Poster Session I

*Al Hamra Convention Center*

Sunday, February 18, 2018 18:30-20:30
I.1 Characterization of Adsorbents Derived from Date Pit Extraction Residues

Haliemeh Sweidan, Naeema Al Darmaki, Yaser Greish and Ali Al Marzouqi
Departments of Chemistry and Chemical Engineering, United Arab Emirates University, Al Ain, United Arab Emirates

I.2 Preparation and Characterization of Alumina NPs - UHMWPE Composites for Hard Tissue Engineering Applications

Omar G. Ayad, Abdel-Hamid I. Mourad and Yaser E. Greish
Departments of Chemistry and Mechanical Engineering, United Arab Emirates University, Al Ain, United Arab Emirates

I.3 Ca^{2+}, Zn^{2+} Sulfate Polycarboxylate Bone Cement: Formation and Characterization

Shafaa Al-Maqdi and Yaser E. Greish
Department of Chemistry, United Arab Emirates University, Al Ain, United Arab Emirates

I.4 Evaluation of a Novel Magnetite-Containing Gypsum-based Bone Cement for the Treatment of Bone Fracture

Fatima Merza and Yaser E. Greish
Department of Chemistry, United Arab Emirates University, Al Ain, United Arab Emirates

I.5 Formation of a Biphasic Calcium Phosphate Sulfate Bone Cement Containing Ibuprofen for Bone Fixation

Maryam Alqaydi and Yaser E. Greish
Department of Chemistry, United Arab Emirates University, Al Ain, United Arab Emirates

I.6 Adsorption of Bilirubin Toxin in the Liver by Chitosan Coated Activated Carbon

Asel A. Mwafy and Ameereh Seyedzadeh,
Department of Mechanical Engineering, United Arab Emirates University, Al Ain, United Arab Emirates
I.7 Neem Gum Modifications for Museum Conservation

Ideisan I. Abu-Abdoun, Reem R. Alteneiji, Amna A. Al Hamadi
Department of Chemistry, University of Sharjah, Sharjah, United Arab Emirates

I.8 Synthesis, Characterization, and Biocompatibility of Thermoplastic Polyurethanes for Medical Applications

Mahmoud A. Mohsin† and Balsam Q. Saeed‡
†Department of Chemistry, University of Sharjah, Sharjah, United Arab Emirates
‡Department of Clinical Science, University of Sharjah, Sharjah, United Arab Emirates

I.9 Machine Learning Algorithm to Quantify Images of Materials

Leora E. Dresselhaus-Cooper, Marylesia Howard, Margaret Hock, B. T. Meehan, Kyle Ramos, Cindy Bolme, Richard Sandberg, Hugh Simons, Keith A. Nelson
Department of Chemistry, Massachusetts Institute of Technology, Massachusetts, USA

I.10 Activity of Gamma-Glutamyl Transferase (GGT) Enzyme as a Prognostic Tool for Heart Failures

Ayoub A Bazzaz,† Susan J. Ali,‡ Noorhan A. Chelebi† and Abdulwadood I. Arif‡
†Department of Basic Sciences, University of Karkuk, Kirkuk, Iraq
‡Department of Chemistry, Faculty of Education, University of Tikrit, Iraq

I.11 Encapsulation of Rosemary Essential Oil on Sodium Alginate and Sodium Alginate/Modified Bentonite Composites

Doha Berraouan, Najla Kaabouch, Samira Salhi and Abdesselam Tahani
Department of Chemistry, Mohamed First University, Oujda, Morocco

I.12 N-doped Graphene Quantum Dots Functionalized Zirconia Based Immunosensing platform for Ochratoxin A Detection

Pramod K. Gupta,†‡ Zishan H. Khan‡ and Pratima R. Solanki†
†Special Centre for Nanosciences, Jawaharlal Nehru University, New Delhi, India-110067
‡Department of Applied Sciences and Humanities, Jamia Millia Islamia, New Delhi-110025
I.13 Latest Advances of Nanomaterials in the Fabrication of Bone and Dental Cements

Yaser E. Greish  
Department of Chemistry, UAE University, Al Ain, UAE

I.14 Electrospray Fabrication of Chitosan Nanoparticles for the Treatment of Hepatocellular Carcinoma

Badriya M. Baig, Yaser E. Greish, Amr Amin  
Department of Biology, United Arab Emirates University, Al Ain, United Arab Emirates

