosity and, therefore, to find out the mechanism associated with the porosity formation. To obtain the heat treatment temperatures, a DTA study was performed. The crystallographic phases were identified by means of X-ray diffraction and scanning electron microscopy. The XRD showed that the $Al_{79}Cu_{15}Fe_6$ alloy was mainly constituted by Al, ω-Al_7 Cu_2Fe, and θ-Al_2Cu phases, generating a porosity of 0.54%. The highest percentage of porosity (60%) was obtained for the $Al_{62}Cu_{28}Fe_{10}$ alloy, heat-treated at 850^0C for 3 hours. SEM images showed that the microstructure was mainly constituted of ı-Al_6Cu_2Fe and β-AlFe phases. Inside the pores, the ı-Al_6Cu_2Fe phase was also found as clusters of fivefold symmetry quasicrystals. According to the microstructural analysis, it was found that the porosity formation mechanism could be related to a reaction that involves the interaction between the Liquid, λ-$Al_{13}Fe_4$, and ω-Al_7Cu_2Fe phases resulting in the formation of ı-Al_6Cu_2Fe phase (ternary peritectic reaction) and a highly porous structure.

Biography

Ignacio A Figueroa joined the Institute for Materials Research at the National Autonomous University of Mexico in 2010 from the Advanced Manufacturing Research Centre with Boeing -Rolls Royce Factory of the Future- in Sheffield (UK), where he was a Research Fellow. He obtained his PhD in Engineering Materials from the University of Sheffield (UK) in 2008. He has graduated more than 40 undergraduate and postgraduate students. He has been awarded with level III of the National System of Researchers (the highest). Distinction in the field of "Technical Creativity or Invention", awarded by the foundation Mexico with Values (Mexico con Valores). The 2015 National Sustainable Energy Award by the Secretary of Energy and the World Energy Council. The National Autonomous University of Mexico-UNAM recognized with the National University Distinction for Young Academics 2016 in the area of "Technological Innovation and Industrial Design". In 2018, CONACYT awarded him with distinction of "Casos de Éxito" (Success Cases). Also in 2018, the Mexican Academy of Sciences awarded him with the 2018 RESEARCH PRIZE in "Engineering and Technology". Finally, in 2021, at the Webinar on Materials Science, Engineering and Technology, he received the "Scientist Award" for his contribution to the progression of his research field.

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Impact of urbanization and development activities on carbon sink and CO_2 mitigating capacity of rubber plantation in Kerala, India

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[1]Rubber Research Institute of India, India
[2]Indian Institute of Horticultural Research (IIHR), India

Urbanization and various development activities are historic changes and are inevitable to a large extent in the scenario of increasing population and modern livelihoods. However, the removal of long duration environment-friendly and commercially important ecosystem especially natural rubber (Hevea brasiliensis- cis- 1, 4-polyisoprene) plantations with fairly good carbon accumulation and carbon sequestration capacity is massive for construction activities in Kerala, the traditional rubber growing region in India. This study intended to account the loss of carbon sink and CO_2 mitigating capacity through the removal of rubber plantation per hectare area. Also, the region-wise variation in carbon sink loss and CO_2 mitigating capacity was also accounted. The estimations have the scope to assess the ecosystem level carbon auditing and decision makers to evolve policy guidelines during urbanization and development activities. Results of the study showed the above-ground (tree biomass, annual litter fall and harvest product sheet rubber) carbon loss for RRII 105, the popular clone in Kerala comes to 157.7t/ha for 23 years (Fig. 1) and 285.1 for 30 years.

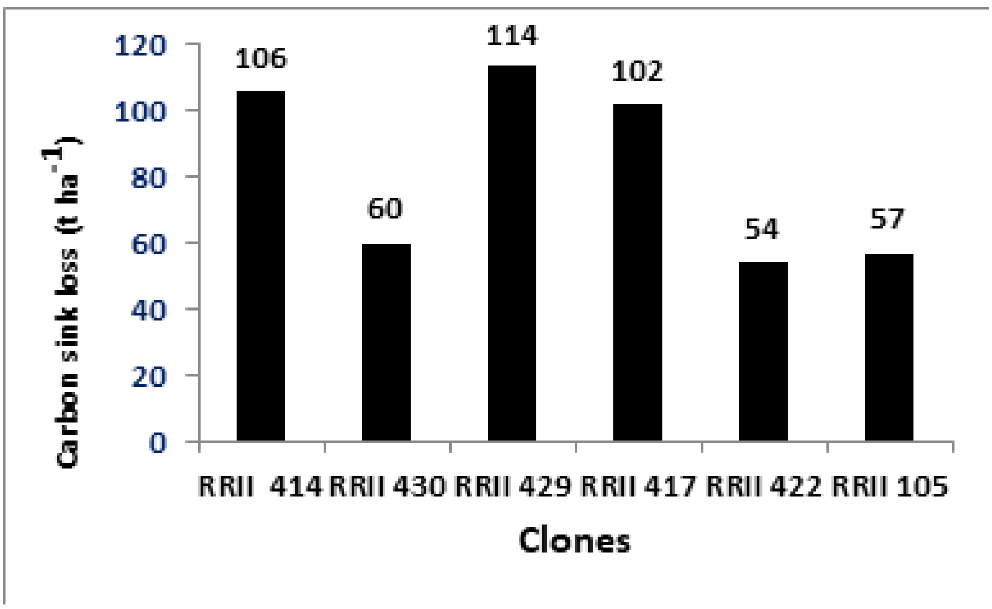

Figure 1. Carbon sink of RRII 400 series clones and RRII 105 at 23 years age.

The newly evolved and speedy establishing modern clones RRII 414, RRII 429 and RRII 417 have 44-50 per cent higher carbon loss. The below –ground (soil carbon sink loss) with per cent soil organic carbon of 1.2 is 43.2. The central region of Kerala showed higher loss and lower loss was in the drought affected northern region than South region because of the difference in tree growth and variations in climatic conditions. The total carbon sink loss (Table.1) for 23, 30 years were 214.2 and 341.5 t/ha respectively. Biomass estimation of trees, organic carbon content in soil and carbon content of tree components and sheet rubber were the methods used in the study. The study proposes for guidelines and policy decisions to take care for maintaining green areas with vegetation and big trees with highest capacity of carbon storage and sequester capacity. Trees with higher lignin are an appropriate option to compensate carbon loss to mitigate the effect of removal of plantations and to become environment friendly. The study pointed out clearly the role of rubber plantation in CO_2 mitigating capacity and the huge loss of carbon stock and is to be seriously considered in the scenario of global warming.

Carbon sink sources	Carbon content (%)	Carbon stock (t/ha)	Carbon sink loss 23 years (t/ha)	Carbon sink loss 30 years (t/ha)
Tree biomass	42	57	57.0	148
Soil	1.2	56.5	56.5	56.5
Litter fall	42.8	2.5	57.5	75.0
Rubber sheet	85.38	2.7	43.2	62.1
Total	-	-	214.2	341.6

Table. 7. Total carbon sink loss from the removal of one hectare rubber plantation (RRII 105)

Biography

Ambily. K.K, Senior Scientist (Soils & Agricultural Chemistry) in Agronomy/Soils Division of Rubber Research Institute of India, Kerala, India. She received Ph. D degree in Chemistry on the topic "Rhizosphere Chemistry and adaptations of Natural Rubber (Hevea brasiliensis) to acidic soil conditions'' from Mahatma Gandhi university, Kottayam, Kerala, India. Received Master's Degree in Analytical Chemistry and graduate degree in chemistry. Presently engaged in research on soil fertility and fertilizer recommendation for rubber and plant nutrition related to yield, potassium and drought tolerance of Rubber plants and environmental studies like carbon sequestration potential of clones. Involved in the development of online fertilizer recommendation programme "RUBSIS- Rubber Soil Information System" for offering online fertilizer recommendation for rubber. .

E-POSTER

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3rd Advanced Materials Science World Congress

March 21-23, 2022

Adv. Materials Science 2022

Mesoporous tungsten oxide films for electrochromic windows

Chi-Ping Li
National United University, Taiwan

Template-assisted sol gel chemistry provides a versatile approach to introduce order and porosity into nanostructured materials. However conventional evaporation induced self-assembly techniques are not easily scaled to produce films with sufficient thickness over large areas at the throughput required by electrochromic windows. Here we demonstrate that the principles of sol gel chemistry may be deployed using ultrasonic spray deposition (USD) for scalable synthesis of nanocrystalline WO_3 films with unrivaled electrochromic performance. Systematic manipulation of sol chemistry enabled the production of mesoporous films with high specific surface area (>100 m^2/g), mean pore sizes of ~5 nm, and narrow pore size distributions. Film thickness is found to be proportional to the sol concentration and number of spray passes, and various combinations are shown to produce films capable of modulating >98% of incident solar radiation in the visible spectrum (450–900 nm). Elimination of haze enables full transmission in the bleached state, while the broadband coloration is attributed to the exceptionally high charge density (>120 mC/cm^2). The materials have good switching speeds which improve with specific surface area, and the long term durability is promising.

Biography

Chi-Ping Li received his PhD of Materials Science from Colorado School of Mines in 2014 and followed by postdoctoral research in National Renewable Energy Laboratory (NREL, USA) in 2015. He joined Department of Chemical Engineering in National United University in Taiwan as an assistant professor in 2018. His research interests are mainly focused on synthesis of nanostructured films, nanocomposite films and nanoparticles. Those materials are used in electrochromic windows, lithium batteries, organic photovoltaics and LED encapsulants. His goal is to overcome the challenges and produce great but low cost materials in the field of green and renewable energy.

Influence of ammonia modification on ultra-pure activated carbons derived from furfuryl alcohol

A. Kałamaga and **R. J. Wróbel**

West Pomeranian University of Technology, Poland

The series of ultra-pure carbonaceous materials were produced from furfuryl alcohol by carbonization process under nitrogen and ammonia atmosphere at 600°C followed by physical activation under carbon dioxide at 1000°C with different times. Sorption capacities were measured by thermogravimetry analysis (TGA) at 30°C. The highest carbon dioxide and ethene uptakes for unmodified samples reached 2.5 mmol/g and 4.2 mmol/g, respectively. N-doped materials were characteristic of significantly lower sorption capacities. X-ray photoelectron spectroscopy (XPS) confirmed purity of materials. In chemical compounds occur solely carbon, oxygen, hydrogen and nitrogen (in modified samples). Lack of impurities e.g. calcium, iron or silica allows to eliminate their influence on sorption processes. In addiction it is possible to determine crucial pore sizes for different adsorbates. By volumetric analysis were obtained pore volume and pore size distribution (PSD). Specific surface areas were calculated from BET equation. The highest SSA for unmodified materials reached 1821 m^2/g.

Using of furfuryl alcohol as a precursor to carbonaceous materials is followed by ecological aspects. It is commonly produced from agricultural waste e.g. corncobs. It is also used to green solvents production.

Ultra-pure carbonaceous materials may find application in expensive areas of science where price of material is irrelevant e.g. purification of atmosphere in spaceships, supercapacitors and lithium-ion batteries.

Biography

Agnieszka Kałamaga graduated chemical technology with a specialization in inorganic chemical technology at West Pomeranian University of Technology in Szczecin in 2021. Currently she is a PhD student at ZUT Doctoral School. She is working on carbonaceous materials for sorption application, especially for carbon dioxide, ethene and butane adsorption.

Bandgap-coupled template auto-catalysis towards the growth of high-purity sp² nanocarbons

Jun Gao[1], **Zhenxing Zhu**[1], **Boyuan Shen**[2], **Yunxiang Bai**[3], **Silei Sun**[1] and **Fei Wei**[1]

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Extraordinary properties and great application potentials of carbon nanotube (CNT) and graphene fundamentally rely on their large-scale perfect sp^2 structure. Particularly for high-end applications, ultralow defect density and ultrahigh selectivity are prerequisites, for which metal-catalyzed chemical vapor deposition (CVD) is the most promising approach.

Due to their structure and properties, CNTs and graphene can themselves provide growth template and non-local dual conductance, serving as template auto-catalysts with tunable bandgap during the CVD. However, current growth kinetics models all focus on the external factors and edges.

Here, the growth kinetics of sp$_2$ nanocarbons would be elaborated from the perspective of template auto-catalysis and holistic electronic structure. After reviewing current growth kinetics, various representative works involving CVD growth of different sp2 nanocarbons are analyzed, to reveal their bandgap-coupled kinetics and resulting selective synthesis. Then our recent progress is reviewed, which has demonstrated the interlocking between the atomic assembly rate and bandgap of CNTs, with an explicit volcano dependence whose peak would be determined by environment. Besides, the topological protection for perfect sp^2 structure and the defect-induced perturbation for the interlocking are discussed. Finally, the prospects for the kinetic selective growth of perfect nanocarbons are proposed. Perfect sp^2 structure is protected by the large formation energy of topological defects, resulting in the relative lack of defective CNT (d-CNT) under proper conditions. Bandgap is significant for the kinetic growth of CNTs. The atomic assembly rate, depicted with turnover frequency (TOF), is prominently lower for metallic CNT (m-CNT) than that for semiconducting CNT(s-CNT), and the latter manifests a volcano dependence on the bandgap that is inversely proportional to diameter, while the peak position of the volcano is shiftable and determined by environment.

Biography

Jun Gao is a Ph.D. candidate in the Department of Chemical Engineering at Tsinghua University. He received his bachelor's degree from Tsinghua University in 2018. His research interests focus on controlled preparation, properties of ultralong CNTs and catalysis.

ACCEPTED ABSTRACTS

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March 21-23, 2022

Adv. Materials Science 2022

Co-processing of biomass-methane-CO_2 for hydrogen production

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Transition from fossil fuels to renewable technologies is extremely challenging as renewable energy sources like solar, wind, and biomass are highly unreliable, subject to variation in geography and local climatic conditions. Transition from fossil hydrogen to renewable hydrogen is bridged by the unique 'natural gas – biomass co-processing. At WVU, hydrogen rich syngas production through renewable hardwood biomass gasification was obtained through synergistic natural gas – biomass co-processing. About 5% methane co-processed with biomass at 850˚C on Fe-Mo/CNF catalyst produces H_2: CO ratio of 6 with a very low CO_2 concentration of < 5% in the syngas. About 60 to 80% hydrogen was obtained in the product gas on the Fe-Mo/CNF, Ni-Mo/CNF, and Mo-Pd/CNF catalysts. Synergistic methane activated biomass gasification could be a promising technology for hydrogen rich syngas production as it requires very low concentrations of methane which could be obtained from flare gas. Flare gas is natural gas flared during commissioning of new wells or maintenance of existing wells in shale gas field. On-site utilization of flare gas with biomass could greatly curb CO_2 emission while producing hydrogen rich syngas. CO_2 utilization in the methane activated biomass gasification was studied by adding 1% CO_2 to the gas feed. CO_2 and CH_4 activation at high temperature was performed on Fe, Ni, and Pd active sites while Mo active sites are responsible for deoxygenation of oxygen rich biomass. *In-situ* conversion of raw biomass co-processed with 5% methane produces H_2-rich syngas on the carbon nanofiber supported catalyst. CNF support is also obtained from the biomass feedstock by impregnation with metals and pyrolysis at 700˚C. This process is 95% renewable with net reduction in CO_2 emissions by recycling of CO_2. Detailed mechanistic investigation through molecular simulations helped ascertain the unique reaction pathway occurring on dual active sites on a transition metal doped β-Mo_2C-CNF catalyst. Application of renewable technologies is on the rise especially in power generation but is still far from being a mainstream source of hydrogen and power.

Finite element investigation of thermal-kinetic-mechanical evolutions during laser powder deposition as an innovative technique for rail repair

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Utilization of laser powder deposition (LPD) as an innovative repair tool for damaged steel components is increasingly growing in recent years. This paper investigates repairing a standard US light rail using LPD. No study has focused on repairing standard US rails thus far. Besides, this is the first time that a three-dimensional finite element model is developed where element-birth-and-kill technique is employed to study thermal-kinetic-mechanical evolutions during the LPD rail repair process. Exploration of hardness versus microstructure yielded a reverse correlation between hardness level and austenite volume fraction. The maximum hardness was found near rail-deposition interface with the minimum austenite concentration, while the topmost deposition layer with the highest austenite concentration showed the minimum hardness. Longitudinal residual stresses at the rail-deposition interface were significantly more than that of transversal and normal. Comparing the residual stress against deposition material yield strength showed a slight exceedance (~5%) of transversal stress from the maximum limit, no exceedance for normal stress, but an extreme exceedance of 50% for longitudinal stress. This fact suggested a high risk of cracking along longitudinal direction at the rail-deposition interface, while there existed only a minor risk of transversal cracking and almost no chance of layer delamination. The simulated results were compared against experimental results obtained via optical and scanning electron microscopy, hardness test, and X-ray diffraction stress measurement, where a maximum deviation of 10% proved the model accuracy. The validated model in this study would be a great backbone for future studies on different process parameters to increase hardness and reduce stress in an LPD repaired rail.

Towards a generic physics-based machine learning model for geometry invariant thermal history prediction in additive manufacturing

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Additive manufacturing (AM) is an emerging manufacturing technology that constructs complex parts through layer-by-layer deposition. The prediction and control of thermal fields during production of AM parts are of crucial importance as the temperature distribution and gradient dictates the microstructures, properties, and performance. Finite element (FE) analyses are commonly conducted to simulate the thermal history of the AM process, but are known to be costly and time-consuming. This paper aims to address the challenge by presenting the essential components of a generic data-driven control framework. The proposed framework utilizes extremely randomized trees and is trained and tested on datasets generated through FE simulations. The datasets contain generic, engineered features constructed based on the physics of the underlying thermal process. The features are transferable between a wide ranges of cases and have achieved mean absolute percentage errors (MAPE) below 2.5% for predicting nodal temperature profiles. In addition, predictions of entire simulations with machine learning (ML) models trained on datasets from different cases have been conducted with MAPE below 5%. The results demonstrate the transferability of thermal histories between several geometries and significantly reduce the need for expensive FE simulations. We believe that these findings are an important step towards real-time optimization in AM.

Microstructural changes in additively manufactured Co-Cr-Mo alloy during cyclic loading

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Cobalt-Chromium-Molybdenum (CoCrMo) alloys are used in applications that require high strength and wear resistance. Examples in biomedical area include artificial hip and knee joints implants that are subjected to repetitive loads during the service. The cyclic loading implies high fatigue strength as fundamental mechanical property, besides those already pointed out. In this regard, it is crucial to understand the mechanism associated with the crack propagation. Therefore, in this work, microstructural changes associated with crack propagation during cyclic loading of a CoCrMo alloy were investigated. Tensile test specimens were manufactured using laser powder bed fusion (LPBF) additive manufacturing technique and examined in the as-build condition. The sample was subjected to cycling loading with constant tension load applied (above the yield strength of the material) and subsequent tension release, an initial linear increase in strain hardening based on the deformation-induced martensitic transformation commonly present in materials with low or negative stacking fault energy. Microstructural changes were followed using electron backscatter diffraction (EBSD) technique. A typical as-build microstructure with a single-phase face-centered cubic (γ) structure, consistent to reported previously. After 5100 cycles, it was possible to trace deformation-induced phase transformation from γ to hexagonal close-packed (ε) structure. Our investigation also revealed that cracks nucleated at the ε-phase formed at grain boundaries. In addition, it was observed that the crack tip was deflected when encountered a grain boundary unfavorably oriented to the crack propagation. Then the crack tip propagated further at the ε-phase inside the grain. Therefore, γ → ε deformation-induced martensitic phase transformation serves as a preferential path to the crack propagation.

Effect of fluoride conversion pretreatment time and the microstructure on the corrosion performance of TEOS-GPTMS sol-gel coatings deposited on the WE54 magnesium alloy

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Magnesium and its alloys have been considered as revolutionary materials for automotive and aerospace applications owing to their unique specific mechanical properties. In particular, the WE54 alloy (Mg-Y-RE-Zr) is conventionally employed in the fabrication of high-performance vehicles due to the presence of Y and RE that confers excellent mechanical response at relatively high temperatures. Unfortunately, the major drawback in the use of Mg alloys is their low corrosion resistance in aqueous environments, which leads to early loss of their mechanical integrity. At present, a promising approach to enhance the corrosion behaviour of these alloys is the synthesis of TEOS (tetraethylorthosilicate) / GPTMS (glycidoxypropyltriethoxysilane) hybrid sol-gel coatings as they offer good corrosion resistance, strong adhesion, flexibility and low cracking tendency. Nevertheless, their protective features could be considerably affected by the high reactivity of the Mg alloys with the acidic sol during the deposition stage, causing the formation of corrosion products at the metal/coating interface. In order to overcome this limitation, it has been suggested the development of a fluoride-based conversion pretreatment that promotes the formation of a magnesium hydroxyfluoride layer with protective characteristics. In this regard, the aim of the present investigation was to evaluate the employment of a fluoride-based pretreatment of the WE54 magnesium alloy on the protection-degradation mechanism of TEOS /GPTMS hybrid sol-gel coatings when in contact with saline environment, giving special attention to the influence of the pretreatment time. The experimental results evidenced that long pretreatment times favoured the formation of a magnesium hydroxyfluoride layer with a higher F/O ratio, which improved the corrosion performance of the sol-gel coatings and the WE54 alloy. However, the presence of undissolved intermetallic particles and Y-rich precipitates on the surface led to structural defects that allowed the corrosive attack to evolute along the immersion time in saline solution.

La-doped $ZnTiO_3$/ TiO_2 and supported on ecuadorian diatomaceous earth as a highly efficient photocatalyst driven by solar light

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Nowadays, there is a great interest in the use of TiO_2 for photocatalytic remediation of wastewater. Doping, heterojunction and immobilization on porous materials are effective methods to improve the photocatalytic efficiency of this semiconductor. In this study, $ZnTiO_3/TiO_2$ (ZTO) and $ZnTiO_3/TiO_2$/La (ZTO/La) nanocomposites were successfully prepared by the sol-gel method and immobilizing on diatomaceous earth (DE). The composition and texture of the prepared composites were characterized by X-Ray diffractometry (XRD), X-Ray Fluorescence (XRF), Diffuse Reflectance Spectroscopy (DRS), Scanning Electron Microscopy (SEM-EDX) and specific surface area (SSA). The adsorption capacity and photocatalytic activity of composites were determined via degradation of methylene blue (MB) in batch reactors. The materials evaluated were prepared in the shape of 0.2 cm (diameter) and 1.0 cm (length) cylindrical extrudates. The results indicated that the ZTO/La-DE composite exhibits a higher efficiency of removal of MB than ZTO-DE and DE under solar irradiation. The Langmuir isotherm model and the pseudo-second-order model were better suited to the adsorption process. The higher degradation percentage of MB obtained was 96% after 150 min of irradiation. The results reflect that synthesized composite could be used potentially for the removal of cationic dye from wastewater.

Design and operation of low energy consumption passive human comfort solutions

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The rapid growth during the last decade has been accompanied by active construction, which in some instances neglected the impact on the environment and human activities. Policies to promote the rational use of electric energy and to preserve natural non-renewable resources are of paramount importance. Low energy design of urban environment and buildings in densely populated areas requires consideration of wide range of factors, including urban setting, transport planning, energy system design and architectural and engineering details. The focus of the world's attention on environmental issues in recent years has stimulated response in many countries, which have led to a closer examination of energy conservation strategies for conventional fossil fuels. One way of reducing building energy consumption is to design buildings, which are more economical in their use of energy for heating, lighting, cooling, ventilation and hot water supply. However, exploitation of renewable energy in buildings and agricultural greenhouses can, also, significantly contribute towards reducing dependency on fossil fuels. This will also contribute to the amelioration of environmental conditions by replacing conventional fuels with renewable energies that produce no air pollution or greenhouse gases. This study describes various designs of low energy buildings. It also, outlines the effect of dense urban building nature on energy consumption, and its contribution to climate change. Measures, which would help to save energy in buildings, are also presented

Multicomponent high-entropy cantor alloys

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All human advances have depended on making new materials, and all materials are alloys, i.e. mixtures of several different starting materials or components. So the history of the human race has been the continued invention of new materials by discovering new alloys. Recently a new way of doing this, by manufacturing multicomponent high-entropy alloys, has shown that the total number of possible materials is enormous, even more than the number of atoms in the galaxy, so we have lots of wonderful new materials yet to find. And multicomponent phase space contains a surprisingly large number of extended solid solutions. The first group of these which was discovered are called Cantor alloys, an enormous composition range with a single-phase Fcc structure, based loosely on the original equiatomic five-component Cantor alloy CrMnFeCoNi. This talk will discuss the previous history of alloying, the discovery of multicomponent alloys, the structure of multicomponent phase space, the fundamental thermodynamics of multicomponent solid solutions such as the Cantor alloys, the complexity of local atomic and nanoscale configurations in such materials, the effect of this on properties such as atomic diffusion, dislocation slip, and the resulting outstanding mechanical properties and potential applications.

Atomic ordering at liquid-metal/oxide interfaces from Ab initio modelling

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Oxide particles, magnesia, spinel and alumina are formed in the liquid light metals inevitably during liquid metal dealing and casting. They play an important role in determination of the properties of the cast parts, and may also act as potential nucleation sites to achieve effective grain refinement. Thus, understanding of the atomic ordering at liquid-metal/oxide (L-M/oxide) interfaces is a prerequisite for controlling the heterogeneous nucleation during casting. Here, we briefly overview recent studies devoting to improve the understanding of atomic ordering at the liquid-metal/oxide interfaces from ab initio molecular dynamics (AIMD) simulations. We identified a formed metal layer terminating the oxide substrates, MgO {1 1 1}, α-Al_2O_3 {0 0 0 1}, $MgAl_2O_4$ {1 1 1} and γ-Al_2O_3 {1 1 1} in the liquid metals. The liquid metal atoms near the interfaces exhibit atomic ordering for L-Al/spinel {1 1 1} as an example. The terminating metal atoms exhibit unusual chemistry: being positively charged and topologically rough, which impact strongly the atomic ordering at the interfaces. The obtained information is helpful not only for obtaining insight into the potency of the oxide particles, further for controlling of the solidification, but also for better understanding of ceramic coating of metals and of metal/oxide composite materials.

Investigation of the characteristics of expanded polystyrene (EPS) foam beads mixture as a lightweight construction material

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This research investigates the natural and the mechanical characteristics of the lightweight expanded polystyrene (EPS) foam beads mixture as a lightweight construction material. to solve problems of construct embankments and abutments of highways on weak soil by reducing the weight of soil. In this research, the mixture was prepared using foam beads, sand, cement and water. The foam beads and sand were mixed with ratio 1:1 by volume and mixed with cement content by percentage 7%, 8%, 9% and 10% of sand weight using the optimum water content. Experimental tests were carried out to evaluate natural properties and mechanical properties such as: unit weight, shear strength parameter, compressibility, and crushing strength. The results found that, the high cement ratio of 10% formed lightweight mass with acceptable crushing strength, CBR and compressibility characteristics. The results show that, the cement contents and curing time effect on the properties of the mixture.

Energy storage and the compressibility of atoms

Jean-Patrick Connerade
Imperial College, United Kingdom

The development of reversible energy storage in 'rocking chair' batteries using Lithium ions usually requires research on special materials for the electrodes. The requirement is essentially that they can act as suitable hosts for the storage of lithium ions. Lithium ions have the electronic configuration of helium and can therefore be categorised as the hardest (i.e. least compressible) of the singly charged ions. Reversible storage therefore requires, in addition to freedom of movement of the ions through the lattice, that the host material should possess the flexibility required to store the ion and subsequently eject it without any recrystalisation, because the latter would imply a change of phase of the host material and hence a loss of energy and reversibility. The storage-recovery cycle often makes use of polaronic distortion of the lattice, which implies the use of 'soft' or highly compressible constituent atoms. It will be shown that these 'soft' atoms belong to a specific class for which the outer electrons are subject to a double-well quantum-mechanical potential. Such atoms belong to a limited class in the Periodic Table. Thus, specific atoms are singled out as the most favourable. A table involving such atoms will be presented.

Advanced laser technology for quantum communications

T.K. Paraiso, R.I. Woodward, D.G. Marangon, V. Lovic, Z.L. Yuan and **A.J. Shields**
Toshiba Europe Ltd, United Kingdom

In this new decade our societies will face rapid changes and will need to adapt to a wide range of new technologies emerging from the quantum world. Among them, quantum communications is set to occupy a central place in our future ways of exchanging and processing of information: by exploiting the laws of quantum mechanics, it allows transferring and manipulating information beyond the capabilities of our conventional technologies. Owing to the threat of quantum computers against conventional public key cryptography algorithms methods, quantum key distribution (QKD) arose as means to establish symmetric encryption keys between distant parties, with information theoretic security.

In the recent years, QKD has demonstrated a high level of maturity, which motivated governments and industry partners to work towards the development of large-scale quantum communication infrastructures. This perspective poses an immediate practicality challenge: how to encode quantum information in a versatile way while preserving the constraints of low-cost production, high power efficiency, small size and high scalability required for a viable integration in our conventional communication infrastructure?

In this talk, we present recent advances in laser modulation technologies that have enabled the development of efficient and versatile light sources for quantum communications. Based-on on appropriate combinations of different features of well-known laser physics, these sources have been used to demonstrate several QKD protocols with state-of-the-art performance. After introducing the concepts of quantum cryptography and advanced laser modulation techniques, we review and interpret the applications and experimental results enabled by this new approach in the light of a complete theoretical framework.