I.15 Fabrication of Starch-PVA Films Incorporated with Oleoresin for Food Packaging Applications

Sudarshan B L,† Divya K,† Madhukar B S,‡ Hemanth Kumar Kandikattu,§ Farhath Khanum⊥ and Sanjay K R†  
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I.16 Solid Acid Catalyst in Esterification Reactions

Shagufta,† Irshad Ahmad† and Rahul Dhar‡  
†Department of Mathematics and Natural Sciences, School of Arts and Sciences  
‡Department of Chemical and Petroleum Engineering, School of Engineering  
American University of Ras Al Khaimah, Ras Al Khaimah, United Arab Emirates

I.17 Nanoparticles Embedded in Graphene Oxide: Toward Photochemical Applications

Nathir A. F. Al-Rawashdeh, Mohannad Theeb Al-Jarrah and Odai Monzer Allabadi  
Department of Math & Natural Science (Chemistry), Higher Colleges of Technology, Ras Al-Khaimah, United Arab Emirates
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Abdulrahman Al-Hagri, Mohammed Faisal, Mohammed Misbah Uddin, Loai Bamatraf Anas Alaidaros, Ahmad Alhamdat, Rengaraj Selvaraj and Mohammed Meetani
Department of Chemistry, United Arab Emirates University, Al-Ain, United Arab Emirates

I.19 Resource Recovery from Scrap Tires through Catalytic Pyrolysis

Rashid Miandad and Ahmad Saeed
Department of Environmental Sciences, University of Haripur, Haripur, Pakistan

I.20 Structural and Electronic Properties of Na$_2$Ti$_3$O$_7$ and H$_2$Ti$_3$O$_7$

Sara A. H. Abass and Nicola Seriani
Department of Physics, Khartoum University, Khartoum, Sudan

I.21 Valorization of Bio-methane Production from Waste Activated Sludge using Newly Synthesized Visible Light Cr$_2$O$_3$/C$_3$N$_4$-(6M) Photocatalyst

Muzammil Anjum, Rajeev Kumar, Samia Qadeer and M. A. Barakat
Department of Environmental Sciences, King Abdulaziz University, Jeddah, Kingdom of Saudi Arabia

I.22 Chitosan Coated Cotton Cloth Supported Zero-Valent Nanoparticles: Simple but Economically Viable, Efficient and Easily Retrievable Catalysts

Fayaz Ali, Sher Bahadar Khan, Tahseen Kamal, Khalid A. Alamry, Abdullah M. Asiria and Tariq R. A. Sobahi
Center of Excellence for Advanced Materials Research (CEAMR), Department of Chemistry, King Abdulaziz University, Jeddah, Kingdom of Saudi Arabia

I.23 ZnO/Au/BN for Photocatalysis and its Antibacterial Effects

Yara Aldrees, Arshia Fathima, Faheem Ahmed, Yasmin Mussa and Edreese Alsharaeh
Department of Life Sciences, Alfaisal University, Riyadh, Kingdom of Saudi Arabia
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Sara AlEid, Arshia Fathima, Faheem Ahmed, Yasmin Mussa and Edreese Alsharaeh
Department of Life Sciences, Alfaisal University Riyadh, Kingdom of Saudi Arabia

I.25 Impact of the Substitution of PbO by PbF$_2$ on Structural Properties and Luminescence of Neodymium-doped Lead Borate Glass

Asmaa Ratep and Ismail Kashif
Department of Physics, Ain Shams University, Cairo, Egypt

I.26 Electrospinning as a Tool in Controlling the Morphology and Porosity: A Electromagnetic Interference Shielding Perspective

Khadija Kanwal Khanum, Pritom J. Bora and Praveen C. Ramamurthy
Department of Materials Engineering, Indian Institute of Science, Bengaluru, India

I.27 Approximation Technique to Determine the Solar Cell Temperature in Mega Solar Power Plants by using Climatological Data

Zia Hameed and Adnan Yousaf
Department of Electrical Engineering, Superior University, Lahore, Lahore, Pakistan

I.28 Analysis of Defect Free Pure Cadmium Oxide (CdO) Nanoparticles

M. Cuba, N. Qamhieh and Saleh T. Mahmoud
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I.29 Dye-Sensitized Solar Cells (DSSCs) based on TiO$_2$/BN/Ag Nanocomposites