3D-printed hierarchical pillar array electrodes for high performance semi-artificial photosynthesis

Xiaolong. Chen and **Jenny. Zhang**
University of Cambridge, United Kingdom

The re-wiring of photosynthetic bio-machineries to electrodes is a forward-looking semi-artificial route for sustainable bio-electricity and fuel generation. Currently, it is unclear how the bio-material interface can be designed to meet the complex requirements for high bio-photoelectrochemical performance. Here, we developed an aerosol jet printing method for generating hierarchical electrode structures using indium tin oxide nanoparticles. We printed libraries of micropillar array electrodes varying in height and sub-micron surface features and studied the energy/electron transfer processes across the bio-electrode interfaces. When wired to the cyanobacterium Synechocysis sp. PCC 6803, micropillar array electrodes with micro-branches exhibited favourable biocatalyst loading, light utilisation and electron flux output, ultimately almost doubling the photocurrent of state-of-the-art porous structures of the same height. When the micropillars' heights were increased from 50 to 600 µm, milestone mediated photocurrent densities of 245 µA cm^{-2} (the closest thus far to theoretical predictions) and external quantum efficiencies of up to 29% could be reached. This study demonstrates how bioenergy from photosynthesis could be more efficiently harnessed in the future and provide new tools for 3D electrode design.

Interface engineering of solid garnet batteries

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Justus Liebig University Giessen, Germany

The solid-solid interfacial contact is a critical issue during the studies of solid-state batteries (SSBs), which greatly affects the electrochemical performance of SSBs, such as the coulombic efficiency, and cycle life. For flexible polymer/garnet electrolytes (PGEs), the interfacial issue mainly comes from the interactions between the inorganic fillers and the polymer matrix. The slow Li^+ transport through the polymer/garnet interface can lead to the low ionic conductivity of PGEs. While for garnet ceramic electrolytes (GCEs), the ceramic bulk with a relative density over 99% shows no obvious grain boundary, leading to the ionic conductivity over 10-3Scm^{-1} at room temperature. Under this circumstance, the interfacial issue could be attributed to the poor interfacial contact between the GCEs and Li metal anodes. It can induce the large interfacial resistance as well as the lithium dendrite growth. In this presentation, I'll focus on the aforementioned interfacial issues, various targeted strategies will be introduced to construct the excellent interfacial structure, thus significantly improving the performance of SSBs.

Studying the residual macrostress and texture development upon low temperature nitriding of Co-Cr alloys

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Low temperature gaseous nitriding of Co-Cr alloys at 400°C with the initial hexagonal close-packed (hcp) crystal structure results in the development of supersaturated hcp phase with the incoming nitrogen atoms. The residual macrostress develops on the surface as a result of volume misfit between the nitrided case and the untreated core. This macrostress affects the nitriding behavior of differently-orientated hcp variants at the surface, in a way that their further transformation to face-centered cubic (fcc) phase is anisotropic. The intent of current research is to investigate the magnitude of this residual macrostress as well as the resulted texture on the surface of nitrided specimen. The stress measurements were carried out using stress analysis method by X-ray diffraction, so-call the Sin2ψ method, on a surface of specimen with the nitrided layer containing expanded hcp phase. The measured (101) lattice spacings against Sin2ψ depicts an oscillation, which can be ascribed to the crystallographic texture. In addition, re-orientation of surface adjacent grains with respect to their orientation in the core is realized using electron backscatter diffraction (EBSD). The lattice elongation perpendicular to the specimen´s surface can be assumed similar to the deformation resulted from the uniaxial tension. In a case of a sever deformation, an obvious texture may be observed for the grains at the surface similar to the fibre texture that can be achieved after the uniaxial tension of hcp materials.

How does the glass beads impact the behavior of the failure pattern in bonded joints?

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New materials and coatings have been introduced in car manufactures to reduce vehicle weight and improve corrosion resistance. In body shop, multimaterial design is joined using structural adhesives. The former epoxy crash adhesive gave adhesive failure on new steel coatings. This kind of failure is not accepted by carmakers. One way to obtain cohesive failure, is by adding glass beads in adhesive formulations. The aim of this work was to analyze how the addition of glass beads to the adhesive layer affects the failure mechanism.

Single lap bonded specimens with mild steels were tested in quasi-static conditions and with different amount of glass microspheres. The results showed that the glass microspheres act as reinforcement particles which introduce stress concentration around the particles and their vicinities. This new phenomenon led the cracks to propagate in the middle of the adhesive layer rather than interfacial. This promote the cohesive failure. This novel effect solved the adhesion issue on difficult surfaces.

Floating photocatalysts to exploit sunlight in water remediation

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In the last decades, the attention to environmental issues and the race to develop eco-friendly processes, has further attracted the field of research towards an inexpensive, simple, and reliable technology. A concerning global issue is freshwater scarcity mainly caused by leaking landfills, industrial waste, and sewage. In this regard, heterogeneous photocatalysis could offer a feasible solution to this problem aiming at the development of photoactive devices suitable for water remediation. Although TiO_2 is still the most used semiconductor due to its chemical and physical stability, good photoactivity and low cost, researchers are willing to replace it with new smart materials because of its suspected carcinogenic nature and limited activity under solar light. Among them, g-C_3N_4 has promising features as photocatalyst for water-remediation considering its visible-light response, simple synthetic pathway, and peculiar layered structure and cheap production cost. To overcome problems related to the use of slurry systems for water purification, new floating substrates were employed to immobilize the photocatalyst. Since their closeness to water-surface, these devices can be fully irradiated by light source, better oxygenated, and easily recovered and reused. Within this framework, synthetic polymers are commonly used as support, however their non-degradability has raised ecological concerns. Instead, an eco-friendly alternative can be the use of natural polymers, such as alginate, which derives from brown seaweeds and can be used for the immobilization of photocatalysts under safe and mild conditions. In the present study, different methods were applied in order to synthesize floating alginates as support for O-doped g-C_3N_4 catalysts, whose activity was improved under visible light by doping with oxygen. These materials were deeply studied for photodegradation of rhodamine B, sodium diclofenac and isoproturon in water under solar light irradiation. Furthermore, floating photocatalyst were subjected to recycle test, in order to verify their activity and stability after several experiments.

Metal-free-based photocatalytic materials: Advances and future perspectives for environmental and energy purposes

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The contemporary world is facing energy shortages and environmental problems, which hinder the evolution of human civilization giving rise to various types of crises. The huge energy consumption and environment pollution related to the traditional industrial processes, along with the increasing need of synthetic chemicals to satisfy the current society requirements, are urgent issues to be addressed for the development of the new foundations for a sustainable future. These critical challenges need solutions which require an important upgrade in energy sources and the conception of new generation processes and manufacturing technologies. Researchers, over the past few decades, have been studying several methods to understand how to overcome these problems. In this context, heterogeneous photocatalysis appears as one of the useful technologies to help these urgent efforts, and it can make a contribution to solve environmental problems and manage the conversion of solar energy into chemical energy in a sustainable way.

Among the semiconductors to be used as photocatalysts, metal-free materials, such as graphene, nitrides, carbides, and conjugated organic polymers, have gained extensive research interest due to their earth abundance, cost-effectiveness, good electrical conductivity, and environmental friendliness. These semiconductors are active for photocatalytic H_2 generation, CO_2 reduction, and for environmental applications, not only for photocatalytic abatement of pollutants, both in gas-solid and liquid-solid regimes, but also for the valorization of substances obtained from biomass to obtain high added value chemicals. All of these applications of the photocatalytc technology are carried out in green conditions, by using water as solvent, at room temperature and atmospheric pressure by using natural solar irradiation as energy source.

In the present work the recent progress from our laboratory research on metal-free photocatalysis will be systematically presented and also compared with the literature research. Opportunities and challenges on metal-free photocatalysts to enhance their activity under natural solar irradiation will be presented. Based on the aforementioned discussions, suitable future research directions and perspectives for the design and development of potential metal-free photocatalysts will be provided.

Ovarian masses-applicable IOTA ADNEX model versus morphological findings for accurate diagnosis and treatment

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A common problem in gynecological practice is the differential diagnosis of the ovarian masses. The clinician must apply the IOTA (International Ovarian Tumor Analysis) ADNEX (Assessment of Different Neoplasia in the Adnexa) model criteria to evaluate the risk of benign, borderline or malignant tumors. The aim of this study was to verify if the IOTA ADNEX model is a practical tool to be used before surgery and if there is a significant difference between IOTA ADNEX criteria and histological findings. A prospective single center study was performed between January 2017 and December 2019 in Obstetrics and Gynecology Hospital "Cuza-Voda", Iasi, Romania. The study included 230 patients between 17 and 74 years old diagnosed with persistent adnexal masses. We applied the IOTA ADNEX model protocol predicting the risk of benign, borderline or malignant masses. The golden standard remains the histological diagnosis of the surgically removed mass. The patients that had been diagnosed using ultrasonography with persistent adnexal masses between 30 and 291 mm were operated on in our clinic. In our study the majority of patients had benign ovarian tumor mass, these being 223 (96.96%) patients, from whom, according to IOTA ADNEX protocol, the correspondence was: 91.8–99.7% at risk of benign tumors, 0.3–4.5% at risk of borderline tumors and 0.3–8.2% at risk of malignant masses. Unexpected findings were obtained from the malignant group that included five patients (2.17%) with the following correspondence: 96.1–99% at risk of benign tumors, 0.6–2.4% at risk of borderline tumors and 1–3.9% at risk of malignant masses. After applying the IOTA ADNEX model criteria, the patients with a suspicion of malignant disease were correctly guided towards surgical treatment in an oncological center. In our hospital, surgical treatment was only proposed to those patients with high suspicion of benign masses.

Several possible phase states in oxide ferroelectrics

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The analysis of phase diagrams, structure and crystal lattices dynamics of oxide ferroelectrics of lithium niobate and tantalate at various concentrations of topological defects was carried out. The structure and dynamics of the lattice in the region optical vibrations were studied by the methods of X-ray structural analysis, quasi-elastic and Raman light scattering spectroscopy. Sound absorption of longitudinal and shear waves and Q-factor of samples were obtained by the radio engineering method and by the Bragg light scattering on sound method. Three types of lithium niobate samples were prepared for the studies - those grown from a stoichiometric melt, grown from a congruent melt and grown from a congruent melt with different rates of pulling out the seed from the melt in order to create different concentrations of dislocations. We calculated the intensity of Raman light scattering in the frequency range 5 - 70 cm^{-1} at the model interaction of 2A1 (TO) symmetry optical vibration with acoustic vibrations relaxing on dislocations. The self-energy part of acoustic phonons was calculated from the Langevin equation. Good agreement of the calculated spectrum with the experimental one was obtained. The high degree of correlation between the parameters makes it possible to dispense with only one parameter in the used model - the concentration of topological defects in the samples. It is shown that there is a critical value of the concentration of topological macrodefects, at which a correlation occurs between dislocations.

Topological insulators: Myths and reality

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Topological insulators (TI) are a new kind of solids. Simply speaking they are bulk insulators with metallic surfaces. All semiconductors with the inverted band structure are the topological insulators. At the moment there are three myths about TI: Myth 1: the beauty of ARPES, Myth 2: topological insulators are the material of the future electronics, Myth 3: Topological protection against back scattering, and Myth 4: Chiral interconnection. The subject of this talk is the critical analyses of these mythes.

Antiphase boundary defects in Strontium-doped Lanthanum Scandate

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$LaScO_3$-based oxides are promising oxide materials for solid oxide electrochemical devices, such as protonic ceramic fuel cells, electrolysis cells, and gas sensors. The substitution of La^{3+} lanthanum with strontium Sr^{2+} should lead to a decrease in the oxygen content in the oxide lattice in order to satisfy the electroneutrality condition. The ^{45}Sc NMR method was used to study the local structure of $La_{1-x}Sr_xScO_{3-\delta}$ oxides (x = 0, 0.04, 0.09). Only one line was found on the ^{45}Sc NMR spectra, which corresponded to the 6-coordinate scandium in strontium-doped lanthanum scandates, and the contribution of the quadrupole broadened part of the spectrum decreased with an increase in the level of doping with strontium, indicating an increase in the local symmetry of the Sc^{3+} ion.

EBSD and TEM study shows the existence of a structural inhomogeneity in a polycrystalline sample of strontium-doped lanthanum scandate was found in comparison with the undoped oxide. Defects, represented as straight or arbitrarily curved lines that did not extend beyond the grain boundaries, were identified as п-type antiphase boundaries.

The atomic structure of possible antiphase boundaries in lanthanum-strontium scandate perovskite, a promising proton conductor, was modelled by means of DFT method. Two structural types of interfaces were modelled: edge- and face-shared. Energetic stability of all interfaces was calculated along with the oxygen vacancy formation and migration energies. Mechanisms of oxygen migration in both types of interfaces were modelled. It was shown that both types of interfaces are structurally stable and permit oxygen ionic migration. Oxygen vacancy formation in face-shared interface is by 0.2 eV lower than that in the bulk. Oxygen migration, however, most likely, will be blocked by some high-energy barriers over the O–O bonds with shared faces.

Biodegradation and incineration as the final stages of the life cycle of polymer packaging in a circular economy

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Changing the profile of world trade in the context of the transition to a circular and low-carbon economy is inextricably linked to global flows of "polymer waste," which lead to "plastic pollution" of the planet and are subject to international regulation (EU Framework Directive 2008/98/EC). Polymer packaging is one of the largest use areas of polymer composite materials. We have found that the biodegradability to polymer composite materials based on a number of synthetic polymers, practically not decomposable in pure form, gives arabinogalactan (AG), one of the most important components of Siberian and Daurian larch - these types of larch contain up to 30%AG. We have established that AG is contained in larch in the form of an aquacomplex - "arabinogalactan-water". Such a complex has a freezing point below -60°C and can be considered as a natural low-temperature eutectic that provides frost resistance to these larch species and the possibility of larch growing in permafrost.

The AG-water complex for larch is the liquid phase that fills its capillary-porous structure and allows larch to survive in conditions of Siberian frosts and permafrost, and provides fatigue strength to its branches and roots. At the same time, larch roots can be considered as a carbon sequestration path, and the alternating wind load for a growing tree ensures the development of its root structure and increases the amount of carbon sequestered in the ground. There are offered industrial versions of arabinogalactans extraction from larch and versions of usage of sawdust with increased content of arabinogalactans as components of composite materials of packaging purpose. An advanced innovative technology has been developed for processing into fuel briquettes both sawdust and their mixtures with waste of synthetic polymers, including those with used plastic packaging.

Application of luminophore-containing compositions for modifying the spectral characteristics of diamonds in X-ray luminescent separation schemes

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Significant losses of diamonds during the enrichment of diamond-containing kimberlites according to the schemes of X-ray-luminescent separation (XLS) are due to the fact that some of the crystals have spectral-kinetic characteristics, the values of which go beyond the ranges of settings of X-ray-luminescent separators. The idea is substantiated and a technology is proposed to reduce the losses of weakly and anomalously luminescent diamonds in the XLS process of diamond-containing material using luminophore-containing compositions that provide an approximation of the anomalous spectral characteristics of non-recoverable diamonds to the standard parameters of natural crystals. With the chosen approach, a simultaneous increase in the convolution and the attenuation time constant of the X-ray luminescence signal is achieved. The effectiveness of the use of the luminophore FL-530, characterized by the presence of a pronounced slow component of the X-ray luminescence signal, and the anthracene luminophore with a large amplitude of the fast component, for modifying the spectral characteristics of diamonds is confirmed. The use of diesel fuel as an organic phase of a luminophore-containing emulsion that provides effective fixation of a luminophore-containing composition on diamonds is justified. The expediency of adding reagents to the organic and aqueous phases of the emulsion has been experimentally confirmed, which provide an increase in the adhesion and retention ability of the organic phase with respect to diamonds and luminophores or reduce the fixation of on kimberlite minerals. A mode of increasing the oleophilicity of the luminophore FL-530 by treatment with hydrophobizing reagents has been developed, which provides an increase in the retention capacity of the organic phase in relation to the luminophore and the efficiency of its fixation on the surface of diamonds.

Effect of phase transformations of a metal component on the magnetic and transport properties of nanocomposites $Co_x(MgF_2)_{100-x}$ and $(CoFeZr)_x(MgF_2)_{100-x}$

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The aim of this work was to establish the effect of structural-phase transformations on the magnetic and transport properties of $Co_x(MgF_2)_{100-x}$ and $(CoFeZr)_x(MgF_2)_{100-x}$ nanocomposites depending on the metal or alloy content in the dielectric matrix MgF_2 on the basis of complex studies by various methods: XRD, XPS, IR-spectroscopy, magneto-optical spectroscopy and electro-resistivity methods.

The percolation thresholds in the system Cox $(MgF_2)_{100-x}$ at x = 37 and in the system with the alloy $(CoFeZr)_x(MgF_2)_{100-x}$ at x = 30 determined from the concentration dependences of the electrical resistance of nanocomposites, coincide with the formation of metal nanocrystals in the dielectric matrix MgF_2. The average size of metal nanocrystals in both systems varies within 10–20 nm.

In magneto-optical studies on the concentration dependences of transversal Kerr effect (TKE) in the visible and near-IR regions of the spectrum in nanocomposites $Cox(MgF_2)_{100-x}$ one maximum is observed at the percolation threshold at x = 37 which coincides with the formation of α-Co nanocrystals. When the content of cobalt x<42 Cox $(MgF_2)_{100-x}$ nanocomposites exhibit a soft magnetic character, and at a higher metal content (x> 42), a hard magnetic character with a coercive force of up to 95 Oe.

In nanocomposites $(CoFeZr)_x(MgF_2)_{100-x}$ two maxima appear on the concentration dependences of transversal Kerr effect in the visible and near-IR regions of the spectrum, one of which corresponds to the formation of hexagonal nanocrystals of the CoFeZr alloy at x = 30 and the second maximum at x = 45 corresponds to the phase transition of nanocrystals from a hexagonal structure to a cubic body-centered structure.

In nanocomposites $(CoFeZr)_x(MgF_2)_{100-x}$, the value of magnetic percolation Xc = 30 coincides with the formation of nanocrystals: below this value x<30 nanocomposites exhibit superparamagnetic properties, and at large values x> 30 become soft magnets with a maximum value of the coercive force Hc <30 Oe.

The effective cold fusion energy production realization on base of the planar X-ray waveguide-resonators use

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The main intricate and energy outlaying problem for realization of nuclear fusion reactions is the Coulomb barrier overcoming, which hinders to the direct nuclear interaction. In thermonuclear apparatus the barrier overcoming is effected by increasing of ions kinetic energy in ionized ensemble. This approach competence to the nuclear fusion reactions realization is beyond questions. A.D. Sakharov and Ya.B. Zheldovich pointed on the principle possibility of alternative approach to the nuclear fusion reaction realization without high temperature application. The idea of cold nuclear fusion was implemented by I.S. Filimonenko. Moreover, the cold nuclear fusion or nuclear transmutation phenomenon is beyond questions, too. However, the magnitude of cold nuclear fusion effect is smaller as the expected one on some hundreds thousands times. Our work proposes an alternative approach to the cold nuclear fusion realization on base of the radiation fluxes waveguide-resonance propagation phenomenon consequence and the wave-corpuscle dualism principle. Our experimental studies showed that the planar extended slit clearance transports X-ray characteristic radiation fluxes without attenuation when its width is smaller as the radiation coherence length half ($L/2=\lambda_0^2/2\Delta\lambda$). This fact was interpreted as the new phenomenon discovery:the wave guide-resonance propagation of radiation fluxes or the radiation superfluidity. The phenomenon is characterized by appearing of the uniform interference field of radiation standing waves. Devices functioned in frame of the phenomenon were called as planar X-ray waveguide-resonators (PXWR). Study of there devices properties showed that independent radiation fluxes can interact in some conditions in result of mutual influence of uniform interference fields of radiation standing waves excited by these fluxes. Owing to the wave corpuscle dualism principle the radiation standing wave uniform interference field can be excited by particles beams with zero rest mass, too. This hypothesis found own experimental confirmation in investigations of low energy neutrons fluxes propagation peculiarities. Analogical interference fields can be formed for atomic and molecular fluxes. Then it will be needed to find conditions for there fields interaction. The suggesting approach allows to evade the Coulomb barrier.

Optimum stimulation period for pulse thermography

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The usage of InfraRed Thermography to measure temperature over the last 70 years. Using an energy source, temperature patterns can be created and amplified. Combining the application of energy and using thermography to measure its effect creates a technique called Active Infrared Thermography (AIRT). Here, the energy can be applied in the form of a transient wave, where the energy is applied during a certain period or in the form of a sinusoidal wave, called lock-in thermography.

The active thermal test energy can be applied in the form of a magnetic flux, hot air flux, or a simple light. Independently of the amount of energy applied, the time during which is applied has a great importance is the test result. Small periods lead to small thermal patterns, longer periods lead to higher temperatures and blurred thermal images. Therefore, it is important to select the adequate period in order to obtain the best result. Particular if is intended to perform a comparison or systematic evaluations.

The application of energy in the form of a pulse wave is one of the fastest and better performing ones. To determine the optimum period for a transient thermal test experimental tests and FEM simulations were performed. Part of the simulation parameters were adjusted by fitting a temperature profile from a simulation to an experimental test.

The results show, concerning Carbon Fiber Reinforced Polymers (CFRP), there is a limit for the maximum detectability. Combining both results we created a simple equation that allows a fast determination of the optimal period for a certain sample thickness.

On the question of material selection and design options analysis for a centrifugal fan impellers

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The comparative stress analysis of various design options of the radial blower impellers used in conveyor dryer for fine-grained raw materials is presented. Several popular materials that can be used for the impeller manufacturing are considered. Finite Element Method (FEM) has been used to evaluate the stresses and strains of impeller within the operational speed range and to select the appropriate material. An advantage of using steel with higher impact toughness for the manufacturing of the fan impeller has been shown. Such materials allow to have greater resistance to shock loads during abrupt starts or stops, hitting foreign objects, etc.

Analysis shows advantages of impeller design with central disk. The maximum operational rotation speed for this design is 1135 min^{-1} according to the yield strength with 15% safety factor, while for basic design without central disk is 1225 min^{-1}. The maximum stress for this impeller design is slightly higher among competitors in blades slot for central disk fitting, but the overall stresses are greatly decreased, especially in contact edges with hub and shroud (by 22-38%) and blades bending deformation is reduced by 51%.

It is shown that the most effective material option from the considered ones for impeller manufacturing is Hardox 450 steel. Aluminium alloy 6061-T6 demonstrates worse results. Using this alloy is limited in practice, because it made it impossible to operate in high temperature conditions. However, the advantage of using aluminium alloy is the possibility of significant lightening of the impeller while maintaining high strength parameters. The worst strength performance has impeller made from ASTM A36 steel.

In design practice it is worth mentioning that Hardox steels have many competitors on the global market. These competitors have almost the same quality indicators and the choice of material is significantly dependent of its availability and price in specific region. Finally the rational choice depends on operating conditions and required fan performance.

The performed research helps better understanding possible week points in different impeller design options and cause of potential failures of the centrifugal fans as well; hence, to improve reliability of such equipment engaged in various industrial plants.

Simulation of quasi-brittle fracture

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Perfectly brittle or just fragile destruction occurs without plastic deformation. Quasi-brittle fracture involves the presence of a plastic zone in front of the crack edge. Purpose: to describe the factors that determine crack resistance in quasi-brittle fracture. It was assumed that the stress-strain state near the crack tip in quasi-brittle fracture can be described on the basis of:

a) known numerous experimental observations, namely: at a certain stage of loading plastic deformations are localized in two, symmetrical with respect to the crack plane, bands (straight lines) of fluidity;

b) the assumption that the stress-strain state near the crack tip is adequate to the stress state of the soft layer, in both cases the development of plastic deformations is maintained by neighboring areas where the yield strength is not reached;

c) radiographic studies of the newly formed fracture surface, which allow to determine the energy costs of quasi-brittle fracture [8], the proposed formulaK_(1c) = $0.5\sigma_в (3h_0)^{1/2}$, де $\sigma_в$ [MPa] – temporary resistance to destruction; h_0 [m] is the height of the irregularities of the newly formed surface.

In this paper, we propose the conclusion that a detailed description of the stress-strain state near the top of the separation crack under conditions of plane deformation is not mandatory. Destruction by crack propagation is unambiguously determined by the coordinates of points A and B.

Most likely the coordinates of the points are as follows:A($0;\sigma_{0.2}$); B($x0;\sigma_{ut}$), де $\sigma_{0.2}$ – is the conditional yield strength [MPa]; σut - maximum, theoretical strength [MPa]; $x_0 = k(\sigma_{ut} - \sigma_{0.2})$ [m]. Determining the proportionality factor k requires additional research. If $\sigma_{0.2} = \sigma_{ut}$, then there is absolutely fragile destruction. As the yield strength $\sigma_{0.2}$ increases with decreasing temperature, the fracture becomes more brittle.

Behavior of power fractional kinetics in condensed matters

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Kinetics of processes in condensed matters may be expressed in the form of ac frequency spectra of real and imaginary components (in the frequency domain) or in the form temporal decay after abrupt termination of exciting steady state field (in the time domain). Universal relaxation law is characterized by fractional power dependence of real and imaginary component of ac response with the same exponent $0 < n < 1$ and widely observed in different classes of materials like amorphous glasses, ceramics, poly-crystalline and single crystals. In this report dispersive media means a system consisting of dynamical pieces characteristic times of which are distributed over wide temporal range according to fractional power law.

One of the interesting feature of power dispersive solids are unexpectedly high relative dielectric constant let them name as colossal dielectric constant materials. There are a few models explaining their huge values, but they aren't directly related to power fractional dispersion. The aim of this report is to describe behavior of power fractional kinetics on temperature and stress on spectra with exponent n within the range of about 0.7-0.9, formulate the kinetics features and universality in temperature and stress dependencies.

Character of temperature behavior of power dispersive systems has been considered depending on a range of exponent n. The model of temperature behavior of dispersive systems is based on thermally activated behavior of efficient dipoles with different relaxation times. According to the model universality of temperature behavior of medium dispersive system has been described.

Strong stress dependence of medium dispersive systems has been revealed. The proposed model shows that increase of real and imaginary parts of complex relative dielectric constant is accompanied with decrease of exponent n with increasing uniaxial stress. Sensitivity of parameters B and n of dielectric spectra and parameters of effective dipoles on uniaxial stress has been estimated for high-resistivity GaSe layered crystals.

Casting laser liquid phase joining as a method of producing multi layered composites

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In modern production, the use of one or another method for obtaining layered composite materials is determined by the properties of the starting materials, the shape of the manufactured metal products, the conditions of its operation and the methods of processing products.

Methods for manufacturing layered composites can be classified based on the nature of the processes at the interface between the components: metallurgical, diffusion, or adhesive. The strongest connection occurs under the conditions of metallurgical processes. However, the size of the transition layer (connection layer) should be as narrow as possible, since otherwise the mixing of the components (especially dissimilar ones) leads to deterioration in the quality of the raw materials used. And, in the end, to a deterioration in the quality of the product as a whole. The solution of this problem is facilitated by the use of a concentrated source of local heating - laser radiation.

In the development of previously developed traditional technologies, this work provides for the creation of a new hybrid method of casting-laser processing for the production of bimetallic and multilayer products, which makes it possible to combine the advantages of using concentrated energy sources with traditional foundry technologies for the production and restoration of machine parts.

The method allows obtaining significant technical and economic results, of which the most important are: an increase in the service life of machine parts by 2.5 - 6.0 times compared to serial products and a reduction of up to 70 - 80% of the cost of high-alloy expensive materials.

Microthermometric study of fluid inclusions from the Penjom, Tersang and Selinsing Orogenic gold deposits, peninsular Malaysia

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Ore-forming fluids in the auriferous district of the Central gold belt in Peninsular Malaysia were investigated for their temperature, salinity, and relationship to the surrounding geology. Field work conducted at mine sites allowed sampling quartz vein specimens which were mounted and polished to make fluid inclusion sections prior to petrography and microthermometry. Cooling and heating experiments were carried out using the Linkam TH600 heating-freezing stage at the Centre for Ore Deposit, University of Tasmania, Australia.

Homogenisation temperatures of quartz-hosted fluid inclusions range from 210 to 348°C (Tersang), between 194 and 348°C (Selinsing), and from 221 to 346°C (Penjom). Salinities range from 2.41 to 8.95 wt % NaCl (Tersang), between 1.23 and 9.98 wt % NaCl (Selinsing), and from 4.34 to 9.34 wt % NaCl (Penjom). Laser Raman Spectroscopy indicated that at the Tersang gold deposit, most inclusions are either pure or nearly pure CO_2-rich (87–100 mol %), except for one inclusion, which contains CH_4 gas (13 mol %). In addition, at Selinsing, most inclusions are CO_2-rich (90-100 mol %). However, an inclusion was found containing minor N_2 (5 mol %) and CH_4 (5 mol %).

Additionally, at the Penjom gold deposit, most fluid inclusions are CO_2-rich (91–100 mol %), whereas one fluid inclusion is N_2-rich (100 mol %) and another one has minor N_2 (5 mol %) and CH_4 (5 mol %). Microthermometric data shows an isothermal mixing of hydrothermal fluids. The three deposits have CO_2-rich fluids indicative of metamorphic origin. Field relationship shows a spatial distribution of sandstone and carbonaceous black shales with magmatic rocks, such as rhyolite, rhyolite-dacite, and trachyte-andesite at the Tersang and Penjom orogenic gold deposits indicative of involvement of magmatic fluids in the system.

Graphene origami based metamaterials

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Mechanical metamaterials have emerged as a new class of functional materials with unusual material properties. An important example of mechanical metamaterials is auxetic material with tunable negative Poisson's ratio. Such materials are attaching considerable interests due to their promising applications in various engineering sectors. Although enormous studies have been performed to present negative Poisson's ratio properties in various materials, research work on the auxetic behavior of graphene reinforced metal nanocomposites is still at its early stage. The present work develops a graphene origami structure to tune the negative Poisson's ratio in graphene reinforced copper nanocomposites. Extensive molecular dynamics simulations are conducted to study the tuning mechanism of negative Poisson's ratio of graphene/Cu composites. The adaptive intermolecular reactive bond order (AIREBO) potential, embedded atom method (EAM) potential, and Lennard-Jones (LJ) potential are employed to simulate the C-C covalent interaction of graphene, the interactions between Cu atoms, and the van der Waal (vdW) interactions between graphene and Cu matrix, respectively. Various graphene origami structures, including Miura pattern, Waterbomb pattern, and Yoshimura pattern, are formed with the assistance of surface hydrogen functionalization in predesigned areas of the graphene sheet. The shape of the graphene origami can be tuned and controlled by changing the content and width of H adatoms in the creases. Afterwards, the designed graphene origami is embedded into a Cu matrix to achieve the tunability of negative Poisson's ratio. Our results demonstrate that a higher content of graphene origami in composites can lead to a larger negative Poisson's ratio. In addition, the ambient conditions have considerable effects on the auxetic behaviors of graphene/Cu metamaterials. A greater negative Poisson's ratio of composites can be achieved in higher temperature and pressure environments. It is also found that bigger folds in graphene origami can help the metal metamaterial to reach more efficient auxetic properties.