Norah Aldosary, Yasmin Mussa, Arshia Fathima, Faheem Ahmed and Edreese H. Alsharaeh
Department of Chemistry, College of Science & General Studies, Alfaisal University, Riyadh, Kingdom of Saudi Arabia
I.30 Synthesis and Characterization of Lead Halide Perovskite for Solar Cell Applications

Amin Reyhan Sadek, Basem Abdel Aziz, Ibrahim Al Ghoul, Adel Najar and Naser Qamhieh
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I.31 Efficient Temperature Sensing using Photoluminescence of Er/Yb Implanted GaN Thin Films

N Hamza Belkhir, A Toncelli, Abdul K Parchur and E Alves and R Maalej
Department of Physics, Faculty of Sciences of Sfax, Sfax, Tunisia

I.32 Fabrication and Characterization of Gd$_2$O$_3$-HfO$_2$ based Memristor Devices for Gamma-Ray Detection

Maguy Abi Jaoude,$^\dagger$ Lama Mahmoud,$^\ddagger$ Baker Mohammad$^\ddagger$ and Hamda Al Shehhi$^\S$
$^\dagger$Department of Chemistry
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I.33 FP-LAPW Study of the Effective Masses and Bonding Properties of Zinc-Blende Cadmium Chalcogenides

S.Ouendadji
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I.34 The Effect of Pressure and Interstitial Substitution on the Electronic Properties of Molybdenum Disulfide

Wadha K. AlFalasi, Noureddine Amrane, Maamar Benkraouda and Naser Qamhieh
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I.35 Bioelectricity Generation from Human Feces by Microbial Fuel Cell using Graphite Electrodes

Hanish Mohammed C. H. and Muthukumar M
Department of Environmental Sciences, Bharathiar University, Coimbatore,TamilNadu, India
I.36 Enhanced Photoelectrochemical Water Splitting on a Stainless Steel 316L Porous-nanostructured Photoanode

Heba H. Farrag, Sayed Y. Nagy, Nageh K. Allam and Ahmad M. Mohammad
Department of Chemistry, Cairo University, Cairo, Egypt

I.37 A Study on the Lifetime and Photostability of Chalcogen based D-A-D polymer OPVs

Vinila Nellissery Viswanathan, Arun Dhumal Rao, Varun Adiga and Praveen C Ramamurthy
Department of Materials Engineering, Indian Institute of Science, Bangalore, India

I.38 Effect of Fluorination on D-A-D type Hole Transporting Materials for Perovskite Solar Cells

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I.39 Photocatalytic Reduction of CO₂ by Employing ZnO/Ag₁ₓCuₓ/CdS and Related Heterostructures

S.R. Lingampalli, Mohd Monis Ayyub, Ganesan Magesh and C.N.R. Rao
New Chemistry Unit, Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore, India

I.40 Utilizing the Potential of Raw and Modified Natural Zeolite for the Process Optimization of Food Waste Composting

Muhammad Waqas, Abdul-Sattar Nizami and Asad Siraj Aburiazaiza
Environmental Sciences, King Abdulaziz University, Jeddah, Kingdom of Saudi Arabia

I.41 Electrochromic Display Device

Sarfraj Mujawar, Bhushan Dhale and Sachin Pawar
Department of Physics, Savitribai Phule Pune University, Pune, India
I.42 Prepreg Waste to Produce Sustainable Non-Structural Aerospace Elements

Aamna S. Almazrouei, Dina Al Jamal, Farah A. Genena and Lamia A. Almarzooqi
Department of Mechanical Engineering, United Arab Emirates University, Al Ain, UAE

I.43 Enhanced Efficiency of Dye-Sensitized Solar Cells using Coffee as Natural Dye on TiO$_2$/RGO Nanocomposite based Photoanode

Edreese H. Alsharaeh, Faheem Ahmed, A. Soliman, Joud Alsadoun, G. Bharatha, Majdi Khasawneh and K. M. Abu-Salah,
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I.44 Synthesis and Characterization of Highly-ordered Cu Nanowires using Electrodeposition Template Method

Monika Nehra,‡ Deepak Kedia,† Neeraj Dilbaghi† and Sandeep Kumar†
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Guru Jambheshwar University of Science and Technology, Hisar, India