Utilization of supercritical carbon dioxide for development of advanced pharmaceutical formulations with valsartan and carvedilol

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Supercritical carbon dioxide ($scCO_2$) is a green medium that allows production of solvent-free formulations without the use of excipients and organic solvents. In this study, it was used for processing of valsartan and carvedilol in order to produce formulations that will increase bioavailability of drugs. Both valsartan and carvedilol are cardiovascular drugs that have low bioavailability (around 20-30%). In addition, biodegradable and biocompatible pharmaceutical polymers (Soluplus®, hydroxypropyl methylcellulose acetate succinate and Eudragit® E100) were tested as carriers of valsartan and carvedilol.

It was shown that proposed one-step process performed at 30 MPa during 2h allowed for plasticization of all tested polymers. All characterization tests (SEM, FTIR, DSC, XRD) indicated that drugs were dispersed in polymeric carriers, whereby amorphous solid dispersions with density in the range from 327 to 667 kg/m^3 and porosity from 12 to 78 vol% were obtained. Controlled release of drugs was influenced by solubility of polymers in the tested release medium that simulate body fluids (HCl and PBS). Dissolution of valsartan and carvedilol from formulations was increased compared to untreated drugs. Proposed process enabled preparation of two-component system that has advanced properties compared to pristine components as well as commercial formulations. The obtained results provide framework for future development of environmental friendly method for production of drug delivery systems.

Restraining oxygen release and suppressing structure distortion in single-crystal Li-rich layered cathode materials

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Li-rich oxides can be regarded as the next-generation cathode materials for high-energy-density Li-ion batteries since additional oxygen redox activities greatly increase output energy density. However, the oxygen loss and structural distortion induce low initial coulombic efficiency and severe decay of cycle performance, further hindering their industrial applications. Herein, the representative layered Li-rich cathode material, $Li_{1.2}Ni_{0.2}Mn_{0.6}O_2$, is endowed with novel single-crystal morphology. In comparison to its polycrystal counterpart, not only can serious oxygen release be effectively restrained during the first oxygen activation process, but also the layered/spinel phase transition can be well suppressed upon cycling. Moreover, the single-crystal cathode exhibits the limited volume change and persistent presence of superlattice peaks upon Li^+ (de)intercalation processes, resulting in enhanced structural stability with absence of crack generation and successive utilization of oxygen redox reaction during long-term cycling. Benefiting from these unique features, the single-crystal Li-rich electrode not only yields a high reversible capacity of 257 mAh g^{-1}, but also achieves excellent cycling performance with 92% capacity retention after 200 cycles. These findings demonstrate that the morphology design of single crystals can be regarded as an effective strategy to realize high-energy density and long-life Li-ion batteries.

Laser-induced graphene-based electrochemical biosensor for clinical application

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Laser-induced graphene (LIG) has recently received increasing attention due to its simple fabrication and low cost. This study reports a flexible laser-induced graphene-based electrochemical biosensor fabricated on a polymer substrate by the laser direct engraving process. For this purpose, a 450 nm UV laser was employed to produce a laser-induced graphene electrode (LIGE) on a polyimide substrate. After the laser engraving of LIGE, the chitosan-glucose oxidase (GOx) composite was immobilized on the LIGE surface to develop the biosensor for glucose detection. It was observed that the developed LIGE biosensor exhibited good amperometric responses toward glucose detection over a wide linear range up to 8 mM. The GOx/Chitosan-modified LIGE biosensor showed high sensitivity of 43.15 $\mu A\ mM^{-1}\ cm^{-2}$ with a detection limit of 0.431 mM. The interference studies performed with some possible interfering compounds such as ascorbic acid, uric acid, and urea exhibited no interference as there was no difference observed in the amperometric glucose detection. It was suggested that the LIGE-based biosensor proposed herein was easy to prepare and could be used for low-cost, rapid, and sensitive/selective glucose detection.

Organic photodiode integration on Si substrate beyond 1000 nm wavelength

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Near infrared (NIR) and shortwave infrared (SWIR) image technologies are of interest for many emerging applications. Above 1100 nm, Si is blind and has no sensitivity. Emerging optoelectronic materials, such as small molecules, polymer, and organic-inorganic hybrids have been demonstrated as promising alternatives to traditional inorganic photodetectors for NIR and shortwave infrared (SWIR) imaging. Among photodetector technologies, organic photodetectors (OPDs) are groundbreaking light sensors with unique photon-to-electron responses at various wavelengths that offer limitless flexibility in field applications due to the tunable design of organic semiconductors.

Organic photodiode integration on the Si readout circuit offers a solution for extending the sensitivity beyond 1000 nm. In this work, we report the way to integrate organic photodiode on Si substrate with metals that are CMOS process compatible as bottom electrodes, such as titanium nitride (TiN), tungsten (W), and aluminum (Al). We report high-efficiency NIR sensor enabled by employing TiN and W as bottom electrodes, with an external quantum efficiency (EQE) of ~50% at 940 nm and ~70% at 1030 nm, a dark leakage current density of 15 nA/cm^2, a bandwidth of 15 kHz at -4V, and a dynamic range (DR) of ~100 dB are achieved. Low resistivity and inert properties of TiN make it forms a good interface with organic active layer, leading to an ideal bottom contact metal for organic photodiode when integrated on Si substrate.

This work highlights the importance of the interface between the bottom electrode and OPD, which needs to be well considered for OPD and Si-CMOS integration with a CMOS compatible process flow, offering the possibility to extend the sensitivity of CMOS image sensor beyond 1000nm, which can be applied in high-performance NIR/SWIR low-cost imaging systems.

Boost antimicrobial effect of CTAB-capped $Ni_xCu_{1-x}O$ ($0.0 \leq x \leq 0.05$) nanoparticles by reformed optical and dielectric characters

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Chemical doping and coating have been considered as efficient semiconductor physics strategies to modulate the physical, chemical, and biological properties of materials for the required applications. In this study, cetyltrimethylammonium bromide (CTAB) stabilizer capped nickel doped cupric oxide ($Ni_xCu_{1-x}O$) nanoparticles (NPs) with different doping concentrations ($0.0 \leq x \leq 0.05$) were synthesized via a one-step rapid and low-cost solvothermal synthesis route. The as-synthesized CTAB-capped $Ni_xCu_{1-x}O$ NPs have been sightseen for their structural/morphological, optical/dielectric, and antimicrobial properties using XRD/SEM/TEM, FT-IR/UV-visible/Impedance spectroscopies, and Agar well diffusion method, respectively. Relevant results show enhanced optical, dielectric and antimicrobial properties with Ni doping due to the smaller size effect. Importantly, *in vitro* examination, the antimicrobial activity of the grown NPs was evaluated against four microbial species, exhibits that the CTAB-capped Ni-doped CuO NPs possess a command antimicrobial toxicity to Staphylococcus aureus (25923-ATCC), Klebsiella pneumoniae (700603-ATCC), and Escherichia coli (25922-ATCC) and an intermediate performance towards Candida albicans (24433-ATCC). The minimum inhibitory concentration (MIC) assay for the obtained CTAB-$Ni_{0.05}Cu_{0.95}O$ sample upon S. aureus or K. pneumoniae pathogens reaches extremely as low as 5 µg-ml^{-1} for all reported CuO NPs. The improved dose-dependent antimicrobial effect has been found to be strongly dependent on the particle size, surface morphology, elemental compositions, and surface bio-functionality of the catalytic nanomaterials. Additionally, Ni-dopant, CTAB-stabilizer, and binding of Cu^+/Cu^{2+} ions with respiratory enzymes collectively produce an excess amount of reactive oxygen species (ROS) in the bacterial culture medium, which determines a predominant antibacterial mechanism for bacterial cells damage. Overall, these inorganic ($Ni_xCu_{1-x}O$) NPs with antimicrobial cationic surfactant (CTAB) have advantages to use as a functionalized disinfection nano-agent to control the microbial infections in the health care sector together with various electronic and photonic medical diagnoses.

Transformation heat transfer and thermo-hydrodynamic cloaks for creeping flows: Manipulating heat fluxes and fluid flows simultaneously

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Although the subject of thermal cloaking has attracted extensive academic attention, most pioneering studies have so far focused on thermal conduction systems or thermal convection in the porous media, which prevents the object from moving. Here, we have discovered that Stokes equations and the energy transport equation do abide by the coordinate-transformation invariant theory if the former is replaced with the pressure Laplace equation. This discovery enables us to rightfully take advantage of the merit of this theory and to analytically design metamaterial thermo-hydrodynamic cloaks. More importantly, since our designed cloaks depend on the viscosity and the thermal conductivity of background flows as well as geometries of cloaks only, but not on boundary conditions of background flows, they can be continuously utilized when objects travel in the media under realistic flow conditions. Besides, we also suggest experimental demonstrations to show the feasibility of our design. Finally, it is our hope that numerical data obtained in the proposed study can (1) facilitate the realization of lab experiments as well as help them identify characteristic flow and thermal parameters, and (2) serve as a stepping stone to further explore other thermo-hydrodynamic metamaterial devices.

2D glassy-graphene device arrays with photodetection and VOC sensing capabilities

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Multifunctional devices are of great interest for integration and miniaturization on the same platform, but simple addition of functionalities would lead to excessively large devices. Here, the photodetection and chemical sensing device is developed based on novel 2D glassy-graphene[1,3] that meets similar property requirements for the two functionalities. An appropriate bandgap arising from the distorted lattice structure enables glassy-graphene to exhibit similar or even improved photodetection and chemical sensing capability, compared to pristine graphene. Due to strong interactions between glassy-graphene and the ambient atmosphere, the devices are less sensitive to photoinduced desorption than graphene. Consequently, the few-layer glassy-graphene device delivers positive photoresponse, with a responsivity of 0.22 A/W and specific detectivity reaching 1010 Jones under 405 nm illumination. Moreover, the intrinsic defects and strain in glassy-graphene can enhance the adsorption of analytes, leading to good chemical sensing performance. Specifically, the extracted signal-to-noise-ratio (SNR) of the glassy-graphene device for detecting acetone is 48, representing more than 50% improvement over the graphene counterpart. Additionally, bias voltage and thickness dependent VOC sensing features are identified, indicating the few-layer glassy-graphene is more sensitive. This study successfully demonstrates the potential of glassy-graphene for integrated photodetection and chemical sensing, providing a promising solution for multifunctional applications further beyond.

Performance of OLED under mechanical strain: A review

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OLEDs with convenient portability, low power consumption and mechanical flexibility have successfully demonstrated their wide range of applications in display, lighting, and medical devices. With the biological requirement and continuous development of electronic technology, the OLEDs have opened up new possibilities for wearable electronic devices. Plentiful reports have revealed the progress of OLED devices with excellent performance of mechanical strain, involving flexible electrodes, processing technology, and advanced fabrication. In this review, the OLED processing methods are systematically discussed, and the development of flexible electrodes has been focused in terms of mechanical strain. In addition, the OLED performance with flexible electrodes also is described. The review provides a comprehensive understanding of OLEDs that can withstand the mechanical strain and achieve commercial maturity.

Method and mechanism research on highway asphalt pavement hot in-place and central plant recycling based on microwave and hot air combining multi-dimensional low temperature heating

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The recycling of waste asphalt pavement materials is a major problem faced by countries all over the world. Our country produces as much as 300 million tons every year, and long-term stacking takes up a lot of land and pollutes the environment. In 2021, the State Council clearly pointed out to promote the resource utilization of waste roads, asphalt and other materials. Hot recycling is one of the important ways. Traditional Hot recycling methods uses high temperature heating to cause asphalt aging and carbonization on the surface of the aggregate, which affects the fusion of new and old materials and asphalt, and is not conducive to recycling. Moreover, traditional hot in-place recycling has limited grading adjustment, large environmental pollution, and low quality of the recycled asphalt pavement; although the central plant recycling can adjust the grading greatly, it is limited by traditional heating. High-quality recycling is still not high, increasing transportation costs. The microwave regeneration heating efficiency is high and will not cause the asphalt to age. The regenerated asphalt mixture has better high temperature stability, crack resistance and fatigue resistance, but its heating cost is higher. Therefore, the research group proposed the method and mechanism research on highway asphalt pavement hot in-place and central plant recycling based on microwave and hot air combining multi-dimensional low temperature heating, from the heating method, mechanism and thermal regeneration method to jointly solve the current problems of thermal regeneration, in line with the national concept of developing a green and low-carbon circular economy, it has a clear leading and pioneering, innovative asphalt pavement recycling technology.

Optimized energy harvesting approach: Infra-red photo voltaic cells

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Optimal energy solution for any specific requirement depends on geographical location, simplicity of mechanism, technical stability, energy harvesting capabilities, and cost. Wind energy though relatively cheap, but termed sporadic due to non-consistent conditions and periodic maintenance requirement for the extraction mechanisms. Solar energy is a rich energy source with the possibility of exploiting anywhere during day time, and a relatively cheap & noiseless renewable energy source. Though solar energy is pollution-free with less impact on the eco-system, it does have limitations, mainly due to its intermittent nature, attributed to sun availability for specific hours (e.g. during daytime only) and the energy conservation efficiency may be considerably low. Sunlight being a shallow source of energy does require a large area for the collection of a considerable amount of energy. We grasped the idea from MIT cutting edge research focused to harness IR spectrum portion within the solar spectrum. In this research work, we have proposed the design of a multifunctional and relatively efficient energy harvesting mechanism that can also work in the near-infrared region. The design is based on nano-meter sized optical waveguide imprints on micrometer sized conventional window glass ensuring concentrated photon absorption in the infra-red region.

Besides conventional SOI optical waveguides, chalcogenides is also implemented. The dispersive and losses effects calculations provide further knowledge about the state of the window panes transparency / opacity.

Besides leading towards a simple way of energy harvesting; the basic platform (window panes) can still be used for enjoying sunlight inside the rooms as well. The research will open more avenues in the field of photo-voltaic power generation.

Structural behavior of reinforced ultrahigh performance concrete under uniaxial loading

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Ultrahigh performance concrete (UHPC) has recently been promoted for many applications in the construction industry due to its superior mechanical properties including the high compressive strength and the sustained post-cracking tensile strength as well as its pronounced durability. UHPC is mostly preferred to exhibit a strain-hardening tensile response in which multiple micro-cracking characterizes the response until reaching the peak tensile capacity. Such feature results in a large deformation capacity (ductility) and gradual cracking. On a material level, UHPC has been found to demonstrate high ductility and slow failure pattern. However, on a structural level, when combined with rebar reinforcement, the response of UHPC has not been clearly established, and some incidents of quick and brittle collapses have been witnessed, particularly under shear loading where a single macro-crack governs the failure in a very abrupt manner. Hence, the tensile behavior of reinforced UHPC members under tension still requires further research. The tension stiffening effect, the cracking patterns under different fiber content ratios and reinforcement ratios, and the ductility need more elucidation. To this end, this study aims at investigating the behavior of reinforced UHPC under uniaxial loading with regard to the effect of fiber content ratio and reinforcement ratio. The fiber content ratio used in this study was 1, 2, 3.5% in volume, and the reinforcement ratio was 0.97, 1.4, 2.18 and 3.41%. The effects of these parameters on the bearing capacity, ductility and cracking pattern are explored. In addition, an analytical model for describing the response of a UHPC tension member is proposed and simplified expressions for calculating the micro-cracks spacing and macro-crack spacing are provided. The response of UHPC tension members can be extended to describe the response of the tension chords in flexural members.

Plasticity and reprocessing of dynamic covalent polymer networks

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Dynamic covalent bond is a chemical bond that can undergo reversible exchange. The corresponding dynamic covalent polymer network (DCPN) has unique processing properties. That is, when the dynamic covalent bond is activated, the localized segment movement can be realized the solid-state plasticity, while long-range chain movement (or macroscopic flow) can lead to reprocessing. Utilizing the solid-state plasticity of DCPN, this study reports a method for preparing transparent glass with complex three-dimensional geometry. Glass is indispensable in many applications, but its processing options are limited by its rigid and brittle nature. By employing the plasticity of the glass precursor, we developed an origami glass process to realize the preparation of transparent glass. Besides, taking the advantage of the macroscopic flow of DCPN, we report a thiourea based thermoset elastomer that can be reprocessed. More importantly, they can undergo selective oxidation during high-temperature reprocessing, resulting in significant chemical strengthening. In summary, our methods expand the scope of material processing and potentially open up its utilities in unexplored territories.

Gardens of mental peace: A literary perspective of horticulture

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It is long held dogmas that contact with nature (landscape, vegetation and water) ameliorates anxieties and fetch general healthcare benefits. Throughout its life, an individual enmeshes within a dynamic confliction of the natural and artificial environment, social life and consciousness. Within this confliction, the well-being rests on the availability of a perfect environment offering peace of mind and happiness. Nerve-shaken and tired people find wilderness, mountains, forests and meadows as fountains of mental peace and happy life. Thus, mental exhaustion drives a thrust to contact with nature to nourish our physical and physiological needs, and comfort. Naturalized spaces and gardens present a powerful symbolic platform for best manipulations in literature. In addition to nourishing exhausted minds, company of plants does offer nice selection of words for poets and literary men. Gardens as rhythmical manifestation of nature serve the best source of linking literature with the horticulture and this can be the best topic to study so that the upcoming generations can be connected with plants in order to secure the fading love for nature in this materialistic world. Therefore, we can hypothesize that a sophisticated use of word either in literature or in poetry is imperfect unless accompanied by nature.

MnS-nanoparticles-decorated three-dimensional graphene hybrid as highly efficient bifunctional electrocatalyst for hydrogen evolution reaction and oxygen reduction reaction

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The search for renewable energy resources has attracted considerable research interests in electrochemical reactions of hydrogen evolution reaction (HER) and oxygen reduction reaction (ORR) that are essential for fuel cells. Earth-abundant, eco-friendly and cost-effective transition metal compounds are emerging candidates as electrocatalysts in these reactions. Herein, we report the growth of manganese sulfide nanoparticles on three-dimensional graphene, through an easy, progressive successive ionic layer adsorption and reaction (SILAR) method, where manganese sulfide nanoparticles (MnS-NPs), diameter of 4-5 nm are homogeneously decorated on the 3D graphene matrix. SILAR has been proven to be a facile, low-cost and eco-friendly method to grow nanomaterials on 3D conductive support and it is clearly different from previous MnS synthetic routes such as spray pyrolysis, microwave irradiation, chemical bath deposition, solvothermal and hydrothermal that required time-consuming procedures and harsh conditions. Transition metals based sulfides are the most extensively studied among nanostructured electrocatalysts for overall alkaline water splitting, with the advantages of being widely available, inexpensive, chemically stable, and highly active yet with low conductivity and sensitivity to half-cell processes issue. Importantly, the active sites of transition metal sulfides based electrocatalysts are nearly always the metal atoms, while exposed S atoms play a vital direct role in the HER process via increasing the number of active sites and changing the coordination environments of adjacent metal atoms. Moreover, the indirect role of S atoms in the HER provides locations for hydrogen adhesion and separation when metal atoms act as active sites. Owing to such beneficial of transition metal sulfides based electrocatalysts with carbon based supportive materials, as formed ,MnS@3DG has indicated marvelous synergistic effects between metal sulfide based nano particles and high surface areal graphene foam with such noticeable intimacy that has markedly improved conductivity to enlist the MnS@3DG nanocomposite as efficient bifuntional electrocatalyst in alkaline electrolyte showing an η HER of just 274 mV at a current density of 10 mA cm^{-2}, much smaller than that of the bulk MnS (800 mV). Even when the current density is increased to 40 mA cm^{-2}, the overpotential is still low as 350 mV. While the oxygen reduction onset potential was 0.9 V (vs. RHE), and the peak potential was 0.75 V (vs. RHE), thus achieving a bifunctional catalytic performance superior to most of the reported manganese-based electrocatalysts in HER and ORR.

Atomic scale study of grain boundaries in low-symmetry two dimensional ReS_2

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Grain boundaries (GBs) are significant microstructures that dominate properties of polycrystalline two-dimensional (2D) materials. Low-symmetry monolayer rhenium disulfide (ReS_2), which belongs to the triclinic crystal system and displays abundant anisotropic properties, provides an ideal platform to investigate diverse configurations of GBs and their orientation-dependent characteristics. Here, we combine aberration-corrected scanning transmission electron microscopy and density functional theory (DFT) calculations to investigate the atomic configurations, electronic band structure and facture mechanics of both atomically stitched and overlapping GBs in chemical vapor deposition-grown polycrystalline ReS_2 monolayers. Our results provide fundamental insights into the impact of GBs on material's electronic and mechanical properties, thus helping establish a more comprehensive understanding between the macroscopic performance and the microscopic structure of 2D materials.

Soil carbon supplementation: Improvement of root-surrounding soil bacterial communities, sugar and starch content in tobacco (N. tabacum)

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Soil carbon supplementation is known to stimulate plant growth by improving soil fertility and plant nutrient uptake. However, the underlying process and chemical mechanism that could explain the interrelationship between soil carbon supplementation, soil micro-ecology, and the growth and quality of plant remain unclear. In this study, we investigated the influence and mechanism of soil carbon supplementation on the bacterial community, chemical cycling, mineral nutrition absorption, growth and properties of tobacco leaves. The soil carbon supplementation increased amino acid, carbohydrates, chemical energy metabolism, and bacterial richness in the soil. This led to increased content of sugar (23.75%), starch (13.25%), and chlorophyll (10.56%) in tobacco leaves. Linear discriminant analysis revealed 49 key phylotypes and significant increment of some of the Plant Growth-Promoting Rhizobacteria (PGPR) genera (Bacillus, Novosphingobium, Pseudomonas, Sphingomonas) in the rhizosphere, which can influence the tobacco growth. Partial Least Squares Path Modeling (PLS-PM) showed that soil carbon supplementation positively affected the sugar and starch contents in tobacco leaves by possibly altering the photosynthesis pathway towards increasing the aroma of the leaves, thus contributing to enhanced tobacco flavor. These findings are useful for understanding the influence of soil carbon supplementation on bacterial community for improving the yields and quality of tobacco in industrial plantation.

Study on soybean oil based thermosetting resin and its composites

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Environmentally friendly polymers based on biomass have been attracting much attention, and one of hot concerns is making low-priced soybean oil into polymers with higher values. Each fatty acid chain in the triglyceride mixture of soybean oil contains a single or multiple double bonds. Epoxidized soybean oil (ESO) with a higher reactivity, which can be used in the synthesis of high bio-based polymers, is obtained through an epoxidation process of double bonds in soybean oil. In our work, the evolution of the curing process of epoxidized soybean oil was simulated by molecular dynamics simulation, and the thermomechanical properties of epoxidized soybean oil cured by a series of different amine and anhydride were predicted, and the relationship between structure and properties was established. Then thermoset reins with more than 90% bio-based carbon content were prepared by the curing reaction between ESO and a derivative of rosin acid, maleopimaric (MPA). Curing behavior and structure-activity relationship were also studied. Acrylated epoxidized soybean oil (AESO) was prepared by ring-opening reaction of ESO with acrylic acid, and an innovative biobased UV coating synthesized from acrylated epoxidized soybean oil and poly(octamethylene maleate (anhydride) citrate) was developed. Carbon nanotubes were modified with poly(acrylated epoxidized soybean oil) to improve their dispersibility in polymer matrixes to obtain ESO-based nanocomposites with good performance. These results could provide new approaches for the preparation of novel bio-based thermoset resins with excellent performance.

New hydrogen atom model and radiation absorption mechanism

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In Bohr model and Schrodinger equation, only the spherically symmetric Coulomb potential in hydrogen atom is considered, but the Lorentz potential caused by proton and electron spin and orbital magnetic moment is not considered. We find that the Lorentz force and Coulomb force coexist, that the electron moves along a circular or elliptical orbit, that the radius of the ground state orbit is twice the Bohr radius and that the rotation frequency is half the Bohr frequency. The "half frequency" problem that perplexed Bohr's life is solved, and the details and mechanism of radiation absorption and release are given. Using the standing wave condition, we obtain the quantization results of the energy levels. It is revealed and proved that the electronic velocity in the atom and molecule is a constant, and the orbital energy level only depends on the rotation frequency, but has nothing to do with the velocity. The source and physical significance of the fine structure constant and Planck constant are given.

Study on composite materials for electro-hydraulic transmission

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In order to reduce the weight and vibration of Electro-hydraulic Transmission, the composite gear was studied, a new type of steel phenol composite transmission gear was put forward, and its optimal design was given. In this method, the polymer composite was placed between the steel tooth and the central hub area along the radial direction of the gear, so as to reduce the vibration transmission rate from the tooth to the hub and the weight of the gear train. In order to minimize the weight of the composite gear, the optimum size of the radial composite zone of the gear was calculated by considering the fatigue strength of steel and composite materials. The results show that, compared with pure steel gears, the average sound pressure levels of optimized and un-optimized composite gears are reduced by 7.2% and 4.6%, respectively, and the average acceleration is reduced by 15.3% and 12.0%.

Novel functional semiconductor-Ionic materials

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Recent research and development on semiconductor-ionic materials (SIMs) with superionic conduction as alternative electrolytes lead to a new trend in low temperature solid oxide fuel cell (SOFC) and proton ceramic fuel cell (PCFC). This can be traced from a radical new invention of single-layer fuel cell (SLFC) or electrolyte-free fuel cell (EFFC), i.e. one semiconductor-ionic component instead of anode/electrolyte/cathode three components can realize fuel cell technology. Such SIMs can integrate the functionalities of fuel cell's anode, electrolyte, and cathode into one component. This could represent a major progress and breakthrough in fuel cell science and technology and lay grounds for a new era of fuel cell R&D and commercialization.

The SOFC technology depends on the electrolyte, yttrium stabilized zirconium (YSZ), but it requires a temperature over 700°C to operate properly due to requirement of sufficient ionic conductivity. The situation could now be improved if replacing YSZ with a SIM with high ionic conductivity to develop semiconductor-ionic fuel cells (SIFCs). The SIFC may demonstrate high performance at temperatures well below 550°C.

Current SIMs may be classified into three types I) Single phase semiconductors, e.g. perovskite and layered structured oxides, SmNiO3, $LiCoAlO_2$, $LiNiFeO_2$, etc. These semiconductors have shown metal or high electronic (hole) conductivity with narrow or zero bandgap to experience a transition to ionic conduction by proton insertion from fuel cell operation; II) Wide bandgap materials, typically, oxygen deficit oxides, e.g. fluorite structure CeO_2-d. The CeO_2-d can change from insulating or electronic conduction to a proton conductor in the fuel cell operation; III) Both semiconductor and ionic conduction form a two-phase heterostructural nanocomposite, where percolation of both electron and ion conducting paths result in comparable or balanced electronic and ionic conduction.

Image segmentation by phase-field models with local information

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We proposed an improved phase-field model with local information for image segmentation. In our approach, a new double well potential function containing local contributions is taken into account. The advantages of the new scheme are in two folders. Firstly, the affection of noise could be reduced in image segmentation with intensity inhomogeneity. Secondly, a more stable boundary evolution could be achieved compared with the traditional way. Segmentation results for several different types of images are reported. We compare the segmentation results with the classical model for two-dimensional images. In the segmentation of three-dimensional magnetic resonance brain images, the accuracy comparisons are presented by the Dice and Jaccard similarity coefficients. Compared with the classical model, our model has higher segmentation accuracy and better stability of boundary evolution.

Synthesis and surface engineering of low-dimensional semiconductors for electronics and energy applications

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Low-dimensional semiconductors, especially two-dimensional (2D) semiconductors, are considered one of the most promising candidates in the field of microelectronics, optoelectronics, and energy, owing to their atomically thin structure that can mitigate short-channel effects, controllable band gaps, and quantum confinement effect. The synthesis of low-dimensional semiconductors, as well as the use of surface and interface engineering for tailoring the electronic properties are essential to broaden their applications. This report summarizes our research on the synthesis and surface/interface engineering of low-dimensional semiconductors, especially two-dimensional transition metal dihalides (TMDC). Element doping and heterogeneous interface engineering are utilized to adjust their physical and chemical properties in order to realize high-performance electronic devices and new energy devices.

Applications of a novel general solution to the inhomogeneous spatial axisymmetric problem in functionally graded materials

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The axisymmetric problem has always been a typical problem in the theory of elasticity, and the inhomogeneous spatial one has an especially wider range of applications. In this work, we present a novel analytical elastic general solution to the inhomogeneous spatial axisymmetric problem. The specific descriptions of inhomogeneity are: Young's modulus of the material is an arbitrary function of both radius and thickness coordinates, and Poisson's ratio is considered as a constant. The elastic stress method is applied to obtain a general stress solution and a relatively concise analytical displacement solution, the degenerate forms of which are both consistent with the existing results.

Based on the general elastic solution, we study an axisymmetric bending problem of functionally graded circular plates subjected to a transverse loading q_0r^n (n is an even number, and r is the radius coordinate) and give explicitly analytical elastic solutions to the case of uniform loadings under simply supported and two types of clamped supported conditions respectively. The final analytic solutions correspond well to the existing numerical results. The distributions of explicit elastic fields related to the inhomogeneous parameter reveal the influence of inhomogeneity on the stress and displacement in FGM circular plates intuitively, which makes it possible to control the elastic performance of FGM plates more accurately

Atomic insights into synergistic effect of 3D graphene nanoplatelet and carbon nanotube hybrids on the mechanical properties of polymer nanocomposites

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The unique three-dimensional (3D) hybrid structures of graphene nanoplatelet (GNP) and carbon nanotube (CNT) hybrid filler can improve dispersion and enhance interfacial properties to achieve excellent reinforced polymer composites. Molecular dynamics simulations have been performed to explore the underlying synergistic mechanism of pillared graphene or non-covalent connected graphene and carbon nanotubes (CNTs) on the mechanical properties of polyethylene (PE) nanocomposites. In order to reveal the synergistic effect of the morphology and arrangement of pillared graphene in enhancing the mechanical properties of polymer nanocomposites, the pillared graphene/PE (PG/PE) model were engineered. Moreover, by constructing the pillared graphene model and CNTs/graphene model, the effect of the structure, arrangement and dispersion of hybrid fillers on the tensile mechanical properties of PE nanocomposites was studied. The results show that the pillared graphene/PE nanocomposites exhibit higher Young’s modulus, tensile strength and elongation at break than non-covalent connected CNTs/graphene/PE nanocomposites. The tensile strength, Young's modulus and elongation at break of the pillared graphene/PE composites all increase first and then decrease as the length of the carbon nanotube increases. The multi-layer pillared graphene/PE composites have a higher Young's modulus than the single-layer pillared graphene/PE composites. Compared with CNTs/graphene hybrid, pillared graphene delivers a more significant synergistic effect and this is attributed to the self-supporting mechanism of pillared graphene. The pull-out simulations show that pillared graphene by CNTs has both large interfacial load and long displacement due to the mixed modes of shear separation and normal separation. Additionally, pillared graphene can not only inhibit agglomeration but also form a compact effective thickness (stiff layer), consistent with the adsorption behavior and improved interfacial energy between pillared graphene and PE matrix.

High aspect ratio contact etching using $C_6F_{12}O$ precursor with low global warming potential

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In the semiconductor industry, the size of nano-electronic devices is getting smaller and more integrated to form complex nanostructures on wafers. In order to manufacture a nano-electronic device, an accurate pattern must first be formed on a silicon substrate. Dry etching technology is mainly used in patterning processes to control the flux of active neutral species and charged particles formed in plasma and to form accurate nano-meter patterns. So far, due to the high chemical reactivity of silicon and fluorine, perfluorocarbon (PFC)-based gas chemistry including CF_4, CHF_3 and C_4F_8 has been used for nanopatterning of dielectric contacts. However, PFC gases generally have a high global warming potential (GWP) of over 8,000 and have a significantly negative impact on the ozone layer. Attempts have been made to replace, decompose, and/or recycle PFC gases with high GWP to reduce greenhouse effects in nano-sized electronic devices. For this, it is necessary to use low GWP gas for manufacturing nano-sized electronic devices in industrial fields. Low-GWP precursors exist as liquid sources with low boiling points or at room temperature for easy recovery. Therefore, to overcome the environmental issues in the manufacturing process for nano-sized semiconductor devices, the process applicability of liquid-PFC (L-PFC) gases (i.e., $C_6F_{12}O$, C_7F_{14}) should be further studied for fabricating nano-sized devices in advance.

In this study, the etching process was performed using $C_6F_{12}O$, one of the precursors with low GWP. In addition, compared the HARC etching characteristics, plasma analysis and surface chemical bonding analysis of the conventional ICP system (13.56 MHz bias generator) and the ICP system with low RF frequency (2MHz) bias generator.

A study on high aspect ratio contac (HARC) etching process through independent control at low frequency bias using ICP system

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As the memory semiconductor market has grown rapidly in recent years, demand and technology development for next-generation memory semiconductors such as 3D NAND flash, RAM, and PRAM are required. In particular, in the case of a NAND flash, the structure is changing from a two-dimensional structure to a three-dimensional stacked-type NAND flash structure according to technological development. As the number of layers increases during the 3D NAND flash process, the HARC (High Aspect Ratio Contact) etching process is an essential process. However, as the vertical process is required, the difficulty of the process increases rapidly, and distortion of the etch profile such as necking and bowing occurs. In the next-generation HARC etching process, the concentration of radicals, ions, and ion energies is referred to as the impact key. However, current studies on the HARC etching process show that ion and radical concentrations and ion energies change simultaneously. Therefore, the concentration of radicals, ions and ion energies, the effects of each are not analyzed independently. Therefore, in this study, we propose a methodology that can independently control the concentration and ion energy of radicals and ions according to process parameters. Plasma analysis was performed using optical emission spectroscopy and DLP. This established radical and ion independent control conditions. The HARC etching process was performed according to low frequency (2MHz) and high frequency (13.56 MHz) under each independent control condition using ICP. Analyze the SiO_2 profile shape by scanning electron microscopy (SEM) after the HARC etching process. It suggests the direction of the HARC etching process by analyzing the correlation between ion and radical concentration and ion energy through plasma analysis and etching process results.

Study of structural, optoelectronic and magnetic properties of Half-Heusler compounds QEuPa (Q= Ba, be, Mg, Sr) using first-principles method

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The structural, optoelectronic and magnetic properties of the Half-Heusler (HH) compounds QEuPa (Q ¼ Ba, Be, Mg, Sr) in the ground state are investigated from the first principles calculations. Stable optoelectronic and magnetic properties of HH compounds are calculated by the FP-LAPW method implemented in the WIEN2k software. The strong correlation between the Eu/Pa f-states is taken into account when studying electronic properties such as the band structure and density of states (DOS). Based on the band structures of the considered compounds, it can be concluded that they are metallic. The dielectric function ε (ω) obtained for QEuPa HH compounds is used to study optical dispersion and absorption. QEuPa compounds absorb the maximum number of incoming photons in the infrared (IR) region. Significant magnetic moment occurs in these compounds due to the splitting of the Eu-$4f^7$, Pa-$5f^2$ and Pa-$6d^1$ localized orbitals.

Kinetics and equilibrium study of the adsorption of silver ions by polymeric composites containing zeolite and methacrylic acid

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Environmental and water pollution caused by heavy metals, especially silver, is considered a threat to humans, ecosystem, and all living species. Therefore, with the development of industrialization, it is a very important effort to remove heavy metals from the environment and wastewaters. For this reason, in the present study, we synthesized two polymeric composites of ethylene glycol dimethacrylate (EGDM), methacrylic acid (MA), and different amounts of zeolite (25 g and 50 g) (PMAZ25 and PMAZ50) by using BPO-DMA initiator system at room temperature (298 K). Fourier Transform Infrared (FTIR) was used to show the presence of functional groups in the synthesized composites, and Thermal Gravimetric Analysis (TGA) was used to test the thermal stability of the copolymeric composites. Batch adsorption method was applied to examine the effect of polymeric composites on silver ion adsorption at different pH values, contact time, initial Ag(I) concentrations, and adsorbent dosage. The adsorption process was found to be most efficient at pH 6. When we tested the most commonly used, Langmuir and Freundlich isotherm models, in the adsorption process in this study, both isotherm models fitted well. The monolayer adsorption capacity of poly(EGDM-methacrylic acid-25 g zeolite) (PMAZ25) and poly(EGDM-methacrylic acid-50 g zeolite) (PMAZ50) was found as 0.116 mg/g and 0.139 mg/g respectively. The adsorption data were also used for the Dubinin-Radushkevich (D-R) isotherm model, and the adsorption energies obtained from this model (EPMZA25 = 15.384 kJ/mol, EPMZA50 = 14.72 kJ/mol) indicated that the adsorption of Ag(I) on polymeric composites could be of ion exchange type. The time dependency experiments indicated that the adsorption rate of Ag(I) onto the polymeric composites was quite fast in the first 60 min and reached adsorption equilibrium after 100 min. Some kinetic models such as the Elovich, pseudo-first-order, and pseudo-second-order models were examined to deeply understand the adsorption kinetics. The kinetic data can be well fitted to the pseudo-second order kinetics model.

Heatsinks behave as an antenna a source of EMI problems

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The active/passive heatsinks have recently garnered much attention due to their benefit to keep the temperature of the electronic device and PCB/ICs in a certain range. A heatsink is expected both to perform a maximum cooling thermally and to have a minimum of the radiation in electromagnetic terms since it causes electromagnetic interference (EMI) in devices around. In this talk, many studies discussing the EMI and thermal performance (TP) of that in the literature are going to be discussed. We will look the natural convection heatsinks for thermal and electromagnetic (EM) performances in details. Especially in devices operating at high frequencies, these structures behave like antennas if their electrical dimensions are comparable to the interval of λ - λ/20 wavelengths. Analysis show that the heatsinks act as both a monopole antenna and a patch antenna. To eliminate the EMI from a heatsink, the grounding, shielding, and filtering techniques are studied. In the literature, the grounding methods are studied up to 2GHz and it is determined that it provides improvement up to 12dB. For 1-40 GHz it is possible to have up to 20dB improvements in EMI by using absorbers and shielding methods. The proposed solution approaches in the literature and their results are compared and the advantages and disadvantages of each approach are discussed. The base height of the heat sink is pre-dominant both from the heat dissipation and electromagnetic emission point of view in comparison to other parameters. Both the feeding point and type of feeding can be destructive or restorative for heat sinks from the antenna behavior point of view as well as its dimensions. In conclusion, heat sink performance in terms of temperature cannot be the only point to be taken into account, but their quasi-antenna behavior should also be taken into account.

Towards micro-mechanic improved design of granular composites

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In composites, macro properties depend on micro-level morphology such as grains and matrix. Advances in 3D printing, combined with strain measurements by Digital-Image-Correlation (DIC) systems, offer manufacturing "tailor-made" morphologies and measuring the strain fields of entire regions.

Analytical tools have been developed, such as Functional-Perturbation-Method (FPM) to account for micro-morphologies and their effect on the macro-level properties. For strength predictions, one can use the FPM and Green's Functions (GF) to obtain deformation fields as a functional of the heterogenous moduli.

Specifically, the heterogeneous strain fields can be approximated using FPM by developing the displacement fields as a Fréchet series about the average homogenous modulus:

$$u = u\big|_{<E>} + \left.\frac{\delta u}{\delta E_P}\right|_{<E>} * \delta E'_P + \frac{1}{2}\left.\frac{\delta^2 u}{\delta E_P \delta E_{\hat{P}}}\right|_{<E>} ** \delta E'_P \delta E'_{\hat{P}} + ...$$

2D eroded Voronoi morphologies were 3D printed as specimens using PolyJetTM technology. The heterogenous moduli field of each specimen was processed into FPM performed with a GF for the case of a uniaxial tensile load. The 2D generalization of [3] for the first two terms of the Fréchet series for the displacements in yields:

$$u_k \approx u_k\big|_{<E>} + \left\{ G^{(0)}{}_{jl}(P,\hat{P})_{,j} \left(u^{(0)}{}_{k,l} \right) \right\} * \delta E'_P$$

Experiments revealed that local material morphology has significant impact on marco-level strength. The strain fields calculated by the FPM and GF were compared to ones obtained from DIC in the uniaxial tension tests. "Hotspots" locations were found to be identical to the ones observed experimentally with one of them being the actual fracture initiation location.

Hot Ecap implementation in zirconia reinforced aluminium chip matrix (Al6061) composite production

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The demand of aluminium in transportation sector is growing rapidly due to the high strength to weight ratio requirement for fuel saving and performance purpose. There is a need to develop a sustainable recycling process without melting phase for the secondary aluminium production that can further save energy, reduce greenhouse gas emission level and global warming. Therefore, the aim of this research is to perform a meltless equal channel angular pressing (ECAP) method was introduced to process the aluminium wastes in the form of chips in order to achieve the aforementioned agenda. In this study, the composites made of aluminium AA6061 chips reinforced with 5%, 10% and 15% volume fraction of ZrO_2 powder were produced under different processing temperature of 450°C, 500°C and 550°C. The experimental results were analysed using the design and analysis of experiments (DOE) principle and assisted by the Minitab 18 software. It was reported that the maximum yield strength and hardness increased to 119.26 MPa and 65.25 VH compared to 100.26 MPa and 50 VH (as-received AA6061), respectively.

Quasispheroidal $LiNi_{0.5}Mn_{1.5}O_4$ coated with Y_2O_3 and distributed over graphene nanosheets enabling high-voltage and high-energy as cathode in lithium-ion batteries

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$LiNi_{0.5}Mn_{1.5}O_4$ is a promising cathode material for lithium-ion batteries with a high-voltage spinel structure. A microwave-assisted chemical co-precipitation method was used to synthesize Y_2O_3 coated quasi-spheres of $LiNi_{0.5}Mn_{1.5}O_4$. The coating of Y_2O_3 and subsequent wrapping of quasi-spheres in graphene nanosheets does not alter the volume or promote the formation of unwanted phases. TGA analysis shows high thermal stability in the material. The material has an initial capacity of 133 mAh g^{-1} at C/10 with a retention of 98% after 100 cycles. In addition, cathode samples show a good capacity of 132 g^{-1} after 20 cycles at higher temperatures (55°C). Oxide coatings protect the particles from ionic leaching but limit the electrical conductivity of the materials. However, graphene enhances the conductivity of the synthesized material and wraps active particles in a conductive channel. Due to the synergistic design of the material and the robust manufacturing technique, parasitic reactions are suppressed without affecting the electrical conductivity. To increase their cyclic performance, the suggested material synthesis approach may successfully be applied to various electrode materials.

Polyolefin coatings reinforced with modified hybrid CeO_2@ ZnO particles for corrosion protection of steel

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This work reported the corrosion protection efficiency of polyolefin coatings, reinforced with modified hybrid cerium oxide and zinc oxide (CeO_2@ZnO) particles. The hybrid particles were modified with benzotriazole (corrosion inhibitor). The modified hybrid particles (CeO_2@ZnO/BTA) were reinforced into polyolefin-based coatings. The structural and morphological analysis results were confirmed by employing various characterization techniques. Transmission electron microscopic (TEM) analysis confirmed the hexagonal morphology of zinc oxide particle and confirmed the formation of hybrid particles. Energy dispersive X-ray (EDX) analysis results further validated the successful synthesis of the modified hybrid particles. Fourier-transform infrared spectroscopy (FTIR) analysis demonstrated the chemical bonding and interaction of the synthesized particles and endorsed the synthesis due to emergence of unique peaks relevant to particles. X-ray photoelectron spectroscopy (XPS) provided the more in-depth analysis of synthesized particles. Thermal gravimetric analysis (TGA) demonstrated the thermal stability of the modified hybrid particles. UV-vis spectroscopic analysis confirmed the self-release of the corrosion inhibitor (BTA) at various pH values and established the fact that the release is pH and time dependent. Electrochemical Impedance spectroscopic analysis (EIS) represented that the coatings reinforced with modified hybrid particles provided better corrosion protection as compared to the reference blank polyolefin coatings, thus making them an attraction for oil and gas and marine applications.

Square planar Ni(II), Pd(II), and Pt(II) complexes with new Schiff base ligand (E)-N-cyclohexyl-2-(2-hydroxy-5-methoxy-3-nitrobenzylidene) hydrazine-1-carbothioamide and solvent DMSO: Synthesis, Characterization, X-ray diffraction and anticancer activity

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The ligand H_2L (E)-N-cyclohexyl-2-(2-hydroxy-5-methoxy-3-nitrobenzylidene) hydrazine-1-carbothioamide has been synthesized by the reaction between 2-hydroxy-5-methoxy-3-nitrobenzaldehyde and N-cyclohexylhydrazinecarbothioamide. This ligand was coordinated to metal ion Pd(II) and Pt(II) in basic medium in a mixture of DMSO and methanol solvent. The square planar complexes [PdL.dmso] and [PtL.dmso] were formed via N-S-O coordinating sites of ligand and the fourth coordination bond was formed via S of DMSO which was used as a solvent. The square planar Na [NiL.OAc] complex was formed methanol solvent, whereas CH_3COO- occupied the fourth coordinating site. The FTIR, UV-Vis, and 1H and 13C NMR spectroscopy methods were used to characterize the synthesized compounds. The CHN elemental analysis was carried out to determine molecular formula. The two complexes structure of palladium [PdL.dmso] and platinum [PtL.dmso] were completely elucidated with single crystal X-ray diffraction analysis. The cytotoxicity of the synthesized compounds L, a, b and c were tested against cancer cell lines, Hela and human normal endothelial cell lines (Eahy926) by MTT assay. The palladium complex [PdL.dmso] showed the highest activity among all the compounds with IC50 = 15.6 μM against Hela. The nickel and platinum complexes a and c showed significant activity against Hela with IC50 = 105.7 μM and IC50 = 166 μM respectively. The ligand showed very poor activity against Hela cell lines. The nickel complex showed the

highest cytotoxicity with IC50 = 5.8 μM and the complexes a, b and ligand, L exhibited the activity with IC50 = 43.3 μM, IC50 = 45 μM, and IC50 = 185 μM respectively against Eahy926. The palladium complex b showed potential activity with a very good selectivity index (SI=2.8) against Hela cell lines. The coordinated complexes showed higher activity than free ligand due to metalation increased lipophilicity. The group 10 metal complexes could be the promising cancer therapeutic agents.

Synthesis of poly(vinyl alcohol)-aided ZnO/Mn_2O_3 nanocomposites for acid orange 8 dye degradation: Mechanism and antibacterial activity

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Zinc oxide is one of the novel metal oxides utilized for diverse applications. The sol–gel and unintended self-propagation procedures were applied to synthesize the porous and high surface area ZnO-based metal oxide nanocomposite. The p-type manganese (III) oxide was successfully coupled with n-type ZnO. The physical property characterization results revealed the surface area, porosity, and charge transfer capability improvement on the poly (vinyl alcohol) (PVA)-aided binary nanocomposite (PVA-ZnO/Mn_2O_3), compared to ZnO. The XRD patterns and TEM image analysis validated the nanometer size range for the materials (15–60 nm). The SEM micrographs and BET spectral details have confirmed the porous nature of the PVA-ZnO/Mn_2O_3 nanocomposite. The supporting results were obtained from the HRTEM (IFFT) and SAED pattern analyses. The EDX and HRTEM analyses were used for the confirmation of elemental composition and reality of the PVA-ZnO/Mn_2O_3 composite, respectively. The presence of the improved charge transfer property for PVA-ZnO/Mn_2O_3, compared to ZnO, was evidenced from acid orange-8 dye degradation. The highest zone of inhibition (14 mm) was recorded on Escherichia coli bacteria for the uncalcined PVA-ZnO/Mn_2O_3 nanocomposite compared to PVA, yet, less zone of inhibition compared to the calcined PVA-ZnO/Mn_2O_3 nanocomposite. The authors recommend the formation of the couple between metal oxides by electrochemical technique analyses as a future work.

Catechol bio-based polymers for surface modification of nanomaterials

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Catechol-based polymers have been received much focus as a result of their unprecedented under-water adhesion. Despite of several attempts, the preparation of catechol based materials requires multi-step protection and deprotection of catechol group. The synthesis poly(N-carboxyanhydrides) containing robust anchoring group requires further investigation owing to their structural versatility and potential applications in medicine. The application of organocatalysis in ring-opening polymerization (ROP) of N-substituted N-carboxyanhydride (NCA) monomers is discussed. Important updates on the dual functionality of Brønsted base to subdue the catecholic functions in dormant form and to promote the ring-opening polymerization (ROP) in a living manner is articulated. Well-defined polypeptoids with predicted molecular weights (Mn, NMR = 4.4 KDa) and dispersities (Đ) of 1.1 are synthesized and further used for the functionalization of manganese oxide and silver nanoparticles. Herein, the synthesis of catechol based polypeptoids and polyethers for surface modification of metallic nanoparticles are highlighted. In this review the recent advances in the synthesis of catechol bearing bio-based polymers and organocatalysis in ROP of N-carboxyanhydrides are elaborated in depth. Furthermore, the application of catechol based amphiphilic block copolymers for surface modification of nanomaterials is discussed. This finding could be used as a platform for the synthesis of biocompatible and water dispersible metallic nanomaterials in nanomedicine.

Nutritional composition and sensory quality of injera prepared from tef (Eragrostis tef (Zucc.) Trotter) complemented with lupine (Lupinus spp.)

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There is currently an emerging problem of protein malnutrition in Ethiopia. This food formulation was done to increase the accessibility of nutrient rich food products for the consumers. This study aimed to investigate the effect of tef, lupine varieties and blending ratio on the chemical composition of injera and sensory acceptability of Ethiopians staple food. The effect of blending ratio and lupine varieties (Australian sweet lupine and Dibettered lupine seed) were studied. The formulations were generated by using mixture design software. Lupine variety and blending proportion had significant ($P < 0.05$) effect on proximate, mineral, anti-nutritional compositions and sensory acceptability of blended injera. The nutritional compositions of formulated injera ranged from 60.37 to 66.97%, 1.76 to 2.05 %, 11.78 to 18.84 %, 2.53 to 4.01 %, 2.83 to 3.16%, 72.55 to 81.32% and 393.19 to 400.91 kcal/ 100 g for moisture content, total ash, crude protein, crude fat, crude fiber, utilizable carbohydrate and gross energy, respectively. The result showed that the crude protein content highly increased as the proportion of lupines increased. Crude protein and crude fat contents were higher for injera blended with dibettered lupine seed variety while crude fiber content was higher for those blended with Australian sweet lupine variety because of the raw material. Mineral content of composite injeras varied from 12.26 to 14.98 mg/100 g, 2.39 to 2.83 mg/100 g, and 145.31 to 163.96 mg/100 g for iron, zinc and calcium contents, respectively. Therefore, this study showed significant increment in protein content of injera and provides insights for use of Lupine-tef flour mixture at home and industry level for enriched injera. As the sensory acceptability scores data indicated for both lupine varieties blended with tef for the production of injeras of up to 15% lupines almost all sensory attributes showed higher scores without significantly different among them but after 15% lupine addition there were observed drop of the sensory acceptability scores in a 7 point hedonic scale.

Investigation of mechanical properties of hybrid natural composite

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Majority of the conventional materials have been replaced by Natural fiber composites due to their high strength to weight ratio, biodegradable, eco-friendly environment. Based on various literature surveys, natural fibers are a very good alternative for the Engineering and Manufacturing industries. The main goal of this work is to investigate the effect of fiber orientation and wt.% composition on mechanical properties. Fabrication of the composite was made from a hybrid polymer matrix reinforced with nettle fiber (NF), sisal fiber (SF), and glass fiber (GF). Different compositions wt.% of nettle and sisal fiber were used with 00/900 and 450 orientations. A 5% NaOH was used for both fibers to remove further lignin, hemicellulose, and other fiber remnants. The total volume fraction of the fiber was 40 wt.%. From this wt.% of nettle and sisal fibers were hybridized as 20NF:10SF, 15NF:15SF, and 10NF:20SF through 00/900 orientation by keeping wt.% glass constant. The mechanical property results for those samples were very good. In this case, the tensile load and impact force was applied in the direction of both fibers sample S5 and S5′. In the case of S5, the load was applied longitudinally to SF. Whereas in S5′ the load was applied longitudinally to NF. Tensile and impact strength of S5 and S5′ were 97MPa, 8.4J, and 91MPa, 6.9 J respectively.

The effects of pore size and percentage composition of air voids on impact energy absorption of Al foam using numerical approach

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Recently, there is a high interest to use lightweight aluminum foams for automotive, railway and aerospace applications. Because of its high ductility and deformability, Aluminum foam is usually used for energy absorption purpose for crashworthiness application. To keep the safety and to avoid occupant injuries it is necessary to absorb the kinetic energy generated during impact. Therefore, to absorb high kinetic energy, the crash box material needs a special material microstructure, which is light in weight and can absorb more energy than the existing one like $CaCo_3$, CBC, SiC. B_4C etc. In particular, the analysis of energy absorption of aluminum foam in automotive for energy absorption applications is limited. The main objective of this research is to analyze, and optimize the porosity size and voids percentage on impact energy absorption of aluminum foam using a numerical approach. For this purpose, first, fifteen CAD Al foam specimens were developed by using Digimat multi-scale material modeling software. Second, cubic elements with circular bubble shape at 5%, 10% and 15% void percentage and at 1.5mm, 2mm, 2.5mm, 3mm and 3.5mm bubble sizes were modeled. Finally, the numerical analysis of impact energy by using ANSYS workbench 19.2 Explicit dynamics by applying initial low velocity was performed. The parameters were compared to each other to optimize the proper percentage composition and cell size for the best of energy absorption applications. The effects of bubble shape, foaming agent and percentage composition on energy absorption were discussed. In this study the analysis was accomplished by determining and comparing the energy absorptions of all the models and finally, comparing with existing foaming agents.

Differential pulse voltammetric determination of hexavalent chromium using nickel hexacyanoferrate modified glassy carbon electrode

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The current boom in the industrial sector of the country is arise scientific concern about environmental contamination by heavy metals such as chromium. The objective of this project is to fabricate a sensitive and selective electrode for differential pulse voltammetric determination of Cr (VI) in water samples and demonstrate its applicability in complex matrices such as tannery effluent. The drop casting method is use for electrode development. Experimental variables that can influence the DPV response of the developed electrode for Cr (VI) including strength of supporting electrolytes, pH of the solution, and concentration parameters were optimized. The figures of merit of the developed electrode were evaluated and the applicability was demonstrated through determination of Cr (VI) in tannery effluent water. The developed electrode was detected a very low level of Cr (VI) in acetate buffer at pH 5 with limit of detection and limit of quantification 0.0885 and 0.2950 μmol L^{-1} respectively. The linear calibration plot is R2 value of 0.999 suggesting a very good correlation between DPV current response and concentration of Cr (VI). The current electrode was simple to develop and can successfully be applied for the determination of Cr (VI) in wastewater samples.

Preparation of skin care product using coccinia abyssinica tuber extract

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Background: Anchote (Coccinia abyssinica) is highly nutritious crop which is mostly cultivated in Wollega Zone, Oromia Regional State of Ethiopia. The term 'anchote' is the local name of coccinia abyssinica. Anchote is traditional food crop which play a pivotal role in nutritional security, especially in the western Oromia Regional state of Ethiopia. It is herbaceous plant species which is usually consumed in cooked form. Tuberous root is the main edible portion of coccinia abyssinica. A number of essential nutrients in anchote such as Calcium, Starch, Zinc, Magnesium, Iron, protein and etc makes it the most important food crop.

Materials and Methods: Coccinia abyssinica tuber extract was prepared by maceration extraction method. Coarsely powdered coccinia abyssinica tuber was placed inside a container; menstruum was poured on top until completely covered the powdered tuber. The container was then closed and kept for three consecutive days. The content was stirred periodically to ensure complete extraction. At the end of extraction, the micelle was separated from marc by filtration. Then, tuber extract of coccinia abyssinica was mixed with ingredients such as thickening agents, humectant, emollient, antioxidant, preservatives and fragrance to prepare a new skin cream. A new skin cream was formulated by mixing ingredients.

Results: Whitish brown semi-solid cream was prepared by mixing ingredients. A newly prepared skin care product was applied to the human skin. The skin became soft, attractive and supple after using this new skin care product. It didn't cause any side effects on the human body.

Conclusions: Calcium, starch and other nutrients in anchote tubers are vital for our skin. Thus, a new skin care product was prepared using tuber extract of coccinia abyssinica (anchote) with the aim of nourishing the skin. The current study revealed that coccinia abyssinica skin care product enrich the body with nutrients and useful minerals. Coccinia abyssinica skin cream offers significant advantages over competing products.

Techno-economic analysis for Li-ion battery recycling in the UAE

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Nowadays, millions around the world rely on portable electronics and electric cars to get around. Numerous modern gadgets are powered primarily by rechargeable lithium-ion batteries. The current study will examine the environmental and economic benefits of recycling lithium-ion batteries at the end of their useful lives. Lithium (Li), Cobalt (Co), and Manganese are the three most precious metals utilized in these batteries. This study is considered as the first comprehensive study and database dedicated to the United Arab Emirates hydrometallurgical recycling technique which was generated utilizing the Argonne National Laboratory's EverBatt cost model. It has been investigated the differences in costs between the various LIBs chemistries. We demonstrate a comparison between the recycling price of the LIBs in the United Arab Emirates and the recycling price of the same battery material in the United States. A number of different battery chemistries have been employed, including NMC (111), NCA, and LCO. The purpose of this study is to quantify the environmental impacts and costs associated with remanufacturing NMC111, NCA, and LCO battery cells and to compare them to the costs associated with manufacturing batteries from virgin materials in order to determine whether battery remanufacturing is feasible. The model is using the cost calculation from BatPaC as well as the environmental impact calculation from GREET to make its decisions. The amount of energy consumed, the amount of trash generated, and the recycling efficiency all have a significant influence on the environmental advantages and economic sustainability of LIB recycling. As a result, EverBatt model was utilized to analyze the particular LIB disassembly procedure in terms of these factors. We will compare the pricing of recycling LIBs at recycling facilities in the United Arab Emirates and the United States. We will examine different recycling process with different recycling fractions ranging from 80% to 100%, as well as varied annual throughput volumes of 8,000, 10,000, and 12,000 tonnes, respectively. Additionally, many prices or different recycling techniques are compared, including pyrometallurgy and hydrometallurgy.

Relationship between silicon, phosphorus content and grain number in mild steels and its corrosion resistance in pickling hydrochloric acid

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The micro-structural effects on the corrosion resistance of three classes of mild steels (A, B and C) suitable for galvanizing industry, according to their silicon, phosphorus content, grain number and size of carbides (Fe_3C) in concentrated hydrochloride acid solution was investigated by a series of known techniques, such as potentiodynamic polarization curves, electrochemical impedance spectroscopy measurements, optical microscope and scanning electron microscopy. Results showed that the corrosion rate of the three classes of mild steel depends on their silicon and silicon/phosphorus combinations contents. It is found also that the corrosion rate depends on grain number and size of carbide content in mild steels. These findings were confirmed by micro-structural characterization and scanning electron microscopy techniques. They indicated that the severe corrosion cavities formed on the carbon steel surfaces and their sizes depended to silicon and silicon/phosphorus combinations contents. These results explained by micro-galvanic corrosion process between cementites and ferrites which became more serious with silicon and silicon/phosphorus combinations contents.