I.45 An Overview of Grain Size Distribution, Geochemistry and Mineralogy of Red Sea and Arabian Sea Sediments

Jawad Majeed, Ibrahim Muhammad Ghandour, Raiea A. Haredy and Ali Saeed Basaham
Department of Marine Geology, King Abdulaziz University, Jeddah, Kingdom of Saudi Arabia

I.46 An Eco-Friendly Microwave-Assisted Click Synthesis, Characterization and Anticancer Screening of Novel 1,2,3-Triazoles Tethering Benzimidazole and Sulfa Drug Conjugates

Mohamed R. Aouad,† M. A. Almehmadi,† Nadjet Rezkı,† Sanaa K. Bardaweel‡ and Mouslim Messali†
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I.47 Eco-Friendly Synthesis of a New Class of Ionic Liquids with Attractive Biological Activity

Mouslim Messali, Nadjet Rezki and Mohamed Reda Aouad
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I.48 Spectral and Optical Characterization of silver nanoparticles biosynthesised by Origanum majorana and Calendula officinalis

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I.49 H₂S Gas Sensor based on Chitosan-WO₃ Hybrid Nanocomposite

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Characterization of Adsorbents Derived from Date Pit Extraction Residues

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Date pits are considered one of the natural sorbents that have been studied for their potential for the removal of heavy metal cations from waste water. A major advantage of this kind of sorbents is its high abundance in the UAE as a natural waste material. In our studies, we have been investigating methods of maximizing the use of this waste in the removal of a model heavy metal pollutant (Pb$^{2+}$) from waste water. In the current study, three types of adsorbents derived from local waste date pits, namely raw date pits (R-DP), the residue date pit powder of Soxhlet extraction (S-DP), and the residue date pit powder of supercritical carbon dioxide extraction (CO2-DP), were characterized and evaluated for their sorption affinity of Pb$^{2+}$ ions from waste water. The sorbents were characterized by TGA, FTIR, and SEM techniques. TGA and FTIR analysis of the three adsorbents confirmed the removal of oil by Soxhlet and supercritical carbon dioxide extraction, while SEM analysis showed the fibrous nature of the sorbents. The differences in the TGA among the adsorbents confirmed that S-DP and CO2-DP contained less organic material than R-DP. In addition the FTIR spectra of S-DP and CO2-DP showed a sharp decrease in the band attributed to O-H in the carboxylic groups of the oil. The results of this study showed that both Soxhlet and supercritical carbon dioxide extraction are effective methods for the extraction of oil from date pits, with supercritical being more selective. In addition, the three adsorbents showed similar adsorption capacities, indicating that extraction of oil has no significant effect on the adsorption capacity of date pit powder.
**Preparation and Characterization of Alumina NPs - UHMWPE Composites for Hard Tissue Engineering Applications**

**Omar G. Ayad, Abdel-Hamid I. Mourad and Yaser E. Greish**

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In order to partially or totally replace defective hard tissues, biomaterial scientists have been looking for synthetic ceramic-polymer composites to match the composition, microstructure and properties of natural hard tissues. This work aims at the study of using alumina ($\text{Al}_2\text{O}_3$) nanoparticles as a reinforcing agent for a polymeric matrix based on ultrahigh molecular weight polyethylene (UHMWPE). Groups of alumina nano-Particles ($\text{Al}_2\text{O}_3$) dispersed UHMWPE samples have been prepared using injection molding technique at different nano-filler concentrations. The mechanical, thermal, and chemical properties of the injection molded samples have been measured to investigate the impact of alumina nano-particle concentration on the characteristics of the produced composites. Different characterization techniques have been used, which include tensile testing, Differential Scanning Calorimetry (DSC), Fourier Transform Infrared Spectroscopy (FTIR), and Scanning Electron Microscopy (SEM). Moreover, the optimally prepared composites were subjected to *in vitro* evaluation using dental stem cells to evaluate their potential as hard tissue partial and total replacements. *In vitro* assessment of composites intended for biomedical applications is an essential step to confirm the non-toxicity of the composites and to ensure the bio-inertness of the components of the injection molded composite is maintained. It has been noticed that the characteristics of the produced composites are dependent on the concentration of the nano-filler.
Zinc polycarboxylate bone cement is one of the commercially available dental cements. It has also been investigated for bone fixation applications. However, it lacks chemical similarity with bone and teeth. Its binding with hard tissues is through the formation of calcium polycarboxylate and/or the displacement of the apatitic phosphate group by the carboxylate group of the cement. On the other hand, gypsum is another bone and dental cement that is listed among the early known cements in the history of bone and teeth cements. Gypsum formation takes place through the hydration of plaster of Paris (POP) with water, while zinc polycarboxylate cements is formed through the reaction of activated ZnO particulates with an aqueous solution of polyacrylic acid. In the current study, powder mixtures containing ZnO and POP with a variable composition between both ingredients were formed by milling. Their interaction with water and 25% and 35% polyacrylic acid solutions were studied. The setting reactions of the formed cements were evaluated. It was revealed that a competing reaction between the Ca$^{2+}$ and Zn$^{2+}$ ions and polyacrylic acid caused a decrease in the affinity of POP to water and a delayed formation of gypsum. The effects of varying the composition of the initial powder mixture on the physical and mechanical properties as well as composition of the final set cements have been evaluated.
Evaluation of a Novel Magnetite-Containing Gypsum-based Bone Cement for the Treatment of Bone Fracture