Characterization of $Na_{0.5}Bi_{0.5}TiO_3$ prepared by hydrothermal method for photocatalytic applications

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Sodium bismuth titanate ($Na_{0.5}Bi_{0.5}TiO_3$, NBT) ceramics have been prepared by using a simple hydrothermal method. Low temperature process of thermal treatment was conducted to obtain a highly dense morphology NBT, using high-purity oxides and carbonates as the initial precursors. The presence of well-crystallized NBT in the rhombohedral phase was also found at hydrothermal temperatures above 180°C. A concentration of at least 10 M NaOH and a reaction time of at least 24 hours were needed to attain maximum perovskite phase. Xray diffraction, Raman spectroscopy, Infrared spectroscopy, and SEM analysis confirm the structure, phase, morphology, and composition. NBT ceramics exhibit the typical characteristics of relaxor ferroelectrics, with a diffusion exponent γ of up to 1.5 to promote their applications in micro-electromechanical and energy harvesting systems. The photocatalytic properties of the hydroth- ermally synthesised powder were evaluated with respect to the degradation of meth- ylene blue (BM). Furthermore, the photocatalyst's stability is excellent. The article carefully discusses the detailed mechanism of photocatalysis.

Effects of high operating temperatures and holding times on thermomechanical and mechanical properties of autoclaved epoxy/carbon composite laminates

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The elevated operating temperature is considered an essential factor affecting the performance of laminated composite structures. Under the intended conditions of use in aircraft engines and nacelles, carbon fiber reinforced polymers are exposed to temperatures ranging from room temperature to 120°C. The present work concentrates on the thermomechanical and mechanical properties of autoclaved woven carbon fiber/epoxy composite laminate subjected to different operating temperatures (60, 120, and 180°C) and holding times (10, 30, and 60 min). Thermomechanical results showed that the rigidity and stiffness of the epoxy resin matrix decrease with increasing temperature. However, all mechanical properties (laminate compressive modulus, laminate compressive strength, and interlaminar shear strength) decreased progressively with operating temperature. Laminate compressive strength and interlaminar shear strength were seen to decline up to 43.74% and 30.60% on the operating temperature of 180°C, respectively, compared to measured values at 60°C. This study indicates that only the compression properties were affected by the holding time, while the interaction between the operating temperature and holding time affects the laminate compressive modulus.

Boundary stabilization of a thermoelastic diffusion system of type II

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In this paper we study the boundary stabilization of a one-dimensional thermoelastic diffusion problem of type II. The system of equations is a coupling of three hyperbolic equations. This poses some new mathematical and numerical difficulties. With the help of the semi group theory of linear operators, we prove the well-posedness of the proposed problem. By using the frequency domain method combined with the multiplier technique, we prove the exponential stability of the solutions. Finally, we present a numerical scheme based on the Chebyshev spectral method and we give two numerical examples to validate the proposed model and to show its capability.

The geometric free-surface profile of granular flows in rotating drums

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The axial and free surfaces are geometric features of tumbling mill flows. Their shape is a characteristic of the particle interactions within the charge body. This means that any modelling scheme capable of predicting these surfaces automatically satisfies the underlying physics of the system and thus can be used as a global continuum signature for breakage and mixing. Elbasher et al (2021) presented a model that successfully captured the shape of the axial free surface by comparing their results to axial free surface predictions from Chou et al (2009). Due to the encouraging results from that work, we leverage off the geometric symmetry between the axial free surface and sigmoid-shaped (S- shaped) free surfaces and present an analytical solution, free from any empirical fitting parameters, to predict S-shaped free surface. These predictions are then statistically compared to those derived from previously conducted Discrete Element Method (DEM) simulations and positron Emission Particle Tracking (PEPT) experiments. This model provides an alternate to complicated numerical routines that fit S-shaped free surfaces to experimental data; these are often prone to regions of numerical instability depending on the nature of the data-set.

Recent advances in microneedle platforms for transdermal drug delivery technologies

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In many clinical applications, the transdermal route is used as an alternative approach to avoid significant limitations associated with oral drug delivery. There is a long history for drug delivery through the skin utilizing transdermal microneedle arrays. Microneedles are reported to be highly efficient and versatile devices. This technique has attracted scientific and industrial interests, due to its outstanding characteristics such as painless penetration, excellent medicinal efficiency, relative protection and affordability. The microneedles have shown considerable potential to create advanced functional devices with remarkable properties for biomedical applications such as delivery of very large substances with ionic and hydrophilic physicochemical properties. In this review we present a summary of recent advances in microneedles-based drug delivery, typical materials used for their construction and fabrication methods that improves the delivery of critical substances through the protective membranes. Further, it explores the practicality of innovative microneedles used as a drug delivery tool. Microneedles are emerging tools that have shown profound potential for biomedical applications. Transdermal microneedle technologies are likely to become a preferred route of therapeutic substances administration in the future since they are effective, painless, and affordable.

A review on polyimide reinforced nanocomposites for mechanical, thermal, and electrical insulation applications: Challenges and recommendations

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In this paper, the application of polymer composites as a candidate material for thermal and electrical insulation was firstly introduced. Polyimide nanocomposites have drawn much attention as mechanical, thermal, and electrical insulation materials because of its superior dielectric, thermal, and corona resistance behaviours. Thus, polyimide nanocomposites are described as substance of polyimide matrix reinforced with certain weight percent content of nanofillers. Several researches have demonstrated the utilization of polyimide nanocomposites in mechanical, thermal, and electrical applications. However, the nanocomposites are noted facing interfacial bonding issues, which have affected their mechanical performance for thermal and electrical insulation behaviours. The dielectric properties and corona resistance lifetime of the polyimide nanocomposites are reportedly deteriorated over a long term exposure to high temperature condition. There has been advancement on improving the mechanical, thermal and electrical characteristics of polyimide nanocomposites for multifunctional insulations. Hence, this paper summaries the influence of nanofillers, such as alumina (Al_2O_3), silica (SiO_2), titanium dioxide (TiO_2), graphene (GN), nanotubes (NTs), boron nitride (BN), and some other fillers on the mechanical, thermal, and electrical properties of polyimide nanocomposites for insulation applications. As the study offers great insight into the improvement and selection of polyimide nanocomposites material for mechanical, thermal, and electrical insulation, the authors concluded the study with advancement, challenges and recommendations for future improvement of polyimide nanocomposites as an insulation material.

Surface dependent properties and tunable photodetection of $CsPbBr_3$ microcrystals

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All-inorganic metal halide perovskites are highly attractive materials for optoelectronics and are typically implemented as thin films, nanocrystals, and single crystals with macroscopic and millimeter-size dimensions. Here, $CsPbBr_3$ microcrystals are fabricated by simple and fast drop-casting of a precursor solution on several substrates that for the growth process are heated to temperatures in the range from 80 to 150°C. The microcrystals have a cubic shape and feature a pyramidal cavity on their top surface that forms due to faster growth at the edges once the growing crystal is attached to the substrate. Distinct heterogeneity in the photoluminescence (PL) and conductivity of the different facets are measured by μ-PL and conductive atomic force microscopy experiments. Toward device applications, the authors contact single microcrystals on conductive substrates mechanically with a micromanipulator tip. They observe diode-like current–voltage curves and good photodetector functionality, obtaining a high responsivity of 150–300 AW^{-1} in the blue–green spectral region under forward bias, and a sharp detection band centered around 540 nm with peak responsivity close to 0.7 A W^{-1} under reverse bias.

Association of some dietary ingredients, vitamin D, estrogen, and obesity polymorphic receptor genes with bone mineral density in a sample of obese Egyptian women

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Although many environmental factors play an important role in bone mass density (BMD) variation, genetic influences account for 60–85% of individual variance. The aim of this study was to find the interaction between some dietary ingredients, vitamin D, estrogen, and obesity polymorphic receptor genes, among a sample of obese Egyptian women. This was a cross sectional study included 97 women (aged 25–60 years). Data on anthropometry, dietary intake, BMD, biochemical, and genetic analyses were collected. Results: Osteoporosis was high among women had dominant Taq1 vitamin D receptor gene while osteoporosis was less common among the homozygous Apa1 receptor gene women. Both genes in their two forms did not show any effect on serum vitamin D. Heterozygous types of osteoporotic women carried both genes revealed a slight but significant decrease in level of serum calcium. Xba1 estrogen receptor gene was identified only in a homozygous type while the heterozygous Pvu11 estrogen receptors gene has been identified among both osteoporotic and non-osteoporotic women, this gene was associated with higher BMI in both groups compared to the homozygous receptor gene. Mutant types of genotype FTOrs99 and FTOrs80 obesity receptors genes were less common (4.44%, 11%) among participants. Both of these genes were associated with the highest value of BMI and caloric daily intake, fat, and saturated fatty acid that were more prominent among osteoporotic women. Conclusion: There is significant association between vitamin D, estrogen, obesity receptors genes, special nutrients, and osteoporosis. Increased BMI, calories, and fat intake lead to rise of genetic predisposition and susceptibility to osteoporosis.

Dosimetric impact of some gamma radiation-induced polymeric materials incorporated silicate using thermoluminescence and ultrasonic techniques

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Polyacrylamide acrylonitrile magnesium silicate {P (Am-AN)-MgSi} & polyacrylamide acrylic acid magnesium silicate {P (Am-AA)-MgSi} hybrid composites were fabricated utilizing gamma-radiation polymerization initiated about 30 kGy. Different types of dosimetric radiation-induced polymeric composites were irradiated by cesium-137 gamma-ray dose to show its possibility for use as a thermoluminescence dosimeter. The prepared polymeric composites showed useful properties such as good dosimetric and thermal stability behaviors. The mechanical behavior of the samples was measured non-destructively by the ultrasonic pulse-echo technique. It was found that the addition of P (Am-AA) with higher elastic moduli to MgSi with lower ones are produced in the {P (Am-AA)-MgSi} composite sample with a midway value for Young's modulus of 7.13 GPa and shear modulus of 2.71 GPa. Dissimilar in the {P (Am-AN).

New improved thermoluminescence magnesium silicate material for clinical dosimetry

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Magnesium silicate has been prepared by a precipitation technique. This composite structure was proven by different tools, XRD, TGA&DTA, FTIR, and XRF. Magnesium silicate was found to have the formulas Mg1.1SiO3.2.1.1H2O. Thermoluminescence (TL) dosimetric properties like (linearity, fading, energy independence) of magnesium silicate in the shape of $MgSiO_3$ have been estimated. A strong TL dosimetry peak associated with gamma radiation arises from 137Cs was developed. Different doses from gamma radiation were measured by thermoluminescence (TL) detection technique for magnesium silicate glasses in unique magnesium elements concentration to assess its dosimetric properties. A single strong peak of about 230°C arises for all irradiated samples. Total integral values of TL output and TL of the principal peak values showing a linear behavior start with 0.5 Gray up to 2 Gray dose range. Correlation of magnesium silicate TL response and different doses showed dose-response improvement concerning low doses linear relationship.

Modified austenitic stainless-steel alloys for shielding nuclear reactors

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In nuclear fields steel alloys are generally used for radiation shielding especially in structure of nuclear reactors. The cobalt element is one of the steel alloys composite elements. The cobalt element is an expensive element; this makes the steels rather expensive, preventing wider selection and application. So the principal aim of this research is preparing cobalt-free stainless steel as shielding to reduce the production cost. Therefore, seven different free-cobalt steel alloys were prepared by using an electro slag re-melting technique. Steel compound ratios were determined by using XRF techniques and the attenuation properties of these alloys were studied by using the software WinXCOM computer program at photon energies 80, 356, 662, 1173, and 1332 keV. Furthermore, the total macroscopic cross-section was determined by using "Geant 4" code for fast neutron radiation shielding. Also the mean free path, half value layer, the atomic effective number and Transmission coefficient of neutron dose calculated. The results prove an excellent cobalt-free steel alloys have good mass attenuation to be used as a proper shielding material in the nuclear field, this clear such as in the sample (0.032 % Ni, 0.009 % Mo, 0.087 % Cr, 0.948 % Mn, 0.002 % Ti, 0.005 % V, 97.01 % Fe, 0.3 % C, 0.035 % P, 0.012 % S) with density 8.28 g/cm^3. Also shielding parameter variations were applied to the steel alloys to investigate the superior shielding properties to gamma rays.

Facile and green synthesis of silver quantum dots immobilized onto a polymeric CTS−PEO blend for the photocatalytic degradation of p-nitrophenol

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Immobilization of inorganic metal quantum dots (especially, noble transition metals) onto organic polymers to synthesize nanometal−polymer composites (NMPCs) has attracted considerable attention because of their advanced optical, electrical, catalytic/photocatalytic, and biological properties. Herein, novel, highly efficient, stable, and visible light-active NMPC photocatalysts consisting of silver quantum dots (Ag QDs) immobilized onto polymeric chitosan−polyethylene oxide (CTS−PEO) blend sheets have been successfully prepared by an *in situ* self-assembly facile casting method as a facile and green approach. The CTS−PEO blend polymer acts as a reducing and a stabilizing agent for Ag QDs which does not generate any environmental chemical pollutant. The prepared x wt % Ag QDs/CTS−PEO composites were fully characterized through X-ray diffraction, Fourier transform infrared spectroscopy, transmission electron microscopy (TEM), thermogravimetric analysis, and UV/visible spectroscopy. The characterization results indicated the successful synthesis of the Ag QDs/CTS−PEO composites by the interactions and complexation between x wt % Ag QDs and CTS−PEO blend sheets. TEM images revealed small granules randomly distributed onto the CTS−PEO blend sheets, indicating the immobilization of Ag QDs onto CTS−PEO composites. The presence of a surface plasmon resonance (SPR) band and the shifting of the absorption edge toward higher wavelengths in the UV/vis spectra indicated the formation of x wt % Ag QDs/CTS−PEO composites. The Ag QDs in the polymeric blend matrix led to remarkable enhancement in the optical, thermal, electrical, and photocatalytic properties of x wt % Ag QDs/CTS−PEO composites. The photocatalytic efficiency of the prepared composites was evaluated by the photodegradation of p-nitrophenol (PNP) under simulated sunlight. The maximum photocatalytic degradation reached 91.1% efficiency within 3 h for the 12.0 wt % Ag QDs/CTS−PEO photocatalyst. Generally, the Ag QDs immobilized onto CTS−PEO blend composites significantly enhance the SPR effect and the synergistic effect and reduce the band gap, leading to a high photocatalytic activity.

Human toxoplasmosis in Mozambique: Gaps in knowledge and research opportunities

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Toxoplasmosis is a parasitic zoonotic disease caused by the Toxoplasma gondii zoonosis that afflicts humans worldwide and wild and domestic warm-blooded animals. In immunocompetent individuals, the acute phase of infection presents transient low or mild symptoms that remain unnoticed. Although the lifelong persistence of the dormant form of this parasite can lead to different toxoplasmosis clinical forms in immunocompetent individuals and immunocompromised patients and be related to neuropsychiatric disorders and neurodegenerative diseases. In immunocompromised patients, Toxoplasma is a life-threatening opportunistic infection, which can result from the reactivation of latent infection or primary infection. Moreover, congenital toxoplasmosis, which results from the transplacental passage of tachyzoites into the fetus during a pregnant primary infection can lead to miscarriage, stillbirth, or ocular and neurologic disease, and neurocognitive deficits in the newborns. Thus, the present review aims to address the current knowledge of Toxoplasma infection and toxoplasmosis in Africa and especially in Mozambique, stressing the importance of identifying risk factors and promote awareness among the population, assessing the gaps in knowledge and define research priorities. In Mozambique, and in general in Southern African countries, clinical disease and epidemiological data have not yet been entirely addressed in addition to the implications of T. gondii infection in immunocompetent individuals, in pregnant women, and its relation with neuropsychiatric disorders. The main gaps in knowledge in Mozambique include lack of awareness of the disease, lack of diagnostic methods in health facilities, lack of genetic data, and lack of control strategies.

Features of the process of compaction of powder aluminum alloys by cold pressing

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A schematic model of the compaction process of spherical particles of different sizes is proposed. In this regard, the process of compaction of granules was considered in the context of three stages. It has been found that in the first stage there is an active compaction, as a result of which the packing of the powder particles becomes tighter. At the second stage, as a result of an increase in the pressing pressure, the contact areas of the particles increase and juvenile friction surfaces are formed, which enhances their molecular interaction and friction resistance. At the transition of pressing from the 2nd stage to the 3rd, the generated pressure strengthens the mechanical contacts and causes the extrusion of particles into the micropores of the pressing. Large differences between pellet sizes improve the extrusion of fine particles.

The analysis of changes in some mechanical parameters of a porous composite material based on aluminum, depending on the applied pressure during compaction, is carried out. With the help of special devices based on compression models proposed by different researchers, the change in the relative density of the porous material depending on the pressing pressure was studied. In conventional and semi-logarithmic coordinate systems, graphical descriptions of the dependences of the relative density of briquettes on the pressing pressure, as well as their initial microhardness on the particle size, are given. In addition, curves were presented that characterize the effect of pressing pressure on both the microhardness of briquettes with different fractions and their shear and compressive strength.

Calculation formulas are given that make it possible to calculate the areas of initial and current pores, depending on the particle size of the constituent fractions, at any moment of load application until the powder is completely compacted.

Comparative analysis of photovoltaic - thermal (PVT) and photovoltaic (PV) modules

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Solar photovoltaic and thermal (PVT) is a hybrid technology that combines photovoltaic (PV) solar cells, which converts solar energy into electricity, with a solar thermal collector, which transfers the unused excess heat from the PV module into the useful thermal energy in the form of heated water or air. The hybrid PVT system proves to be more energy efficient with improved electrical efficiency due to cooling of PV cells and obtained thermal energy due to heat absorbed from heated PV cells. Nevertheless, the utilization of these systems does not grow rapidly due to the controversial operational problems. In this work, the operational problems of PVT technology are investigated. The comparative analysis of properties of PVT modules and general PV module has been conducted.

The operating temperatures of solar cells in PV and PVT modules under the dependence of ambient temperature and other parameters theoretically and experimentally have been investigated. On the base of comparison of operating temperatures of solar cells in PV and PVT modules, the efficiency of PVT hybrid module has been analyzed.

It is demonstrated that when the ambient temperature is low, the temperature of PVT module can be higher than the temperature of the general PV module, due to the decreased convection cooling of PVT in comparison with the PV module. The ambient temperature, below which the PVT module is hotter than the PV module, is called “critical”. As a result of this process, the electrical efficiency of the PVT module becomes smaller than the efficiency of the PV module. This effect is called the “reverse” process. It has been concluded, that to overcome this operational problem, the PVT system and its functionality must be optimized taking into consideration the weather conditions under which the PVT system will be used.

Enhancement of photoluminescence properties of nano-sized Pr^{3+} doped $LuPO_4$ powders by incorporating of Y^{3+} ions

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The work explores the enhancement of photoluminescence properties of nano-sized $LuPO_4$:Pr^{3+} phosphor powders synthesized by sol gel process with incorporation of yttrium ions inside of this single matrix to obtain $(Lu_{1-x}Y_x)$ PO_4:Pr^{3+} (x=10, 20, 30, 40, and 50 at. %) powders. Under UV excitation at 270 nm the emission spectra of LuPO4:Pr^{3+} nanopowder do not present any characteristics emission band attributed to $4f^15d^1$->$4f^2$ transitions of Pr^{3+} ions, while a large emission band has been observed which due to defects created in $LuPO_4$ cell by doping considering the ionic radius of Pr^{3+} is larger compared to the ionic radius of Lu^{3+}, this band extinguishes gradually at the time insertion of the Y^{3+} ions until its total disappearance (for x=40 at. %).It was found that the emission spectra of (Lu1-xYx)PO_4:Pr^{3+} nanopowders under λex=230nm presents only the characteristics emission bands of Pr^{3+} ions with a remarkable influence of the rate of Y^{3+} ions on the intensity of this bands. Furthermore, it was observed that the improvement in the luminescence properties of $(Lu_{1-x}Y_x)$ PO_4:Pr^{3+} nanopowders is very remarkable in visible range.

New design of quad-band polarisation-insensitive metamaterial absorber based on dual-T shaped resonator array for C-, X- and Ku- bands microwave applications

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Multi-band metamaterial absorbers (MMAs) are increasingly becoming the main devices for many electrical systems. Optimizing the electromagnetic qualities of this type of absorber in the microwave regime is a relatively complex operation. In this paper, a quad-band Metamaterial Absorbent MMA covering the microwave bands is provided. The proposed MMA for analysis and design is formed by an (16×16) array of metamaterial base cells. Each cell has an interconnected circular T-C shaped split ring resonator (CTC-SRR) etched on the top face of FR4_Epoxy substrate for electrical dimensions ($0.18\lambda_0 \times 0.18\lambda_0$) where λ_0 is calculated at the lower frequency of 4.6 GHz in the C-band. The electromagnetic qualities of our MMA are expired by the behavior of each basic cell which represents a left hand medium and a negative permeability ($\mu<0$) for magnetic resonances at the frequencies 4.6 GHz, 9.2 GHz, 11.3 GHz and 15.8 GHz. The obtained results simulations performed by the High-Frequency Structure Simulator (HFSS) computer show an insensitive-polarization quad-band behavior for our proposed MMA. The spectral responses of the absorber cover the C-, X- and Ku-bands for important absorption coefficients of the order of 96.22%, 93.25%, 98.46% and 92.37%.

From metallic to semiconductor conversion of single – walled carbon nanotubes by chlorination

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In this research, single-walled carbon nanotubes (SWCNTs) were treated with strong $HClO_4$ acid. Then investigated first by UV–vis-NIR absorption, Fourier transform infrared (FTIR) and Raman spectroscopy; and secondly by numerical calculations based DFT using generalized GGA and LDA as implemented in SIESTA code. The results show significant changes in the behavior of metallic nanotubes and DFT calculations (GGA and LDA) show that adsorption of chlorine atoms on the metallic (9,9) carbon nanotubes wall generates an energy gap in the electronic structure of these nanotubes, confirming the experimental results. This highlights a conversion of metallic nanotube to semiconductor.

Enthalpy behavior of ZnO zinc blende structure under isobaric and isothermal ensembles a MD computation

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In this work we used Parallal Molecular Dynamics and DL_POLY_4 (calculations ran on RAVEN supercomputer of Cardiff University) to analyze enthalpy behavior of ZnO Zinc Blende structure under different pressures and temperatures. Our system is formed from 5832 atoms of ZnO (2916 atoms of Zn^{+2} and 2916 atoms of O^{-2}), the interatomic interactions are modeled by Coulomb-Buckingham Potential for short and long-range, the range of temperature is 300-3000K and for pressure is 0-100GPa. Although no more data under previous conditions our results are in the vicinity of available experimental and theoretical information. This work is very important in nanoscale of time and space and in different sectors of industry.

Phosphido-Bridged Trinuclear Platinum Clusters: A DFT Study

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The compound H(PEt3)3Pt3(μ-PPh2)3 is the unique example of a 46e− phosphido-bridged triangular cluster, but its X-ray assigned stereochemistry appears questionable. In particular, the H-free P3Pt3(μ-P)3 metal core is identical to that of the 44e− cation [(PEt3)3Pt3(μ-PPh2)3]+ in two salts of the same publication. Also, the lack of a distortional effect due to the upright and strongly-bound hydride ligand is suspicious and intriguing aspects emerge from the inconsistent electronic structure. Although H(PEt3)3Pt3(μ-PPh2)3 is fully validated by IR and NMR spectra, DFT optimizations never reproduced the proposed experimental structure but highlighted a different stereochemistry still consistent with the spectroscopic response. Here, a formal Pt(II) ion is essentially isolated and has square-planar coordination, completed by two trans-axial ligands (H and Et3P) out of the Pt3 plane. Given the chemical reliability of the in silicomolecule, the crystals of the experimental structure have likely contents other than the hydridic cluster and a co-crystallized Ph2PH molecule. As a working hypothesis, the Pt-H and P-H linkages of the distinct components may have reacted together with H2 release, and subsequent cristallization of the salt whereas the ion pair [(PEt3)3Pt3(μ-PPh2)3]+/[Ph2P]−. This would explain the equal geometries of the putative 46e− cluster and the H-free 44e− cation. In the lack of any experimental X-ray dataset, the proposed crystal formulation could not be fully validated, but in the paper various aspects support its reliability.

Modulational instability and chaotic-like behaviors in repulsive lattices

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In this work we study the dynamics of modulated waves in a mono atomic granular medium. We start by comparing each grain of the medium to a ball, and the interaction between various balls like linear elastic interactions we established that the dynamics of the system of pendulum used by Fermi-Pasta-Ulam can be governed by a discrete nonlinear Schrödinger equation. Like second advanced, we also established under which conditions this system could be prone to a modulational instability. The long-time dynamics of modulated waves is examined using numerical simulations which are corroborated with analytical results leads to the generation of nonlinear modulated waves which have the shape of a soliton.

Energy potential assessment and characterization of fuel briquettes made from Cameroonian agricultural crop residues

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Scope and objectives: For sustainable development purposes, it may be advisable to substitute fuelwood for fuel briquettes in household cooking in countries with high agricultural potential as Cameroon. The objectives of this study are firstly to assess the theoretical energy potential which could be recovered from agricultural residues for fuel briquettes production; prepare and characterize fuel briquettes using banana peels, rattan waste, coconut shells, palm oil shells and sugarcane bagasse; finally analyse the benefits and barriers of briquetting conversion of these residues in Cameroon.

Methods: The Residues-to-Product Ratio (RPR) method was used to calculate the energy potential. Fuel briquettes were prepared through a conventional method and evaluated by proximate analysis using American Society for Testing and Materials (ASTM) standard, European Committee for Standardization (CEN) standard and Thermo-Gravimetric Analysis (TGA).

Results: The study carried out shows that briquetting conversion of these residues could produce 7 706 260 tons.yr^{-1} of fuel briquettes, the energy potential value is about 106 PJ.yr^{-1}. Results of mass reduction study show that the losses are more important for banana peels (97.98%) and sugarcane bagasse (96%). Bulk density of briquettes produced is in the range 0.470–0.851 cm^3/g; results of proximate analysis show that high calorific values of briquettes produced are 14.25, 16.98, 30.07, 32.16 and 25.93 MJ/kg for palm oil shells, banana peels, rattan waste, coconut shells and sugarcane bagasse respectively; ash content has values in the range 7.44–11.95%, and moisture content is relatively higher than other agricultural residues especially banana peels and sugarcane bagasse.

Conclusion: It is concluded that availability of agricultural residues in that country gives an important potential for briquette production from biomass crops resources. It would interest to valorise this potential considering political, logistical and seasonal crop constraints.

Interplay role between dipole interactions and hydrogen bonding on proton transfer dynamics

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In our work, we examine the role of dipole-dipole interactions on proton dynamics and properties of defects in hydrogen bonding systems. These interactions created by protons and heavy ions allow us to generalize the original Antonchenko-Davydov-Zolotaryuk model. One of the particularities of our model is the shape of the dipole-dipole interaction, which better expresses and explains real systems compared to the classical harmonic interactions usually used. It emerges that the characteristic parameter of the dipole- dipole interaction β is of capital importance in the study of the coupled differential equation of hydrogen bond systems, at the points where its variation drastically changes the dynamics and qualitatively modifies the solutions of the system. The number of solutions obtained and the study of their behavior at the slightest deviation β, imply the use of the theory of bifurcations. This theory allowed us to obtain 23 phase portraits, each trajectory of which determines the possible displacement of the proton. For each orbit of the phase portraits obtained, this under very precise conditions, all possible exact parametric representations of the solutions are identified. It is clear that their interpretation shows a much richer variety of solitons. It appears that β influence differently the proton in function which he has a subsonic, sonic or supersonic speed, but its variation makes it possible to obtain several exact parametric representations of the solutions (periodic solutions, peakon, kink and antikink, compacton, etc.) and singular straight lines. However, due to their robustness, we have chosen the compacton-type solutions having the shape of the kink (Kinkon) to determine the dynamic quantities of the system such as the energy and momentum of the kink (k) and the anti-kink (ak), physical quantities such as mobility and conductivity, in order to better appreciate the validity of the model and the theories we have proposed.

Material, waste, energy and environment

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Material science is the study of material; while material is everything outside nothing i.e. material science is the study of everything outside nothing. Every tangible thing in the universe is a material. Materials are used every day by human for living. Materials can be useful or waste.

Over the years, materials are being transformed using technology available at the material time to make living more comfortable; but as technology continue to advance, materials made with old technology are been abandoned generating waste. Also when an equipment fails or stops to perform it primary function, it’s been abandoned or dumped. This action over the years keep increasing the amount of waste in our environment. As we keep using and developing materials, we keep abandoning old materials causing waste to increase. In most part of the world, waste is beyond control causing environmental hazard.

Ojelola K. et al (2020) studied the waste generation and it management in the most populous city in Africa (Lagos, Nigeria) with the objective of transforming waste in useful products. With aim of transforming waste, Taiwo Alare et al. (2020) presented a model of smart waste cycle which included bioenergy generation, refining and recycling. A lot has been done by researchers on waste transformation especially in the area of biofuel and wastewater purification. It is difficult to know amount of solid waste available in geographical location and in order to reduce via transformation the amount of available waste should be known to ensure efficient operations. In other to increase the exactness of waste data, Taiwo Alare and Kehinde Alare (2021) developed a mathematical formula to calculate amount of solid waste in a location.

As material is a necessary tool in production, in order to reduced cost of production Olanrewaju Akinnawo and Taiwo Alare (2021) used waste in production of a paper cutting machine which tend to reduce the cost by 80%. As material scientists, it is high time we stopped wasting waste.

Prediction of the reflection intensity of natural hydroxyapatite using generalized linear model and ensemble learning methods

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Laboratory data acquisition and analysis of X-ray diffraction (XRD) data involves a lot of tedious human engineering and is time-consuming. To put in context, a summation of the material synthesis procedure leading to the analysis of the structure of the material can span several days. To curb this challenge and to enhance innovations in engineering pedagogy, this article investigates an alternative method that uses supervised learning algorithms based on ensemble techniques and a generalized linear model (GLM) for predicting reflection intensity (XRD patterns) of raw and natural hydroxyapatite under varying sintering temperature conditions given Bragg angles as input to the machine learning algorithms. For the experiment, we trained GLM and ensemble learning models (CatBoost, LightGBM, and two variants of XGBoost based on manual and genetic algorithm for tuning of the hyperparameters). The results show that most instances of the XGBoost yielded a robust performance that surpasses all other approaches, when predicting X-ray reflection intensities ascribed to the biomaterials subjected to varying sintering temperature conditions. In addition, the results show that all the ensemble techniques significantly outperform the GLM, this indicates that the former exhibits better generalization capacity. The ensemble learning techniques and the GLM presents a reduced computational complexity.

Heavy metals contamination in two species of medicinal plants in the Iranian market

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Global threat resulting in heavy metal contamination of medicinal plants is considered a serious concern. The quantitative evaluation of four heavy metals, lead (Pb), cadmium (Cd), zinc (Zn), and copper (Cu), was investigated frequently sold medicinal plants in the markets of Iran. Two medicinal plants, Mentha piperita L. and Zataria multiflora Boiss. Were selected from six different herbalists of six districts of Shiraz, Iran. The dissolution of the sample was performed by a conventional wet acid digestion method, and heavy metal levels were determined using Polarograph. Statistical Analysis was used by SPSS.21. According to the achieved results in M.piperita the levels of Zn, Cd, Pb, and Cu were in the range of 2.66 ± 0.76 mg/kg, 0.017 ± 0.009 mg/kg, 0.092 ± 0.069 mg/kg, and 0.237 ± 0.080 mg/kg, respectively. The concentrations of Zn, Cd, Pb, and Cu in Z. multiflora samples were 1.46 ± 0.74 mg/kg, 0.019 ± 0.004 mg/kg, 0.11 ± 0.05 mg/kg, and 0.41 ± 0.17 mg/kg, respectively. There was a correlation between Zn with Cu in our finding (r = 0.9). Based on these results, we found that the concentration of heavy metals in these two medicinal plants was not more than the standard concentration reported for similar plants. It appears that these plants are generally safe in usual doses. The finding of this study can be used to determine standard heavy metals limits in M.piperita and Z.multiflora in future studies.

Synthesis of 45S5 bioactive glass-ceramic using the sol-gel method, catalyzed by low concentration acetic acid extracted from homemade vinegar

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In this paper, two different type of 45S5 bioactive glass-ceramic were compared. Both of them were prepared using the sol-gel method, with two different catalysts: 2 M nitric acid (NACBG) and 10 mM vinegar. Homemade vinegar (HMV) extracted from apples which contained up to 5% acetic acid, as an affordable and low concentration catalyst, was used for the synthesis of 45S5 bioactive glass ceramic called Homemade Vinegar Catalyzed Bioactive Glass (HMVCBG). The substitution of 2 M nitric acid by 87 mM acetic acid strongly reduces the concentration of the acid solution necessary for being a catalyst. The effect of these two catalysts on the structure, morphology, and properties of the bioactive glass-ceramics were investigated. Scanning electron microscopy (SEM) with energy dispersive X-ray spectroscopy (EDXS) and Brunauere Emmette Teller (BET) were used to assess surface characteristics and specific surface area, which showed more uniformity and more specific surface area in HMVCBG. Crystallinity and composition were analyzed by X-ray diffraction (XRD), X-ray fluorescence (XRF) and Furrier transform infrared spectroscopy (FTIR) which showed some crystalline phases in BG. In-vitro bioactivity was studied in Phosphate Buffer Saline (PBS) and SEM results showed that HMVCBG has a more uniform hydroxyapatite layer and formation occurs more quickly. This due to the fact that hydroxyapatite is dissolved at a lower rate at higher pH values and it takes longer to form at a higher pH. HMV can form more numerous porosities and a more specific surface area because of higher pH of acetic acid. Hence, PBS solution penetrates to the depth of HMVCBG and hydroxyapatite nucleation form in more spots in the depth of HMVCBG. Thus, HMVCBG has a higher bioactivity level than NACBG.

Analysis and examination of aluminum sheets suitable for automotion body: Ultrasonic testing, signal processing, simulation

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There are many changes in the automotive industry, today. All aluminum sheets used in the automotive body must have good weldability. In this article, we will test the spot welding on 6 types of 5XXX and 6XXX aluminum sheets. These sheets have been selected as the best sheet suitable for the automotive body after welding test on all sheets. This test was examined by ultrasound. The signals obtained from the ultrasound wave test do not have accurate results for better sheet determination. For this purpose, signal processing was performed on the obtained signals in order to detect sheet defect. By simulating these sheets, a comparison is made between the experimental test and the simulation, which can be used to make the best decision about the chosen sheets. The status charts of these sheets have been reviewed and it is easy to select the sheets that have been tested in the shortest time. Generally, findings indicated that the best suitable sheets in automotive bodyare type of 5XXX aluminum sheets.

Inulin enriched wheat bread: Interaction of polymerization degree and fermentation type

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Inulin enrichment of wheat bread is important in improving its nutritional quality. Despite the preference of inulin enrichment of wheat bread, its efficiency may be frustrated by the inulin loss through bread making process. In this study, we aimed to investigate the nutritional and technological functionality of inulin enriched wheat bread. The different fermentation process [common yeast (Y) and mixed fermentation based on sourdough (MFSD)] were used to leaven wheat breads enriched with inulin at three different degree of polymerization (DP) as short chain, long chain and native. Inulin was replaced at 10% w w^{-1}. Despite the gluten dilution impacts induced by inulin replacement, it has been alleviated by long chain inulin incorporation and MFSD in which no significant difference has been observed regarding its specific volume and textural assessment by the control sample. The most fructan hydrolysis occurred through baking process of wheat breads containing short chain inulin in the presence of MFSD reaching losses up to 41% after baking process. Inulin loss ratio is dependent to the type of fermentation process and polymerization degree of inulin. Results obtained in this study may provide further insight to inulin enrichment of wheat bread from technological and nutritional points of view.

Neurotoxicity of silver nanoparticles in the animal brain: A systematic review and meta-analysis

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Objective: About 30% of all nanoparticle products contain silver nanoparticles (AgNPs). With the increasing use of AgNPs in industry and medicine, concerns about the adverse effects on the environment, and the possible toxicity of these particles to primary cells and towards organs such as the brain and nervous system increased. In this paper, the toxicity of AgNPs in neurons and brain of animal models was investigated by a systematic review and meta-analysis.

Methods: The full texts of 26 relevant studies were reviewed and analyzed. Data from nine separate experiments in five articles were analyzed by calculating the standardized mean differences between viability of treated animals and untreated groups. Subgroup analysis was conducted. In addition, a systematic review provided a complete, exhaustive summary of all articles.

Results: The results of the meta-analysis showed that AgNPs are able to cause neuronal death after entering the brain (standardized mean difference (SMD) = 2.87; 95% confidence interval (CI) 2.1–3.61; $p < 0.001$). AgNPs sized smaller or larger than 10 nm could both cause neuronal cell death. This effect could be observed for a long time (up to 6 months). Neurons from embryonic animals whose mothers had been exposed to AgNPs during pregnancy were affected as much as animals that were themselves exposed to AgNPs. Toxic effects of AgNPs on memory and cognitive function were also observed. Studies have shown that inflammation and increased oxidative stress followed by apoptosis are likely to be the main mechanisms of AgNPs toxicity.

Conclusion: AgNPs can enter the brain with a long half-life and it can cause neuronal death after entering the brain. AgNPs can manifest proinflammatory cascades in the CNS and BBB. Some toxic effects were detected in the cerebral cortex, hypothalamus, hippocampus and others. Studies have shown that inflammation and increased oxidative stress lead to apoptosis, the main mechanism of AgNPs neurotoxicity, which can be caused by an increase in silver ions from AgNPs.

Comparison of strength and mechanisms of stabilized samples of coarse and fine-grained soils with cement kiln dust

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Road pavement soils have not had sufficient resistance in most road construction projects. Therefore, instead of substituting high-strength soils for base soils, cement kiln dust like stabilizers can be used that are not only inexpensive but also environmentally friendly. In this research, stabilization of coarse-grained sandy soils (SP) and silty fine-grained soils (SM) using different percentages of 5, 10, 15 and 20% of cement kiln dust has been investigated. Standard compaction and uniaxial compressive strength tests as well as direct shear test with two types of soil mentioned with different percentages of cement kiln dust at the time of curing and 7, 14 and 28 days have been performed. The results show that by adding 20% of CKD to sandy soil, the resistance has increased 11.3 times than of the base soil, while with the same percentage of CKD, the uniaxial strength of silty soil has increased by 9.8. Therefore, the CKD stabilizer for coarse-grained sands has a greater effect than fine-grained, which can be attributed to the better locking of sand grains in the effect of increasing the CKD than silty soil. Also, microstructural experiments including XRD, SEM, EDAX, FTIR have been performed for stabilized samples and base soil and the results have shown that changes in the peak Formation of CSH gels and coherent structure related to sandy soil have been observed that confirms this issues.

Assessment of heavy metals in agricultural and background soils around future copper mine, using enrichment factor and Geoaccumulation index, Iran

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Heavy metals are pollutants released into different parts of the environment such as soil and plants due to natural and anthropogenic origin. There is a possibility of water, soil, and plant pollution in Darreh Zereshk area in the near future. To assess the soil contamination and determine the origin of selected heavy metals, enrichment factor (EF) and geoaccumulation index (Igeo) were conducted. To aim this purpose a total of 30 agricultural soil samples and 12 background soil samples were collected from Darreh Zereshk area in central Iran which is going to be one of the richest copper mines in Iran and the Middle East. Accordingly, total and soluble concentration of heavy metals (Cu, Pb, Zn, Mn, As, Fe, Ni and Cr) and some Physico-chemical properties of soils were determined. According to the Igeo result Dareh Zeresh village is moderately to heavily contaminated with Cu (2.16), Hasan Abad and Bishe villages are moderately contaminated (1.21, 1.04) and Darreh Gazeh and Dehshir villages are uncontaminated to moderately contaminated (0.01, 0.13), which can be justified by the presence of rich copper deposit in the area and the distances of each village from that. High EF factors for Cu, Zn and especially for Pb as it is not an essential micronutrient, indicate a considerable enrichment caused by pollution. Contamination of the agricultural soils is more severe for Pb, Cu and Zn and less severe for As. The origin of Ni and Cr does not seem to be anthropogenic.

An investigation into the laser forming process of perforated tubes

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Tube bending is always a challenge in conventional bending. Usually, an internal plug is inserted inside the tube, and bending happens. However, a laser beam can also be used for tube bending. The laser beam is irradiated on the tube surfaces and may result in 2D or 3D tube bending. The laser tube bending process (LTBP) process is a thermal non-contact process for bending tubes with less springback and less thinning of the tube. In this work, the laser forming process of perforated tubes is studied numerically. For this purpose, the finite element simulations are performed in ABQUS software. In addition, the effects of process parameters such as laser output power, laser scanning speed and laser beam diameter on the characteristics of laser formed tubes are studied.

The characterization and mineralogical studies of thorium ore deposit in Choghart, Yazd, Iran to evaluate beneficiation prospects

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This paper investigates the mineralogical characterization of a thorium ore taken from the Choghart iron mine, Yazd, Iran. The mineralogical studies revealed that the main thorium content mineral of the ore was thorite; and it was mainly disseminated as a valuable mineral in different forms in minor quantity along the edge or within the intergranular spaces of gangue silicate minerals and magnetite. The XRF analysis of a radiometric sorting concentrate sample indicated that the sample contained approximately 0.25% thorium oxide, 66.28% silicate compositions, 9.14% iron oxide, and significant amounts of rare earth elements. Sink and Float tests of different sizes of the sample using diiodomethane and bromoform resulted in a 2.22% concentrate with 85.7% thorium recovery. Liberation degree studies by SEM-EDX and image processing indicated that a size range of (-125,+75)μm was the optimum liberation size, and it was recommended for further beneficiation tests.

Ventilation prediction for an industrial cement raw ball mill by BNN- a "conscious lab" approach

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In cement mills, ventilation is a critical key for maintaining temperature and material transportation. However, relationships between operational variables and ventilation factors for an industrial cement ball mill were not addressed till today. This investigation is going to fill this gap based on a newly developed concept named "conscious laboratory (CL)". For constructing the CL, a boosted neural network (BNN), as a recently developed comprehensive artificial intelligence model, was applied through over 35 different variables with more than 2000 records monitored for an industrial cement ball mill. BNN could assess multivariable nonlinear relationships among this vast dataset and indicated mill outlet pressure and the ampere of the separator fan had the highest rank for the ventilation prediction. BNN could accurately model ventilation factors. Since improving the milling efficiency has an essential role in machine development and energy utilization, these results can open a new window to the optimal designing of commination units for the powder technologies.

High density polyethylene-bismuth oxide nanocomposite: A dental shield applied in radiography centers

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Due to the importance and approach of lead-free radiation shields, which has received serious attention in recent years, in this research, radiation shielding characteristics of High Density Polyethylene/Bismuth Oxide (Bi_2O_3/HDPE) nanocomposite against the gamma rays of 241Am source with 59 keV photon energy was investigated by MCNP, XCOM simulations and experimental methods.

First, the quantities of linear attenuation coefficient (μ), mass attenuation coefficient (μ/ρ), Half-Value Layer (HVL) and Tenth-Value Layer (TVL) related to different weight percentages of the composite were simulated using the MCNP code. Then, the simulation results were validated with XCOM software data, which indicated the high accuracy of the simulation.

The simulation results showed that by increasing the energy of the incident photons, the attenuation coefficient of the photons was decreased. At the end of the simulation phase, 60 wt% Bi_2O_3/HDPE composite with density of 2.01 g/cm^3, μ=5.9193 cm^{-1}, μ/ρ=2.945 cm^2/g, HVL=1.2 mm, TVL=3.9 mm was selected to fabricate a jaw shielding material at 59 keV. With increasing the Bi_2O_3 weight percentage in the polymer matrix, the effective atomic number and density of the composite will be increased accordingly, thus the amount of attenuation coefficient will be increased and the HVL and TVL values in the mentioned energy will be decreased.

In the experimental phase, 60 wt% Bi_2O_3/HDPE nanocomposite was fabricated via soloution method. Then, various tests such as FESEM and XRD were performed on the samples, which indicated good dispersion states of bismuth oxide nanoparticles in the polyethylene substrate. After fabrication of the samples, the quantities of μ, μ/ρ, HVL and TVL were measured. Results showed an acceptable correlation with simulated values with MCNP code and XCOM software.

SnO_2 nanoparticles/ reduced graphene oxide nanocomposite for fast ethanol vapor sensing at a low operating temperature with an excellent long-term stability

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Pristine SnO_2 nanoparticles (NPs) and its composite with reduced graphene oxide (SnO_2 NPs/rGO) have been successfully synthesized using a facile hydrothermal method. Prepared samples are characterized by X-ray diffraction, high-resolution transmission electron microscopy, X-ray photoelectron spectroscopy, Brunauer–Emmett–Teller analysis, and Raman and photoluminescence spectroscopy. The results show that the average crystallite size of SnO_2 NPs with tetragonal rutile structure decreased from about 14 to about 8 nm during the formation of SnO_2 NPs/rGO nanocomposite. The resultant SnO_2 NPs/rGO nanocomposite exhibits high surface area of 128.52 m^2/g and large pore volume of 0.14 cm^3/g with uniform pore size of 4.39 nm. The existence of electronic interactions caused by the formation of p–n heterojunctions between p-rGO and n-SnO_2 NPs is confirmed by analysis results. SnO_2 NPs/rGO nanocomposite sensing responses toward 600–1700 ppm of ethanol vapor at 130℃ are about 14–33 times higher than those of pristine SnO_2 NPs at 210℃. The nanocomposite sensor exhibits very low response time of below 3 s, good selectivity, and excellent long-term stability with the response decay of about 4% after 4 months. The improved sensing characteristics in SnO_2 NPs/rGO nanocomposite can be attributed to the formation of p–n heterojunctions, small particles size, large specific surface area, and high porosity.

Evaluation of the effects of nanoparticles on the therapeutic function of platelet: A review

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Objectives: Nanotechnology and nanoparticles can be used in the blood disease monitoring and therapy. Nanoparticles have various effects on blood components and can reduce or improve the function of therapeutic platelet during the storage time. This review study was performed to evaluate the impacts of nanoparticles with various sizes and charges on platelet function and storage time. The present review contains the literature reported between 2010 and 2020. The data have been used from different sites such as PubMed, Wiley, Science Direct and on-line electronic journals.

Results and discussion: The literature survey demonstrated that among various properties, size and charge of nanoparticles were critical on the function of therapeutic platelet during the storage and inhibition of their aggregation. Overall, this study described that nanoparticles with smaller size and negative charge were more effective in increasing the survival time, inhibition of aggregation and improving the function of the therapeutic platelet.

Summary Based on the current review, it confirmed that nanoparticles such as dendrimer, Au, Ag and iron oxide nanoparticles with smaller size and negative charge have significant advantages for improving the efficacy of platelets during the storage chain and inhibition of their aggregation.

Nanotechnology, big things from a tiny world

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Gathering knowledge and technology for hello tomorrow…. Science and technology impact our daily lives, our societies, our planet. We powering deep technologies for better tomorrows and building the future of Humanity together. We believe that nanotechnology can have a global impact and solve the world's major issues…. Nanotechnology is science, engineering, and technology conducted at the nanoscale where the atoms and molecules behave differently at the nanoscale. Making materials at the nanoscale to take advantage of enhanced properties such as higher strength, lighter weight, increased electrical conductivity, and chemical reactivity compared to their larger-scale equivalents. However, there is a major bottleneck in transforming these technologies into impactful products ... but no worry this will be our mission. Our mission is to BUILD a bright TOMORROW.

Mechanical properties and microstructure evolution in arc stud welding joints of AISI 1020 with AISI 316L and AISI 304

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The mechanical properties and microstructures of dissimilar arc stud weldments of AISI 316L/AISI 1020 and AISI 304/AISI 1020 were investigated. Welding currents of 400, 600 and 800A and welding time of 0.2, 0.25, 0.3, 0.35, 0.4 and 0.45 second were employed. Maximum torque strength of 77N.m was registered with 600A and 0.25 second for 316L/AISI 1020 joints with failure occurred away from the fusion zone (FZ) within the stud shank. Whereas for AISI 304/AISI 1020 joints, the maximum torque strength was 68Nm recorded with 600A and 0.35 second and the failure occurred at FZ. For both dissimilar joints, the presence of chromium carbides and equiaxed grain structures are the direct caused for the augmentation of hardness at the FZ. The microstructure of FZ was completely re-solidified of the austenite phase.

Morphological, magnetic, optical, surface potential and H_2S gas sensing behavior of polypyrrole nanofibers

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The effect of the oxidant-to-monomer (O/M) molar ratio on the morphological, magnetic, optical, and surface potential performance of polypyrrole nanofibers (PPy NFs) has been studied. PPy NFs were prepared by chemical polymerization of pyrrole at 5°C, then the structure of nanofibers with various diameters was determined by field-emission scanning electron microscopy (FESEM). X-ray diffraction analysis and energy-dispersive x-ray spectroscopy were used to determine the composition of the PPy NFs in the prepared nanostructures. The magnetic hysteresis loop of PPy NFs showed soft ferromagnetic behavior. The surface potential of PPyNFs was measured by Kelvin probe force microscopy, revealing that the sample with a MO:Py: $FeCl_3$ molar ratio equal to 1: 5.6: 4 showed excellent surface potential behavior. The H_2S gas sensing performance of the PPy NFs thin films with each molar ratio was also tested, revealing an enhancement with increasing oxidant concentration.

Green synthesis and characterize of silver nanoparticles by using leaves extract of Polyalthia Sclerophylla and their cytotoxicity studies

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This study was conducted to synthesize and characterize Silver Nanoparticles (AgNPs) using a rapid green synthesis approach. The crude extract of leaves of Polyalthia sclerophylla (CEPS) were used as a reducer and silver nitrate ($AgNO_3$) as an initiator. Two samples were prepared and named as AgNPs-a and AgNPs-b, respectively. The prepared samples were carried out to characteristic their chemical, physical and biological properties. The first technique that used to confirm the formation of AgNPs were ultraviolet–visible spectroscopy (Uv-vis) and Energy Dispersive X-Ray Analysis (EDX). Scanning electron microscopy (SEM) and scanning transmission electron microscopy (STEM) were used to identify the morphology and size of the particles. Mg-63 human cells were used to study the cytotoxicity of the AgNPs using the Alamar blue assay. The results have been shown that, the wavelength of AgNPs-a was 436 nm, while the AgNPs-b showed at 441 nm. Prepared samples were shown spherical in their shapes according to SEM and STEM images. The size of the particles was not same, whereas, the diameter size range of AgNPs-a were from 48nm to 68 nm, while the AgNPs-b showed range from 59 nm to 77 nm. Prepared samples showed availability for the Mg-63 cells more than 89% for all concentrations after 24h. Present study has been demonstrated non-toxic prepared samples with nano-sizes which can be used safely in the medical and biological fields.

In vivo kinetic release of five metal ions (iron, titanium, nickel, copper and chromium) from fixed orthodontic alloys in Erbil city-Kurdistan region/Iraq

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The orthodontic kinetic release of metal ions was studied in order to have a conclusive in-vivo data for variation of metal ion concentrations with time (month) at normal oral temperature 37°C, which affects the saliva quality and quantity, pH, chemical and physical characteristics of food and liquid. The superficial break down and release of metals from the alloy brackets were investigated by scanning electron microscopy (SEM) and energy dispersive X-Ray spectroscopy (EDS) images. The kinetic release experiment of the metal ion concentrations (Nickel, Chromium, Titanium, Iron, and copper) in the saliva uptakes follow a pseudo-second-order kinetic model, the release rate of metal ions was in series $Fe^{2+} > Ti^{2+} > Ni^{2+} > Cu^{2+} > Cr^{3+}$ and the highest saliva pH and flow rate were detected after one month for fixed orthodontics appliance was (7.16 ± 0.55) and (0.88 ± 0.55) respectively.

Triazole analogues as potential pharmacological agents

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Background: A large number of studies have recently reported that, because of their significant biological and pharmacological properties, heterocyclic compounds and their derivatives have attracted a strong interest in medicinal chemistry. The triazole nucleus is one of the most important heterocycles which has a feature of natural products as well as medicinal agents. Heterocyclic nitrogen is abundantly present in most medicinal compounds. The derivatization of triazole ring is based on the phenomenon of bio-isosteres in which substituted the oxygen atom of oxadiazole nucleus with nitrogen triazole analogue.

Main text: This study focuses on recent synthetic procedure of triazole moiety, which comprises of various pharmacological activities such as antimicrobial, anticonvulsant, anti-inflammatory, analgesic, antitubercular, anthelmintic, antioxidant, antimalarial, antiviral, etc.

Conclusion: The study highlights the current status of triazole compounds as different multi-target pharmacological activities. From the literature survey, triazole is the most widely used compound in different potential activities.

A systemic research based study on a survey of customer's choice of toothpaste in the Rajasthan population

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Objective: The customer's choice of toothpaste may seem a light topic to be discussed but sheds light on the knowledge of dental hygiene among the customers of various ages, ethnicity, geographical locations and brands. This survey discusses the factors that influence the customer's choice as well as the most common brand preferred among various age groups and also what the customers desire in their toothpastes.

Methods: A survey was conducted among 300 people from different parts of India. The questionnaire used was kept consistent and covered various aspects from dental hygiene to toothpaste preferences to help with further studies of toothpaste qualities to generate customer satisfaction.

Results: Various pie charts give information regarding the questions answered by the people, and further evaluation and studies on them have been done to give detailed results.

Conclusion: This information can help understand the type of oral hygiene methods that patients feel comfortable to approach and use. It can also help to understand the knowledge level of patients regarding dental hygiene and thus make products with appropriate features to make it more approachable to the customers.

Geotechnical characterization of red mud waste material for road construction

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Red mud waste material is a by-product generated during the extraction of alumina from bauxite ore by Bayer process. Million tons of red mud is being produced/piled near by the producing industry in India which is increasing day by day and causing serious issue related to proper disposal as it has very limited application. Accordingly, study on red mud was carried out to explore the possible application in road construction. Physical/chemical characterization was carried out to examine the morphology and chemical constituents. Toxicity characteristics leaching procedure (TCLP) test was also carried out to know the hazardous nature of the material. Stress-strain behavior was analyzed and compared with other similar materials along with other geotechnical characteristics. To study the stress- settlement behavior, laboratory physical small scale plate load test was carried out simulated with traffic loading and the same was validated by numerical finite element method. It was observed that red mud has lattice and impervious microstructure of silt and clay size fine particles. It mainly contains manganese, chromium, vanadium, barium, lead, copper and zinc with traces of other elements. Concentration of heavy metals was within the permissible limit which indicated that it is a non-hazardous material. It has high values of dry density (21.28 kN/m^3), California Bearing Ratio (25%) and angle of internal friction (44°) compared to soil which makes it suitable for road construction. It was observed that its stress-strain behavior is similar to conventional materials (soil). Modulus value indicates that it is a stiff material which leads to less settlement as an embankment fill constructed at maximum dry density and optimum moisture content.

Adsorption and equilibrium studies of methyl orange on tamarind shell activated carbon and their characterization

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Biomass-derived carbon with high surface area and tunable pore structures are attracted due to their applications in several fields. A facile one-step approach for preparing activated porous carbon from tamarind shells and ammonium chloride is presented here. The activated carbon from the tamarind shell (ACTS) was characterized using FTIR, TGA/DTA, and SEM to understand the functionalities present in the material's surface, stability, and surface morphology. The ACTS material was employed as an adsorbent to remove synthetic dyes and a potential applicant in removing organic compounds from industrial wastewater. The effect of dosage with the concentration of dye materials is studied using Langmuir and Freundlich isotherm models. The Langmuir model showed a better fit with a maximum adsorption capacity of 24.3 $g.L^{-1}$.

Electromechanical bandgaps in piezo-embedded mechanical metamaterials

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Elastic mechanical metamaterials are the exemplar of periodic structures. These are artificially designed structures having idiosyncratic physical properties like negative mass and negative Young's modulus in specific frequency ranges. This unusual dynamic behavior is frequency contingent, which modulates wave propagation through these structures. Locally resonant units in the designed metamaterial facilitate bandgap formation virtually at any frequency for wavelengths much higher than the lattice length of a unit. Here, we analyze the band structure of piezo-embedded negative mass metamaterial using the generalized Bloch theorem. The addition of the piezoelectric material at the resonating unit increases the complexity of the solution. The results elucidate, the insertion of the piezoelectric material in the resonating unit provides better tunability in the band structure for simultaneous energy harvesting and vibration attenuation. Non-dimensional analysis of the system gives physical parameters that govern the formation of mechanical and electromechanical bandgaps. Thus, broader bandgap generation enhances vibration attenuation, and energy harvesting can be simultaneously available, making these structures multifunctional.

Hybrid organic-inorganic perovskite-based electronic devices

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The success of the organic-inorganic hybrid perovskite materials for the solar cell since 2009 has also extended to other applications such as memory devices, ultrafast switches and light - emitting diodes (LED), field-effect transistors, lasers, detectors, etc. Herein, we leverage the unwelcome ion-migration in perovskites to unlock new opportunities for resistive switching using layered Ruddlesdsen-Popper perovskites (RPP) and explicate the underlying mechanisms. The ON/OFF ratio of RPP-based devices is strongly dependent on the layers and peaks at $n^{-}=5$; demonstrating the highest ON/OFF ratio and minimal operation voltage. Long data retention even in 60% relative humidity and stable write/erase capabilities exemplify their potential for memory applications. Impedance spectroscopy reveals a chemical reaction between migrating ions and the external contacts to modify the charge transfer barrier at the interface to control the resistive states. Our findings explore a new family of facile materials and the necessity of ionic population, migration and their reactivity with external contacts in devices for switching and memory applications. In parallel, we unravel the potential of the D_2O as a solvent additive to enhance the PCE ~ 21% in triple cation based perovskite solar cells with stronger stability. Ultrafast optical spectroscopy confirms trap states passivation increased carrier recombination lifetimes and enhanced charge carrier diffusion lengths in our deuterated samples. Fourier transform infrared spectroscopy and solid-state nuclear magnetic resonance (NMR) spectroscopy validates $N\text{-}H_2$ group as the preferential isotope exchange site. Furthermore, first-principles density functional theory calculations reveal a decrease in PbI6 phonon frequencies in the deuterated perovskite lattice. This stabilizes the PbI6 structures and weakens the electron-phonon coupling, yielding higher electron mobility. Importantly, these findings prove that selective isotope exchange opens new opportunities for tuning perovskite optoelectronic properties.

Image encryption using microcontroller

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The encryption of RGB color image using microcontroller ATMEGA 32 is studied in the present paper via synchronization with one-dimensional chaotic map. Two microcontrollers are used to execute encryption and decryption algorithms under synchronized condition to demonstrate the cryptosystem. Both the microcontrollers run the dimensional logistic map and they become synchronized through open plus closed loop (OPCL) coupling. Under synchronized condition, the stored data of the input image in one microcontroller is encrypted with its generated chaotic sequences and transmitted to the remaining microcontroller, known as the receiver. The receiver microcontroller decrypts the encrypted data and stores in its memory. After decryption of the full image data it is forwarded to LCD display to visualize the decrypted image. The strength of security of the algorithm is analyzed by a number of cryptanalysis techniques like, correlation coefficient, histogram analysis, information entropy, NPCR, UACI, MAE, etc. should give clear indication of the objectives, scope, results, methods used, and conclusion of your work.

Experimental studies on coir geotextile reinforced low volume rural roads

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This paper proposes the practical implementation of improvement of weak subgrade soil by using coir geotextile. The test track is subjected to various tests to study the improvement in structural behaviour of the reinforced pavement. The total length of the road was divided into three sections.

This was done to analyse the performance of coir reinforced pavements with sections of different thickness and types of coir geotextiles. Coir geotextiles with mass density 740 gsm (designated as CGT1) and 365 gsm (designated as CGT2) of widths 6 m and 8 m were used. The study explores the improvement in elastic modulus that could be attained by the subgrade reinforced with coir geotextiles through field experiments like geogauge and static plate load tests. The culmination of this work is the preparation of design guidelines for coir geotextile reinforced low volume roads. Hence baseline design inputs that are obtained from the above mentioned tests were used for the numerical analysis using KENPAVE software. The data reveal that the elastic modulus of the subgrade has multiplied appreciably when reinforced with coir geotextile, which would help in increasing the service life of the pavement. The same has been reflected in the distress survey results also. The improvement attained is 1.41 and 1.25 times of the elastic modulus of the parent soil, with coir geotextile of mass per unit are 740gsm and 365gsm, respectively. The modified subgrade elastic modulus has been inputted in the KENPAVE software and analysed in order to prepare a design chart for coir geotextile reinforced low volume roads.

Electrophoretic study to detect the biomolecules using graphene-based field effect transistor

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Graphene based sensor devices have been investigated significantly and results of different chemicals decorated on a graphene sheet were identified by the transfer characteristics. The GFET based device was fabricated by the mechanical exfoliation method with an inbuilt reference electrode acting as an electrolyte gate electrode. Devices show good transfer characteristics, which depend on the surface morphology of the material and substrate. During fabrication of the device, the substrate morphology was disturbed in appropriately by the contamination of the surface. In the present study, monolayer Graphene Field Effect Transistor (GFET) was driven with hydrophobic Hexamethyl Disilazane (HMDS) layer. Fabrication of GFET device on the hydrophobic substrate enhances the effective ambipolar behaviour. The fabricated devices were used for direct adsorption of single- and double-stranded DNA. Detection of disease-related gene expression by DNA hybridization is one of the useful diagnostic methods. In this study a monolayer graphene field effect transistor (GFET) was used for the detection of a particular single-stranded DNA (target DNA). The VDirac was shifted to the negative direction in the probe DNA immobilization. In recent cases of cancer therapy, such as DNA based therapies, messenger RNA (mRNA) is also used as alternatives. mRNA has a good capability to classify cancer subtypes. The device can support mRNA detection and provides the best platform for cancer detection. Furthermore, the monolayer GFET is driven by an inbuilt top-gate for detecting the pH of the contacting buffer solution. The fabricated devices are also used to detect the protein samples decorated on the channel surface. Detection of protein is the most important diagnostic method for immune regulation and metabolism. The GFET device detects the effect of hydroxide ions on a graphene surface. The sensitivity of the device was estimated the device performance. Fabrication of this kind of compact GFET device with inbuilt gate enables low-cost, real-time sensitive amperometric sensors, which enhances the effective sensing and user-friendly in the platform of biosensing applications.

Biomaterial material based devices for controlled release of agrochemicals

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Explosion in population is a big threat. This has resulted in food scarcity. Rain deficiency has caused soil desertification. Smart materials based controlled release devices can solve the problem of desertification. Such materials can be used effectively for the sustained and controlled release of agrochemicals and can provide alternative to traditional chemical fertilizer treatment due to their ability to release the agrochemicals under controlled conditions. These materials can also conserve the moisture in the soil for a long period. They are of great importance in reducing the underground water pollution as well as soil pollution. Thus, such materials are of great importance from Farmer's economy point of view and provide a better way to solve problems related with agricultural issues. The present work includes the fabrication of polymeric materials of natural origin for their applications in agricultural sectors.

Synthesis and characterization of shear thickening fluids for soft armours applications

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Body armour for the military has traditionally been designed to provide protection against fragmentation and ballistic threats. Armours have traditionally been protected based on steel which gives rise to extremely heavy structure and weight, provides logistical problems and discomforts due to transport to a battle site. Soft Armour is a ballistic protection technology that provides security for people in vulnerable environments. Presently, high performance fibres have been used to make soft ballistic body armors for the realization of lightweight, flexibility and comfort. But inclusion of these fibers has resulted in significant improvements in the cost of body amours. The Shear thickening fluid (STF) has attracted attention for impact protection due to its unique properties subject to impact. STF is a non-Newtonian fluid and shear thickening behaviour is triggered by a sudden increase of shear rate to the STF, which causes colloidal dispersions to concentrated exhibiting an abrupt increase in viscosity. In this perspective, the present research work is focused on the preparation and characterization of a novel shear thickening nanocomposite fluid to improve the stab resistance and to resist the penetration of bullets in soft wearable armours. The present work endeavours towards the development and characterization of ZnO nanoparticle dispersed shear thickening fluid. The shape and size dependency of the nanoparticles on the shear stress behaviour of shear thickening fluid (STF) was studied. The optimized composite STF was coated on polypropylene (PP) woven fabric and further characterized for its stab and ballistic impact resistance.

Graphene-silver nanoparticles loaded cement based material improves the mechanical, antimicrobial properties

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Modern architecture was based upon new and innovative technologies of construction, particularly the use of glass, steel and reinforced concrete. Modern infrastructure requires structural components with higher mechanical strength and greater durability. Now a day's researcher in concrete technology working on innovative composite material incorporation with nanomaterials to improve cement-based materials mechanical properties. Some such nanomaterials include nano-silica (nano-SiO_2), nano-alumina (nano-Al_2O_3), nano-ferric oxide (nano-Fe_2O_3), nano-titanium oxide (nano-TiO_2), carbon nanotubes (CNTs), graphene and graphene oxide despite the many available studies on the evaluation of the influence of nanomaterials on the properties of cement-based composites, the effects of some nanoparticles have not yet been fully recognized. Among the unrecognized nanomaterials is graphene-silver nanocomposite. The literature devoted to this subject is limited. This paper reviews state-of-the-art research carried out on the effect of graphene-silver nanocomposite on the properties of cement-based composites. Detailed descriptions of the processing, microstructures (hydration products), properties (hydration, workability, mechanical and functional properties, and durability). Foremost new property we found in this material, which enable the antimicrobial activity in cement based composite material.

Vibration based micro-scale piezoelectric energy harvesting system

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The growth in the field of VLSI has given a new range of portable electronic gadgets to mankind and connected the whole world with communication devices. The success of portable electronics devices is based on energy needs and power consumption. The energy need is accomplished with the batteries. The advancement in fabrication industry is doubling the number of transistors in every 18 months, while the energy density of batteries is comparatively flat during an equivalent period. Moreover, batteries contain heavy metals that are toxic and hazardous.

The alternative to traditional batteries is to make use of the parasitic mechanical vibration energy available locally in the atmosphere. Industrial devices, cars, structures, and human movement release mechanical vibrations which could be excellent sources for collecting small amounts of power without impacting the source itself. The use of piezoelectric, electromagnetic and electrostatic transducers can convert mechanical vibration energy into electrical energy. Piezoelectric transducers offer more viable option because of their high energy density. Important factors governing the performance of piezoelectric energy harvester are choice of material, volume, shape, resonance frequency and output power.

The objective of this research work is to design a piezoelectric energy harvesting system with a wide bandwidth and a current amplification energy harvesting circuitry which would be capable enough to autonomously power micro-scale devices throughout their lifetime. Through the simulative analysis it has been concluded that the stress generated on a cantilever is more than any other mechanical structures. A bimorph cantilever harvester is constructed with silicon substrate and zinc oxide as piezoelectric material. Volume of the bimorph is 341.4mm^3 which is significantly less than micro-scale maximum volume of 1000mm^3. The studies concluded to have a thin film and a longer device which could provide higher power and better matching of resonance frequency with ambient vibration sources. The output power of 0.5mW across a 4MΩ resistor produced by the bimorph piezoelectric cantilver energy harvester at around 90Hz resonance frequency.

A novel piezoelectric energy harvester has been proposed in this work based on a conventional seesaw mechanism. See-saw harvester is linear in design compared to other broadband energy harvester which have nonlinearity in structures with magnets, stoppers introduced. The displacement, charge and voltage sensitivity of the proposed harvester is improved by 76%, 12% and 8% respectively. The bandwidth of the proposed structure is also large as compared to the conventional design. The proposed design has a better sensitivity bandwidth product per unit volume of 33.23%, 10.20% and 22.70%, in terms of displacement, charge and voltage respectively.

UWB MIMO Antennas

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The overlapping of narrowband communication systems with the UWB spectrum makes radio signals interfere. Therefore, the proposed antenna is designed with triple-band rejection capability. The antenna consists of four feedlines and a common ground surface which acts as the main radiator. The four elements of the antenna are kept orthogonally to exploit polarisation diversity, resulting in high isolation. The presented antenna is having size=44×44 mm^2 and printed on FR4 substrate. A spiral slot was introduced in the ground surface which behaves similarly as a band-stop filter (BSF) and rejects the X-band for Uplink Satellite Communication. For rejecting WiMAX and WLAN band, the modified trident shape of the microstrip line is used. Also, Defected Ground Structure (DGS) is used for the isolation (>23 dB) enhancement. The proposed antenna is used for small handheld communication devices.

A planar Ultra-Wideband (UWB) wearable Multiple Input Multiple Output (MIMO) antenna is designed for on-arm wearable Wireless Body Area Network (WBAN) applications. This antenna is designed on a 100% cotton cloth substrate. The two-port MIMO antenna has a dual spinning wheel shape like radiators with the partial ground and microstrip feedings. The two partial grounds are connected to a rectangular strip to have common ground. The complete surface area of the antenna is 40 × 70 mm^2. In comparison with recently published papers in the same research area, the bending and SAR analysis are also done to estimate the performance of this wearable antenna, which is the novelty of this research work. For entire UWB bandwidth, S–parameters, gain, efficiency, and diversity parameters (Channel Capacity Loss (CCL) and Envelope Correlation Coefficient (ECC)) and far-field simulations are done for all cases such as flat, bend, on body antenna, which demonstrates the appropriateness of the presented antenna to be operated to the human arm.

Investigation on corrosion properties of bright Zn-Ni alloy coated mild steel

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Electrodeposition is a renowned surface-modification method to get better surface characteristics, both functional and decorative properties of a broad diversity of materials. Recently, zinc and its alloy coatings are finding several applications, as a sacrificial metallic coating for the protection of mild steel. Zn-Ni alloy coating is the most commonly exploited in commercial applications and it exhibits significantly higher corrosion resistance ability and superior surface morphology than pure zinc. It is used as a replacement for toxic and expensive cadmium coatings. Literature survey revealed that zinc-nickel alloy coating without brightener is dull, unattractive and uneven and has comparatively less corrosion resistance ability. Hence, brighteners are gaining significance. They are found to adsorb on cathode surface (Mild Steel) and thereby modify the surface characteristics of the coating. Adsorption of brightener affects the nature of coating resulting in refined coating, which in turn alters the surface properties especially corrosion resistance of steel.

A new brightener CG was synthesized by condensation of Cysteine Hydrochloride and Glutaraldehyde. Electrodeposition of Zn-Ni alloy from Sulphate bath was done in presence of CG. Corrosion studies were carried out using Electrochemical Impedance spectroscopy and Potentiostatic techniques. Surface morphology was studied using SEM, Reflectance spectroscopy and X-Ray Diffraction.

Brightener CG was successful in giving bright zinc-nickel alloy deposits. Corrosion techniques confirmed increase in corrosion resistance and protection ability of bright zinc-nickel coatings. Surface studies revealed enhancement of fine grained nature of zinc-nickel alloy crystallites. XRD studies depicted the presence of η and γ- phases of pure zinc and zinc-nickel alloy respectively in the deposits. CG is accountable for increasing the corrosion resistance ability of bright zinc-nickel depositsince refined grain structure is closely associated with corrosion resistance property. It changes the orientation of Zn-Ni alloy crystallites which is accountable for brightness. CG can act as an efficient brightener and can be commercially used.

Aluminum metal–organic framework nodes support single-site nickel (II)-hydride catalyst for chemoselective hydrogenation of nitro and nitrile compounds

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The development of chemoselective and heterogeneous earth-abundant metal catalysts is essential for environment-friendly chemical synthesis. We report a highly efficient, chemoselective and reusable single-site nickel(II) hydride catalyst based on a robust and porous aluminum metal-organic frameworks (DUT-5) for hydrogenation of nitro and nitrile compounds to the corresponding amines under mild conditions. The nickel hydride catalyst was prepared by the metalation of aluminum hydroxide secondary building units (SBUs) of DUT-5 having the formula of $Al(\mu_2\text{-}OH)(bpdc)$ (bpdc = 4,4′-biphenyldicarboxylate) with $NiBr_2$ followed by the reaction with $NaEt_3BH$. DUT-5-NiH has a broad substrate scope with excellent functional group tolerance in the hydrogenation of aromatic and aliphatic nitro and nitrile compounds under 1 bar H_2 and could be recycled and reused at least 10 times. By changing the reaction conditions of the hydrogenation of nitriles, symmetric or unsymmetric secondary amines were also afforded selectively. The experimental and computational studies suggested reversible nitrile coordination to nickel followed by 1,2-insertion of the coordinated nitrile into nickel-hydride bond occurring in the turnover limiting step. The zeroth-order dependence of the reaction rate on the pressure of H_2 allowed progressing all the reactions under ambient hydrogen pressure. This work highlights the potential of MOF-based single-site earth-abundant metal catalysts for practical and eco-friendly chemical feedstocks production due to their low cost, excellent stability and reactivity, and the usage of cheap and atom-economical reductant hydrogen.

Impact of surface functionalization on GaN/ZnO nanostructure based hetero-interfaced UV photodetectors

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The pandemic COVID-19 is causing significant economic, healthcare and social disruption world-wide. The protective vitamin-D synthesis by the Ultraviolet-B (UVB) radiation in human beings found to be major break-through for the betterment of mankind. Therefore, it is inspiring to emphasis on utilization of UVB and fabricates energy efficient and durable ultraviolet-photodetectors (UV-PDs). Henceforth, the presented study showcased the fabrication of unique tapper ended GaN-Nanotowers (GaN-NTs) based highly efficient UV-PDs. Thereby, hexagonal stacked GaN nanocolumnar structure (nanotowers) exhibits higher photocurrent generation which significantly enhances its responsiveness towards UV and leads to outstanding performance of the device. The fabricated detector display low dark current (~ 12nA), high ILight/IDark ratio (> 104), fast time-correlated transient response (~ 433μs). A very high photo responsivity (R) of 2.47 A/W in self-powered (zero applied bias) mode of operation is reported. While in photoconductive mode, the R is observed to be 35.4 A/W@-3V along with very high external quantum efficiency (EQE) is ~ 104%, lower noise equivalent power (NEP) ~ 10-13 WHz-1/2 and excellent UV-Vis selectivity. Besides this, the role of increased thickness of AlN-buffer layer and GaN-NTs height is also realized in terms of enhanced performance PDs. This variation in device geometry leads to augmented R, low NEP, and a high EQE of 88.6 to 484.77 A/W@-3V to -6V, 1.76 × 10−13 W.Hz 1/2, and 1.85 × 105 %, respectively. Moreover, for further improvisation, a hybrid interface of ZnO/GaN with unique geometry of nanostructure over nanostructure is also explored. These ZnO-NRs hybridized GaN-NTs based UV-PDs demonstrated enhancement in R value from 477 A/W to 1204 A/W@-6V. Furthermore, an impact of sensitization of chemically synthesized novel GQDs on a ZnO-NRs/GaN-NTs heterostructure-based UV-PDs is also realized. The fabricated device demonstrates an excellent R of 3200 A/W at −6 V and displays an enhancement of ~671% and ~ 265% compared to its bare counterpart (GaN : 477 A/W and ZnO/GaN: 1204 A/W). In addition, the fabricated heterostructure UV-PD exhibits a very high EQE of 1.2 × 106%, better switching speed, and signal detection capability as low as ~ 50 fW.

Estimation of service life of polymer composite in nuclear environment for shielding application

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When one puts a product into service, the ability to predict its lifetime or failure rate would be highly beneficial. The composite part should be tested in real time and in environments similar to those in which the part will be exposed.

For applications, such as space applications, in radiation environment, it is expected to have about 20 to 30 years durability. In case of polymer composites, the reactive intermediates like free radicals present in the polymers are capable of initiating chemical reactions resulting in scission and cross-linking on irradiation. It may result in failure of material under application. The decomposition study has been carried out to predict the stability of developed materials under ionizing radiation conditions.

The lifetime estimated for all developed material is found around 20 to 45 years at 50°C which is desired for a device under a nuclear environment.

Accurate predictions are highly dependent on the testing methodology, the type and form of the composite used, and the processing history.

Here we have discussed a thermal decomposition method to predict the life span of polymers.

Synthesis and utilization of bio-waste derived activated carbon for enhancement of tribological properties

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Critical climate change and environmental pollution not only demand the use of biodegradable material, but also the utilization of biowaste to convert them into value-added products. Bio-waste materials being natural materials are available in huge stock and are landfill materials. Dumping these bio wastes material in an open environment, provide a safe passage for bacteria growth, which in turn leads to bacterial disease. However, these waste materials could be of economic value when used in a sensible manner. The two such bio wastes eggshell and coconut shell were utilized. There two-fold application, one such application is using eggshell to convert into nanoparticles and other is two use these two in combination two produce activated carbon, which would further be utilized in the composite fabrication. In the present work the eggshell and coconut shell, synthesized activated carbon was utilized for fabrication of activated carbon epoxy composite. The attributes of activated carbon are identified through different characterization techniques (TEM, XRD, FTIR),

The composites were studied for their hardness, moisture absorption and erosion wear behaviour at variable impingement angles (30°, 45°, 60°, and 90°) and impingement velocities (101 m/s, 119 m/s, and 148 m/s). It was observed that addition of activated carbon particles has enhanced hardness and wear resistance of the composite. Composite with 2 wt% particulate reinforcement was found to be the optimum percentage of reinforcement which was subjected to 82.4% less material loss i.e., erosion rate at 45° impact angle compared to neat polymer. It may be concluded from observation of results that, the present work is indicative of potential application in automobile body parts, pipelines carrying solid particulate matter etc.

Magnetic nanoparticles on drug delivery applications

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Nanotechnology, as a promising technique, has succeeded in overcoming a wide variety of technological impasses in unprecedented ways. Surprisingly, the convergence of nanotechnology and biology has provided a powerful impetus for research in a new area known as nanobiotechnology. In order to realize the potential of nanobiotechnology in the form of different functional agents for biomedical applications, nanoscale particles have been considered a significant class of biomaterials. The perfect concept of simultaneous therapeutic and diagnostic applications have been made feasible on a single so-called "theragnostic" agent by using the special properties of nanoparticles. Magnetic nanoparticles (MNPs) have drawn a lot of interest as a possible theragnostic device.

Magnetic nanoparticles have been used as contrast agents in MRI, gene transfection, gene consignment, and to bind cytotoxic drugs for selective drug delivery for the past few years. The magneto-structural properties of the magnetic particle are critical for biotechnological applications. Because of the nanoscale size, the nanoparticle can quickly pass through thin veins and enter the cellular membrane. The particle's ferromagnetic and superparamagnetic properties allow it to be tampered by an external magnetic field and directed to the defined goal. The modified superparamagnetic nanoparticles' surface has hydrophilic functionalized groups that help with drug binding and biocompatibility. The poor retentivity of superparamagnetic nanoparticles when the applied external magnetic field is eliminated is a significant aspect. Furthermore, nanoparticles' capacity to monitor their size ranging from a few nanometres to hundreds of nanometres enables them to be similar to a biological organism of interest. Due to their peculiar properties of being biodegradable and biocompatible, superparamagnetic iron oxide nanoparticles (SPION) have gotten a lot of attention as scaffolds for constructing theragnostic agents.

The present study discusses on the potential application of solvothermal synthesized magnetic nanoparticles for stimuli based drug delivery.

Variation in magnetic properties of CRNO AISI M-43 grade electrical steel post laser and TIG welding

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A cold rolled non-oriented (CRNO) electrical steel of M-43 grade is widely used in medium capacity rotating electrical systems and domestic appliances are investigated for observing the variation in magnetic property and losses, post TIG and laser welding. The investigation is made on the toroidal core samples welded on 6 sides around the outer periphery using TIG and laser welding. The welded toroidal core samples are observed for estimating the variation in magnetic properties and power loss density at different ranges of magnetic flux density. Additionally, the grain size analysis and micro-hardness testing of the weld samples is performed. Significant increase in losses is observed for TIG welded M-43 grade samples. The microstructural investigation also revealed the existence of relatively coarse grains in the weld region of TIG welded samples as compared to the laser welded samples. The maximum increase in hardness of around 62.3 HV as compared to the base metal is observed for the TIG welded samples. The B-H curve obtained for M-43 grade TIG welded, laser welded and non-welded samples. The hysteresis losses are found to be increasing as a result of internal stresses generated due to the welding process. It is evident that the laser welded samples revealed much controlled grain size variation as compared to TIG welded.The etched samples are observed under Scanning electron microscope (SEM), the laser welded sample with polygonal shaped ferritic grains. The maximum grain size of 52.1 μm is at the base metal (BM) region. However, coarse sized grains of maximum size 120.8 μm is at Heat Affected Zone (HAZ) region and 187.5 μm in the Fusion Zone (FZ) for TIG. The grain size measurements are performed using the Image J software.

Designing high efficiency materials for energy generation and storage

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Designing new materials with high efficiencies based on earth abundant nontoxic materials for renewable energy technologies is key to mitigate the climate change and develop prosperous sustainable society. With this idea in mind we are designing new materials useful for hydrogen economy, Li and Na ion battery cathodes, photovoltaic and thermoelectric applications using state-of-the-art density functional methods.

Li-rich materials with simultaneous anionic and cationic reduction is one among the most promising class of cathode materials for high-capacity Li-ion batteries. The recent studies on the Li-rich Li_5FeO_4 with defect antifluorite-type structure show that Li_5FeO_4 can enable high capacity by simultaneous reduction of Fe and oxygen atom without any obvious release of oxygen gas. In the present study we have substituted Fe site with Ti in different concentrations ($Li_5Ti_xFe_{1-x}O_4$ with x = 0.125, 0.250, 0.375, 0.500, 0.625, 0.750, 1.00) and investigated the structural, electronic and Li-diffusion properties using density functional theory calculations. The polyanionic compound Na_2MnSiO_4 is regarded as one of the promising cathode materials for Na-ion batteries due to good specific capacity along with its attractive prospect of utilization of two electrons in the redox processes. So, in this study we have performed the thermodynnamic and electronic structure analysis of Na_2MnSiO_4 using first principles density functional theory calculations. The intermediate ground state configurations for Na_2MnSiO_4 during Na de-intercalation were found using the cluster expansion method and are used to obtain the 0 K voltage profile as a function of Na concentration. This material shows an average voltage of 4.2 V and the finite temperature analysis at 300 K using Monte Carlo simulations indicates that this material undergo two phase mixing when desodiate beyond 1.5 Na/f.u. The involvement of oxygen in the redox reaction apart from the transition metal is identified using the Bader charge analysis. Relevant Na diffusion pathways and their corresponding calculated energy barriers are compared with the partially Fe substituted Na_2MnSiO_4 to understand the effect of Mn-site substitution on the process of Na migration through this material

Compared with the remarkable achievement of using perovskites in photovoltaic applications, the role of antiperovskites in solar cells has not been adequately identified and reported. So we have predicted the crystal structures of the antiperovskites Be_3PN, Mg_3PN, Ca_3PN, Sr_3PN, Ba_3PN and Zn_3PN using structural optimization with stress as well as force minimization by considering 32 potential structural variants into the calculation. We found that all these compounds are having direct bandgap behavior with low carrier effective mass, high optical absorption, well separated electron-hole pair etc. Due to the iso-structural as well as isoelectronic nature of these materials with tunable bandgap value apart from the above mentioned other advantageous optoelectronic properties suggest that these materials are suitable for higher efficiency tandem solar cell applications.

Multinary aliovalent substituted semiconducting half Heusler alloys are expected to have low thermal conductivity due to increase in the phonon scattering centers and thus it is expected to increase the thermoelectric figure of merit. So we have studied electronic structure, lattice dynamics, and thermoelectric (TE) transport properties of a new family of pentanary substituted TiNiSn systems using the 18 valence electron count (VEC) rule. The substitution of atoms with different mass creates more phonon scattering centers and hence lower the lattice thermal conductivity. The calculated lattice thermal conductivity for Hf containing systems $La_{0.25}Hf_{0.5}V_{0.25}NiSn$ and non Hf containing system $La_{0.25}Hf_{0.5}V_{0.25}NiSn$ are found to be 0.2 and 0.36 W/m-K, respectively and they can attain maximum ZT value of 0.78 at 500 K and 0.76 at 450 K, respectively. Based on the calculated results we conclude that one can design high efficiency thermoelectric materials by considering 18 VEC rule with aliovalent substitution.

In order to identify potential materials for hydrogen storage application worldwide attention has been focused on hydrides with high gravimetric and volumetric capacity to have sustainable energy system. If one can find hydrogen storage materials where hydrogen is present in both negative and positive oxidation state within the same structural frame work then one can accommodate hydrogen with high volume density because of the attractive interaction between oppositely charged hydrogen. So, it is fundamentally as well as technologically important to identify compounds in which hydrogen is in amphoteric nature and understand the necessary criteria for its origin. We have identified several hydrogen storage materials with hydrogen in amphoteric state using van der Waals interactions corrected density functional calculations and explain such behaviour.

Device design optimization of highly efficient perovskite solar cell

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In order to provide experimental guidance, a theoretical study was performed on transparent conduction oxide (FTO)/TiO_2/ interface defect layer 1/$CH_3NH_3SnI_3$/interface defect layer 2/Cu_2O/ back contact solar cell. The simulation was performed under the illumination of 1000 W/m^2, at 300 K and an air mass of AM 1.5G. The diffusion lengths of electron and hole were set to 260 nm and 560 nm in absorber layer, respectively. The set value is very near to recently observed experimental values. The device performance is severely influenced by the thickness of absorber layer, acceptor density, defect density and work function of various back contact electrode materials. Oxidation of Sn^{2+} into Sn^{4+} was considered and it is found that the reduction of acceptor concentration of absorber layer significantly improves the device performance. Further, optimizing the defect density (1014 cm^{-3}) of the perovskite absorber layer, encouraging results of the Jsc of 40.14 mA/cm^2, Voc of 0.93 V, FF of 75.78% and PCE of 28.39% were achieved. This theoretical simulation provides an appropriate direction for devolving photovoltaic technology.

Phytofabrication of silver and cupric oxide nanoparticles using Simarouba glauca and Celastrus paniculatus extracts and their enhanced apoptotic inducing and anticancer effects

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Objectives and scope: Silver (AgNPs) and Cupric oxide nanoparticles (CuONPs) were phytofabricated utilizing leaf extract of Simarouba glauca (SG) and aerial extract of Celastrus paniculatus (CP) to evaluate anticancer effect and also to verify the apoptosis, cell cycle analysis.

Methods used: Free radical scavenging assays like DPPH, ABTS and NO; MTT assay, flow cytometry and caspase-3; EAC model with biochemical and haematological parameters.

Results and discussions: Characterization was validated using FTIR, SEM-EDX, TEM, XRD and UV-Vis analysis. The green synthesized AgNPs and CuONPs showed potent antioxidant potential with IC50 value of about 34.01+0.64 µg/mL contrasted to ascorbic acid. The anticancer activities on cancerous cell lines like MCF-7 and HT-29 cell lines revealed that AgNPs and CuONPs synthesized using S. glauca and C. paniculatus indicated IC50 values ranging from 70.85+0.67 to 240.6+0.57 µg/mL. They could not effectively prohibit the growth of immortalized normal human breast epithelial cell lines (MCF-10A). To be more precise for anticancerous effect, molecular mechanism was examined in MCF-7 cell line treated with CuO-CP NPs by cell cycle analysis that depicted 75.28 % of cell arrest in Sub G0/G1 phase and 71.29 % of cells were gated in late apoptotic phase of Annexin V and propidium iodide (PI) compared to control cells. The cytotoxicity induced by apoptosis was further confirmed by fluorescent images. The synthesized nanoparticles also demonstrated less hemolysis efficiency and are evidenced by SEM images. We have also evaluated the *in vivo* antitumor efficacy of CuO-CP NPs treated against Ehrlich ascites carcinoma (EAC) bearing C57 mice for the first time and examined by variations in growth parameters, biochemical assays (like lactoperoxidase, reduced glutathione and myeloperoxidase), hematological profile, and histopathological analysis in comparison with control.

Conclusion: The green synthesized nanoparticles exhibited effective control of cancer cells in both *in vitro* and *in vivo* laboratory conditions and thus can be evaluated for lead compound and scale up for industrial usage.

Air-stable and high mobility based electron transport semiconducting material hexachloro- hexa-azatrinaphthylene

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In the last few years, organic semiconductors (OSCs) have attracted a considerable amount of attention due to their wide potential applications in various electronic devices such as organic field-effect transistors (OFETs), organic photovoltaic devices (OPVs), organic light-emitting diodes (OLEDs), and organic solar cells (OSCs). Unlike their inorganic counterparts, organic semiconducting materials are cost-effective, lightweight, and flexible and provide the versatility of chemical synthesis. However, one of the major challenges for the development and fabrications of organic semiconductors for industrial applications is their air instabilities. From the theoretical point of view, the air-stability of the organic semiconducting material depends upon its low-lying frontier molecular orbitals and the energy gap in between them. A new n-type organic semiconductor based on the haxachloro-hexaaza-trinaphthylene compound is reported. The electronic structure and charge transport properties of the compound is calculated in the framework of density functional theory (DFT). The electron- withdrawing group (-Cl) on the end position of the compound could help to lower the LUMO energy level and improve the air-stability and charge carrier mobility. The large electron affinity (2.60 eV) and low LUMO energy (-3.63 eV) suggests that the compounds were to be air-stable and N-type organic semiconductor. Moreover, lower values of the electron- injection barrier as compared to those of the hole-injection barrier implied that the investigated compounds were basically N-type semiconductors. The computed electronic coupling of LUMO of the compound was found to be comparatively larger in the transverse- channel (86.6 meV) than other channels. The computed large electron and hole mobility was found to be 3.54 $cm^2V^{-1}s^{-1}$ and 0.014 $cm^2V^{-1}s^{-1}$. Further, Hirshfeld analysis depicting the distribution of surface charge in between the molecular layers of the crystals revealed that the principal interactions were mostly due to the Cl...H/H...Cl and Cl...Cl contacts of the compounds.

Controlling non-equilibrium processes for fractal growth

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Fractal structures are commonly found in nature. This work demonstrates the growth of tin oxide (SnO_2) fractals on large-area glass substrate. Growth of fractals with fractal dimensions varying from 1.52 to 1.86 were successfully grown. The shape of fractals changed from rhombohedra to fern-like to sword-shaped fractals. The flux, temperature and pH of the solution is understood to play an influential role in the final shape of the fractals. The fractal structures have significant surface roughness and therefore have many adsorption sites. These sites are interconnected by the inherent nature of fractals and therefore may exhibit better charge transport properties. The experiments are underway to optimize the charge transport observed in fractals and investigate their gas sensing response. A better understanding of the growth of fractals may lead to better predictions of material failure in fields like lithium-ion batteries or in alloy formation. Better properties may also lead to applications in gas sensing, potential SERS-substrates, wound healing phenomenon, etc. Thus, growth of fractal structures and a control over their morphology is the fundamental step to be addressed. The present work is an effort in this direction.

A novel fabrication of superhydrophobic surfaces on aluminium substrate by picosecond pulsed laser

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Superhydrophobic surfaces have emerged because of their unique properties like corrosion resistance, self-cleaning, anti-icing and being anti-bacterial. A simplistic and highly effective ultra-fast laser technology was used to fabricate superhydrophobic surface on aluminum substrate. Compared to other laser systems, picosecond laser systems have smaller thermal affected area on the aluminum substrate. They also offer high efficiency, not as much of waste materials and cover enormous areas for mass production. Tilted groove patterns of various angles with respect to horizontal were textured on the substrate by using picosecond laser pulses. The laser parameters, such as hatching distance (HD) and scanning speed (SS), can be varied by keeping the laser power as constant for the various tilted angle of the groove pattern. The textured surfaces were initially super hydrophilic when kept in polyethylene zip lock cover and which also exhibits super hydrophobicity of maximum 155.5° when observed after 15 days. The morphology of surface was characterized by scanning electron microscope, EDX and X-ray diffraction.

Effect of Ar^+ ion implantation to enhance non-linear optical property on the L-Proline-doped Potassium hydrogen phthalate single crystals

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Single crystals of semiorganic potassium hydrogen phthalate crystals and L-Proline amino acid doped potassium hydrogen phthalate crystals were implemented with 10KeV Aa ions at various fluencies of 1 x 10^{15} 5 x 10^{15}, 1 x 10^{16} and 5 x 10^{6} ions / cm^2 to enhance their nonlinear optical property. The study reveals that Ar ion irradiation indicated the role of defects which could have influenced the non linear optical behavior.

Photoconductive laser spectroscopy and sub-bandgap defects in the metal-oxide semiconductors

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The emergence of high performance large-area electronic materials enabled the display technologies, which have transformed the way people interact with mobile devices such as smartphones and tablets. The most promising family of materials for this application are the metal-oxide semiconductors (MOS). Properties, which make MOS desirable, include their optical transparency, bandgap modulation, and high electron mobility. The journey from lab curiosity to market for MOS has taken place in a short time span, and current applications of the technology include flat panel displays, sensors, and logic devices. One of the chief problems of MOS is the tendency to form sub-bandgap defects, which can have a detrimental effect on device performance. Gaining an in-depth understanding of the behavior of these sub-bandgap defects will be key to unlocking better device performance or perhaps even discovering beneficial applications for sub-bandgap defects. We developed an alternative spectroscopic technique, the photoconductive laser spectroscopy that is able to identify distinct spectral signatures of sub-bandgap defects in MOS used in thinfilm transistors (TFTs). These sub-bandgap peaks are not normally visible in previously reported spectra measured by using available spectroscopic techniques. Negative bias illumination stress (NBIS) has a strong effect on the stability of the TFT performance. It is assumed that during NBIS, the deep neutral sub-bandgap defects in the MOS activated and modulate the threshold voltage of the TFT. I will talk about the photoconductive laser spectroscopy technique, which we developed, its sensitivity and effectiveness to identify and study, the modulation of sub-bandgap defects in the metal-oxide semiconductors.

Sensing film materials development for FET-based pH sensors

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Ion-Sensitive Field-Effect-Transistor (ISFET)-based chemical/biochemical sensors are used for measuring ion concentrations analyte solutions. Most commonly, they are used as pH sensors, where the current through the transistor changes with respect to the ion concentration at the sensing region (gate). ISFET is a solid-state device, which makes it rugged for the measurement of ion activities in analytes, with the aid of a reference electrode and it has been widely used for pH measurements. PH is one of the most important parameters in agricultural, environmental, bio-medical and potable water studies. ISFET has attracted much interest due to the feasibility of facile integration with readout circuits. It is an alternative to the conventional glass membrane electrode-based pH sensors, where it enables measurements in ultra-small volumes with fast response. This work deals with the design, modelling, fabrication and characterization of ISFET-based pH sensors.

The most critical element in ISFET-based pH sensors is the sensing film deposited over the gate region of the sensor. In this work, the sensing films are deposited using pulsed-DC magnetron-assisted reactive sputtering technique. Various process parameters for deposition of the film were optimized through several experiments. The deposition process for three sensing films were optimized, namely, AlN, Al_2O_3 and TiN, and their material characterization was carried out using various techniques. ISFET-based pH sensors were fabricated using well established, CMOS compatible unit processes. In this work, three variants of ISFET-based pH sensors have been fabricated with AlN, Al_2O_3 and TiN as the sensing films, using self-aligned process. The devices were encapsulated using the Dam-and-Fill technique and packaged using thick-film alumina technology. The sensors were characterized for pH sensing applications. Moreover, drift and hysteresis studies were performed for each sensor and low drift and hysteresis values were obtained for the fabricated ISFETs.

Maximum power point in a single step in solar photovoltaic panels

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Solar PV system arises as viable option in the critical power system era, its low efficiency energy conversion attribute necessitates an efficient power conversion system. The nonlinearity of I–V (current–voltage) characteristic and its alteration for an assorted insolation and temperature values may enable the alteration in terminal voltage. This may deviate maximum power point due to which the available maximum power delivery to load can be differed. Literature of this field reiterated that the uniform insolation and partial shading condition demands undeniable need of maximum power point tracking. Nonetheless through investigation in this direction furnishes the availability of a bunch of such techniques; each of them possesses its own pros and cons. This ubiquitous trait of available maximum power point tracking (MPPT) techniques unfolds the complexity in its precise selection. To diminish such complexity this article offers a novel idea in DC-DC converter hardware alteration instead of software (algorithm) to reach maximum point in a single step. A high precise capacitor with low electro static resistance is connected in parallel with a DC-DC converter (any type) with a single semi-conductor switch. This arrangement enables user to know the entire curve region with maximum operating point, thanks to highspeed microcontrollers. The converter is then in turn to operate accurately at that particular point, which removes the oscillation around MPP point. A hardware prototype of 1 kW lab scale setup has been developed and experimental results shows 18% improvement in MPP tracking capability (which generates 18% more energy than exist), which we see as a game changer for PV industry. The detailed circuit, and its economic analysis will be given in the full-length article.

Materials for non-conventional solar cells developing cost effective sustainable green energy

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Solar power is the key to a clean energy future. The sun provides more than enough energy to meet the whole world's energy needs, and unlike fossil fuels, it won't run out anytime soon. That's why we're investing heavily in solar plants and why we are now offering solar kits to the society. Solar panels produce electricity by transforming the continuous flow of energy from the sun to electricity. As a renewable CO_2-free power source, the environmental impact of solar power is significantly smaller than other power generation methods. The photovoltaic process that transforms sunlight into electricity doesn't require any fuel and has no variable costs. Silicon is, by far, the most common semiconductor material used in solar cells, representing approximately 95% of the modules sold today. As a renewable energy source, the only limitation of solar power is our ability to turn it into electricity in an efficient and cost-effective way. With a higher efficiency, fewer panels, or modules, need to be installed to reach a desired power target. This means less labor, less land and less hardware. That game changed a couple decades ago with the advent of thin-film solar cells and other cost-effective solar cells that forced the industry to focus on lower costs rather than high performance. Now that solar cells are less expensive to manufacture, the industry has entered a third phase with the goal: increasing efficiency while keeping low-cost manufacturing. A several such solar cells will be discussed during the presentation.

Artificial intelligence techniques in Healthcare: Opportunities and challenges

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Artificial intelligence (AI) is gradually changing medical practice. With recent progress in digitized data acquisition, machine learning, and computing infrastructure, AI applications are expanding into areas previously thought to be only the province of human experts. We summarize the latest developments of applications of AI in biomedicine, including disease diagnostics, living assistance, biomedical information processing, and biomedical research. This talk aims to keep track of new scientific accomplishments, understand the availability of technologies, and appreciate the tremendous potential of AI in biomedicine. It can be asserted that the application of AI in biomedicine is still in its early stage, just like AI itself. New progress and breakthroughs will continue to push the frontier and widen the scope of AI applications, and fast developments are envisioned soon. This talk aims to:

- Outline recent breakthroughs in AI technologies and their biomedical applications
- Identify the challenges for further progress in medical AI systems
- Summarize AI's implications in healthcare.

Flying robot path planning techniques and its trends

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A Flying robot is a system capable of vertical take-off and landing to perform some specific task with no direct human intervention. Flying robots are distinct from other robots by their ability to fly with no direct human control and are capable of making a decision based on the situation. Drones, Aerial robots, Unmanned Aerial Vehicles (UAV) are few examples of flying robots. Path determination of flying robots is one of the most critical aspects of robot Routing design. Path planning is a technique which tells flying robot how to fly, where to fly and to find a collision-free optimal path. Numerous techniques have been put forward over the past few years to find an optimal path for flying robots. This work discusses on new trends led by artificial intelligence and safe human-robot interaction for optimal path planning of aerial robots. Furthermore, a comprehensive study is carried out on various 2D and 3D path planning algorithms done to date and different algorithms are classified based on important criteria for optimal path planning for flying robots.

Effective sensitization of Yb^{3+} ions on Yb^{3+}/Nd^{3+} co-doped fluoroborate glasses for NIR luminescence applications

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Nd^{3+}/Yb^{3+} co-doped fluoroborate glass samples were fabricated by melt quenching. The infrared luminescence of the Nd^{3+}/Yb^{3+} codoped fluoroborate glass was characterized by XRD, SEM, FT-IR, optical Absorption, Photoluminescence and time resolved luminescence. There is an effective mutual energy transfer process between Nd3+ and Yb^{3+} in prepared glasses was observed. Excitation was made using a laser diode tuned to 808 nm wavelength. The broad emission range from 850 to 1400 nm is due to both Nd^{3+} ($^4F_{3/2}\rightarrow{}^4I_{9/2}$, $^4F_{3/2}\rightarrow{}^{4I}{}_{11/2}$ and $^4F_{3/2}\rightarrow{}^4I_{13/2}$) and Yb^{3+} ($^2F_{5/2}\rightarrow{}^2F_{7/2}$) transitions. The dependence of NIR emission, lifetime, and the energy transfer efficiency (ηETE) with the concentration of Yb^{3+} was studied in detail. The Photoluminescence spectra along with donor decay curves have been used to establish the energy transfer mechanism between Nd^{3+}/Yb^{3+} ions. The results represents that the sensitization of Yb^{3+} is possible through 4f-4f transition of Nd^{3+} ions in prepared glasses. The photoluminescence properties of the Nd^{3+} singly doped and Nd^{3+}/Yb^{3+} co-doped prepared glasses indicate their suitability as multiple pump channel sources for Yb^{3+} fiber laser systems. Those results prove that Nd^{3+}/Yb^{3+} codoped prepared fluoroborate glass is the potential infrared laser gain material.

Effect of isothermal aging at 750℃ on microstructure and mechanical properties of UNS S32101 lean duplex stainless steel

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UNS S32101 lean duplex stainless steel (LDSS) is utilized in the present investigation which has a two-phase microstructure consisting of austenite (γ) and ferrite (δ) in near equal proportions. Aging at high temperature results in formation of σ phase reducing ductility and also corresponding depletion of Cr from the adjoining matrix. The effect of long-term aging on the microstructure and mechanical properties is still an active area of research for lean DSSs. In the present work effect of aging at 750°C (up to 480 h) on microstructure and mechanical properties has been systematically studied. Scanning electron microscopy (SEM) revealed that the precipitates were distributed along ferrite/austenite (δ/γ) interfaces and ferrite/ferrite (δ/δ) boundaries. Nitrides (mainly Cr_2N) were observed in initial phases of aging and σ phase afterwards, mostly at longer aging times. The decrease of Ni and Mo and increase in N in UNS S32101 steel delayed the precipitation of σ, but could not avoid it completely. The room temperature absorbed impact energy of specimens decreased gradually as the aging time increased. The lowest value of absorbed impact energy was found to be 24±2 J after 480 hours of aging, which was only ~11% as that of solution annealed specimen. Fractography also showed that the fracture morphology changed from fibrous (ductile) to dominant brittle (which involved predominance of cleavage facets along with long, wide cracks i.e., delamination fracture) with increasing aging time. Tensile tests also showed a decrease in ductility and an increase in yield stress/ultimate tensile strength with aging time.

Highly sensitive photonic crystal fiber on hybrid layer of metal / 2D materials

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Platinum Diselenide, $PtSe_2$ is gaining popularity due to its intriguing optoelectronic, thermoelectric, and semiconductor properties. They are non-toxic, chemically inert, and allow for high biomolecule absorption, making them ideal for use in sensors to improve sensing. Here, we proposed Photonic Crystal Fiber (PCF) based Surface Plasmon Resonance (SPR) sensor for enhanced refractive index sensing at mid infrared wavelengths. To achieve this, Tri-Path PCF (TP-PCF) was coated with a gold/$PtSe_2$ hybrid layer, which allows light to freely pass through the cladding and interact with the plasmonic material, resulting in a significant coupling effect. Finite Element Method is used for numerical examination and exhibits maximum wavelength sensitivity of 42,000 nm/RIU and maximum wavelength resolution of 2.4×10^{-6} within the analyte range from 1.33 to 1.38, which almost covers the unknown analytes of chemical and bio.

Environmental pollution cleaning using organic smart material by photocatalysis

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Complex aromatic organic dyes and pigments are the vital waste which damages the human health as well as aquatic life. Researchers are working to overcome this serious issue from many years, but to developed cost-effective and eco-friendly method is unsolved challenge. Of late, inorganic based photocatalysis helps to treat industrial wastewater up to some extent. Various inorganic semiconductor photocatalysts with high efficiency have been reported with different dyes degradation study.

We have synthesized PQ an intermediate require synthesizing Pentacene which is well known organic semiconductor from last couple of decades. After complete characterization using spectroscopic and microscopic techniques, we explored PQ for Industrial Dye degradation and Photocatalytical H_2S splitting for the first time. We also synthesized composite system of PQ-TiO_2 with inorganic semiconductor photocatalyst. Recently a report of PQ-MoS_2 photocatalyst also covers the water splitting area. This organic PQ photocatalyst have high potential in photocatalysis field which can be utilized for the clean environment and for water treatment.

Greener synthesis of zirconia nanoparticles and their applications

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Zirconia in nanoscale has been found useful as nanocatalyst, nanosensor, nano adsorbent. Additionally, its biomedical applications in dentistry and drug delivery, and interesting biological properties such as anti-microbial, anti-oxidant, and anti-cancer activity have further motivated the researchers to explore different synthetic pathways. In this work, greener synthesis of zirconia nanoparticles was carried out suing using green tea leaves and zirconium oxychloride. The prepared nanoparticles were characterized with UV-visible spectroscopy, transmission electron microscopy and powder XRD, and scanning electron microscopy. Powder XRD pattern and microscopic studies confirm the formation of nanocrystalline material having the size in the range of 15-40 nm. Keeping in view biomedical applications of zirconia, antibacterial and antifungal activities of prepared nanoparticles were investigated. These studies have shown promising results.

Seasonal variation of manakudy estuarine water chemistry, south west coast of India

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Toxic trace elements from rivers are either weathered naturally from soils and rocks or introduced anthropogenic from point or non-point sources, in labile or particle form, to be debouched into the sea through estuaries. The chemistry and ecology of an estuary system differ significantly from those of a fluvial or marine one. Twenty water samples were collected around the Manakudy estuary and examined throughout the pre and post monsoon seasons. To acquire a better knowledge of the geochemical behaviour of physico-chemical parameters, main ions, and trace elements, as well as variations in associated chemical fluxes. With respect to the mean values during both monsoons, the principal ion sequence of abundance is Na>Mg>K>Ca>NO_3>SiO_4>P>NO_2. When compared to Cu, Cr, Cd, and Co, the mean concentrations of Fe, Zn, Mn, and Pb are 4128, 42, 36, and 5.18g/l in premonsoon and 2064, 31, 37, 25, and 6.17g/l in postmonsoon, respectively. The contamination factor (CF) and potential ecological risk index (PERI) were used to calculate the toxicity level of trace metals in water. Based on CF values, Cu was found to be the most polluting metal in estuary water. Premonsoon water has a moderate to high danger, whereas postmonsoon water has a moderate to significantly high risk. The interconnected components of water quality attributes that influence the estuarine water environment include physico-chemical parameters, main ions, and trace elements. As a result of geogenic and anthropogenic processes enriching and overloading these components, species diversity, metabolism, and habitat population are negatively impacted. To reduce the overloading of contaminants in the Manakudy estuary water, strategic management plans should be established.

Heart disease prediction and detection using association rule ming techniques

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Data science mining methods are utilized in the field of medication for different purposes. Mining affiliation rule is one of the intriguing points in information mining which is utilized to produce continuous itemsets. It was first proposed for market bushel examination. Analysts proposed varieties in methods to create incessant itemsets. Creating huge number of incessant itemsets is a tedious cycle. In this paper, the creators contrived a strategy to anticipate the danger level of the patients having coronary illness through incessant itemsets. The dataset of different coronary illness patients is utilized for this exploration work. The information mining strategies-based frameworks could vitally affect the workers' way of life to anticipate heart sicknesses. There are numerous logical papers, which utilize the strategies of information mining to anticipate heart infections. Nonetheless, restricted logical papers have tended to the four cross-approval methods of dividing the informational index that assumes a significant part in choosing the best procedure for foreseeing coronary illness. Pick the ideal blend between the cross-approval methods and the information mining, order strategies that can upgrade the exhibition of the forecast models. This paper means to apply the four-cross-approval methods (holdout, k-overlay cross approval, separated k overlap cross-approval, and rehashed irregular) with the proposed techniques Extended Support Vector Machine and Extended KNN to work on the precision of coronary illness expectation and select the best forecast models. It investigates these procedures on a little and huge dataset gathered from various information sources like Kaggle and the UCI AI archive. The assessment measurements like exactness, accuracy, review, and F-measure were utilized to quantify the presentation of forecast models. Experimentation is performed on two datasets, and the outcomes show that when the dataset is epic (50000 records), the ideal mix that accomplishes the most noteworthy precision is holdout cross-approval with the neural organization with an exactness of 71.82%. Simultaneously, Repeated Random with Random Forest considers the ideal blend in a little dataset (303 records) with a precision of 89.01%. The best models will be prescribed to the doctors in business associations to help them anticipating coronary illness in workers into one of two classifications, cardiovascular and non-heart, at a beginning phase. Successive itemsets are produced dependent on the picked indications and least help esteem. The separated successive itemsets assist the clinical professional with settling on indicative choices and decide the danger level of patients at a beginning phase. The proposed strategy can be applied to any clinical dataset to anticipate the danger factors with hazard level of the patients dependent on picked factors. An exploratory outcome shows that the created technique distinguishes the danger level of patients effectively from continuous itemsets. The early recognition of heart illnesses in representatives will further develop efficiency in the business association.

Amelioration of structurally disturbed soil through microbe-manure amalgams

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Less precipitation, high temperature, and minimal natural vegetation are characteristic of regions having arid climate. The harsh environment massively destructs the soil structure of that area by burning soil organic carbon, leading to deteriorated soil nutritional quality, creating a huge threat to agricultural production and food security. Direct application of organic wastes not only substitutes lost organic carbon but also restores soil structure and fertility. Organic amendments i.e., farm manure (FM), poultry manure (PM), molasses (MO) and Exo-Poly Saccharides (EPS) producing rhizobacterial strains i.e., M2, M19, M22 amalgams were used as treatments. To assess the impact of treatments on soil carbon and structure restoration to hold more water and nutrients, a 42-day incubation experiment using completely randomized design (CRD) under the two-factor factorial arrangement was conducted. Macroaggregation (0.25 to >1 mm), carbon retention in macroaggregates, active carbon (dissolved organic carbon, a mineral associated organic carbon, microbial biomass carbon), total organic carbon, the carbon mineralization activities, and water retention capacities were observed highest in soils that were treated with (FM+M2, FM+M22, PM+M19, and MO+M19). Finally concluded that organics mineralization by microbial actions release organic glues that not only imparts particle aggregation but also conserve organics as aggregate entrapped carbon. Amalgamated application of microbe-manure combinations directly impacts soil structure and organic carbon contents, but in an indirect scenario it improves fertility and productivity of soil.

Chloroform-Injection (CI) and Spontaneous-Phase-Transition (SPT) are novel methods, simplifying the fabrication of liposomes with versatile solution to cholesterol content and size distribution

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Intricate formulation methods and/or the use of sophisticated equipment limit the prevalence of liposomal dosage-forms. Simple techniques are developed to assemble amphiphiles into globular lamellae while transiting from the immiscible organic to the aqueous phase. Various parameters are optimized by injecting chloroform solution of amphiphiles into the aqueous phase and subsequent removal of the organic phase. Further simplification is achieved by reorienting amphiphiles through a spontaneous phase transition in a swirling biphasic system during evaporation of the organic phase under vacuum. Although the chloroform injection yields smaller Z-average and poly-dispersity-index the spontaneous phase transition method overrides simplicity and productivity. The increasing solid/solvent ratios results in higher Z-average and broader poly-dispersity-index of liposomes under a given set of experimental conditions, and vice versa. Surface charge dependent large unilamellar vesicles with a narrow distribution have poly-dispersity-index < 0.4 in 10 μM saline. As small and monodisperse liposomes are prerequisites in targeted drug delivery strategies, hence the desired Z-average $<$ 200 d.nm and poly-dispersity-index < 0.15 is obtained through the serial membrane-filtration method. Phosphatidylcholine/water 4 μmol/mL is achieved at a temperature of 10◦C below the phase-transition temperature of phospholipids, ensuring suitability for thermolabile entities and high entrapment efficiency. Both methods

furnish the de-novo rearrangement of amphiphiles into globular lamellae, aiding in the larger entrapped volume. The immiscible organic phase benefits from its faster and complete removal from the final product. High cholesterol content (55.6 mol%) imparts stability in primary hydration medium at 5 ± 3 ◦C for 6 months in light-protected type-1 glass vials. Collectively, the reported methods are novel, scalable and time-efficient, yielding high productivity in simple equipment.

Internet of things and cloud computing survey

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Internet of things and cloud computing play a vital role in the area of Information Technology now adays. Both of these technologies are essential for the upcoming developments and research in computing domain. This paper will rectify a survey of both these technologies playing a vital role so far. Some observations and comparisons are notified here for the information and verification

Fabrication of organic semiconductor based humidity sensor and its environmental applications

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The compound lophine, 2, 4, 5-triphenyl-1H-imidazole, has been used to fabricate humidity sensors. The sensors were tested in different humidity environments, and at various applied frequencies. The SEM images showed inter-woven spiky needles, pores, pore-channels of diverse shapes and sizes. The H_2O molecules interacted with N and NH sites in the aromatic ring of the compound and thus altered the electrical properties due to the imidazole scaffold's electron acceptor and trifling donating nature. The conduction mechanism is based on Grotthuss hydroxide transfer and prototropic mobility. The calculated dielectric constant of the material was 1.69. In 45-95 %RH limit, the devices capacitance was increased from 11 pF to 460 pF and 7.29 pF to 18.9 pF at applied frequencies 1 kHz and 10 kHz, respectively. The response/recovery time was 39/20 seconds, respectively. The maximum hysteresis was 0.44 % (at 1 kHz) and 1.09 % (at 10 kHz). The R2 values (goodness of fit) 0.98 and 0.99 for chemisorbed and multi-layered physisorbed layers are close to unity and thus considered the best linear-fit. The sensors showed a strong affinity to moisture at ambient conditions with low hysteresis. Fabulous improvement in the device's sensitivity has been noted over the reported sensitivity of devices based on ceramic materials.

Lead-free double perovskites for thermoelectric and optoelectronic applications: Ab initio study

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Energy consumption is increasing day by day in today's world so it is the matter of concern for the scientific community to find the alternative power generation mechanisms by minimizing the whole world's reliance on traditional power generation methods. Thermoelectricity and optoelectronics have emerged as an attractive area of research for finding efficient non-traditional power generation mechanisms. In this scenario, it is a matter of immense potential to find more efficient materials for optoelectronic and thermoelectric power generation. Currently, the structural, electronic, optical, phononic and thermoelectric properties of double perovskites A_2NaBCl_6 (A=Cs,Rb,K and B=Bi,Sb) have been studied in details using density functional theory (DFT) within the frame work of generalized gradient approximation(GGA). The results of $Cs_2NaBiCl_6$ and $Cs_2NaSbCl_6$ are consistent with already reported data whereas $Rb_2NaBiCl_6$, $K_2NaBiCl_6$, $Rb_2NaSbCl_6$ and $K_2NaSbCl_6$ have been reported for the first time. The structural stability, thermal stability, large Seebeck coefficients and figure of merit (close to unity) of these lead-free double perovskites suggest various thermoelectric device applications. High absorption coefficient, high optical conductivity and low reflection coefficient suggests the applications of these compounds in solar cells as a source of low cost eco-friendly power generation schemes.

Contribution of carbon mesopores towards the improved performance of ionic liquid-based EDLCs at different temperatures

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During the presentation an important role of mesopores investigated in electric double-layer capacitors (EDLCs) operating from 24°C down to−40°C by using carbons with hierarchical porosity will be discussed. Home-made carbons were prepared using different precursors as the carbon source, while a binary mixture of imidazolium-based fluorinated ionic liquids was used as a solvent-free electrolyte. It will be shown that short-range graphene layers produced with 8-nm silica nanoparticles lead to the creation of transport channels which better accommodate ions. We explain these findings per coulombic interactions among the ions and between the pore wall and the ionic species under confinement and electrochemical polarization conditions. Further, it will be shown that a microporous carbon performs better than hierarchical carbons at room temperature; however, owing to the large fraction of mesopores, the latter exhibit far higher capacitance down to−40°C. While the ordering of ions in confinement is more critical at room temperature and dictated by the micropores, low temperature performance of supercapacitors is determined by the mesopores that provide channels for facile ion movement and keep the bulk ionic liquid–like properties.

Dispersion of singled walled carbon nanotube in water in presence of direct current field

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The dispersed solution of Single-walled carbon nanotubes (SWCNT) have been utilized in different industrial and laboratory applications such as electrodes of batteries, super capacitors, gas sensors etc. There are many difficulties and challenges to make a stable suspension of SWCNT as they tend to self-associate into clusters. These clusters have to be dispersed before they could be used for different applications. In this research, an effort has been made to reduce the agglomeration of SWCNT by sonication in presence of Direct Current field (DC). It was found that sonication under DC field has increased the degree of dispersion. Furthermore, the result shows that SWCNT can be dispersed with or without use of any surfactants by sonication in presence of DC field. The use of surfactants could increase the impurity content of dispersed solution which was reduced by our modified method of dispersion. In addition, it is shown that our modified method can be used to study dispersion with minimal use of expensive chemicals like SWCNTs.

Kinetic study of removal of fluoride and nitrate, synthesis and characterization of layered double hydroxide

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Layered double hydroxides (LDH) are a class of naturally occurring and synthetic anionic clays classified under the hydrotalcite-like compound. Fluoride (F-) is an essential micronutrient for the calcification of bone and dental enamel formation. But excessive intake causes skeletal and dental fluorosis. The contamination of F in surface and groundwater could come either from natural geological sources and industrial wastewater. Nitrate (NO_3^-) is a widely spread groundwater contaminant. It causes severe health & environmental problems like blue baby syndrome and eutrophication. LDH can be synthesized by using the co-precipitation method. Magnesium dichloride hexahydrate ($MgCl_2.6H_2O$), Aluminium chloride hexahydrate ($AlCl_3.6H_2O$), Potassium Hydroxide (KOH), Potassium Carbonate (K_2CO_3), Deionized water were used to synthesize LDH. It is a comparatively economically feasible synthesis method. The synthetic product can be identified by using the Powder X-ray Diffraction (PXRD) method by using the values at 7.5916(003), 3.8011(006), 3.1390(009) (JCPDS-22-700) and Fourier Transform Infrared Spectroscopy (FTIR) peaks at 558 cm^{-1}(Mg-O stretching), 876 cm^{-1}(Al-O stretching), 1411 cm^{-1} (C-O stretching), 3200- 3500 cm^{-1} (O-H stretching). LDH was stirred with F- and NO3- for 0 - 4 hours respectively. After each 10 minutes time interval, remaining anion concentrations were measured respectively. Finally, the best fitted kinetic model was found for each. Removal of fluoride has been successfully followed Pseudo second-order kinetic model and the kinetics of fluoride removal is not affected by initial concentration and amount of adsorbent quantity. The highest efficiency of removal of fluoride has been found with 4.00x103 mg L^{-1} of LDH and the initial fluoride concentration was 10.00 mg L^{-1}. Removal of nitrate has successfully followed the Pseudo 1st order kinetic model. The efficiency of F removal is 87.58%, while nitrate removal efficiency is 85.38%.

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