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Bone fractures are usually treated with bone cements and or mechanical fixation depending on the extent of fracture. Gypsum-based bone cements have been studied as stand-alone cements or as composites with inorganic and organic components, which are usually added to improve the strength and bioactivity of the cement. In the current study, magnetite nanoparticles have been added to Plaster of Paris (CaSO₄•H₂O; POP) during its hydration to gypsum cements. The effect of adding up to 20 wt% of magnetite NPs to POP on the setting reactions of the gypsum-based composite made thereafter has been investigated. Moreover, the variation of compressive and tensile strengths of the magnetite-gypsum composites and the morphological changes observed as a result of the addition of magnetite NPs has been studied. Due to the high surface area of the magnetite NPs by virtue of their size (< 50 nm), improved mechanical properties of the gypsum composites were observed. It is estimated that NPs act as true fillers within the porous gypsum matrix. Despite these observations, no signs of chemical interaction between magnetite and POP during the hydration of the later were observed as studied by infrared spectroscopy and thermogravimetric analysis. These cement composites are highly believed to be superior to pure gypsum bone cements due to the improved mechanical properties and the presence of magnetite as a source of iron for an enhanced treatment of bone fractures.
Formation of a Biphasic Calcium Phosphate Sulfate Bone Cement Containing Ibuprofen for Bone Fixation

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A wide range of bone cements have been clinically used for the past five decades since the early discovery of the first polymethylmethacrylate bone cement in 1969. Polymeric bone cements have been in use since then despite their chemical structure mismatch with bone. Instead, bone-like cements based on calcium salts such as calcium phosphates and calcium sulfates have been heavily investigated. Gypsum cement is one of these candidates, whose formation takes place through the hydration of plaster of Paris (POP). On the other hand, the apatitic nature of bone has been imitated via the use of a self-setting calcium phosphate cement that produces stoichiometric or calcium-deficient hydroxyapatite (HAp) bone cement. In the current study, a biphasic cement containing calcium sulfate and calcium phosphate has been studied. POP and monetite (CaHPO$_4$) were used as starting reactants to produce gypsum and bone-like Ca-deficient HAp biphasic cement. The combined concurrent setting reactions have been investigated using setting time and composition studies using x-ray diffraction, infrared spectroscopy, thermogravimetric analysis and scanning electron microscopy. Moreover, the setting reaction through the addition of a simulated body fluid (SBF) instead of pure water has been also investigated. Moreover, the effect of varying the proportion of monetite in the composite cement on the mechanical properties of the produced mixed cement composites has been studied and correlated with the setting reaction mechanisms. Finally, the ability of optimally selected biphasic bone cements to in situ deliver Ibuprofen for an enhanced healing of bone fractures was followed by studying the kinetics of Ibuprofen release with time in a phosphate buffer medium.
Liver failure is a widespread disease that influences millions of people worldwide each year. Due to the alarming rate of the spread of liver failure, new strategies are applied for the diagnosis, treatment, and containment of this disease. The aim of this work is to develop activated carbon (AC) from raw date pits to be used in the adsorption of bilirubin toxin from the blood stream of acute liver failure patients. This was accomplished through physical activation and to further enhance the capacity of adsorbance, the AC is coated with chitosan gel, which contains several groups on its chains that act as interaction sites for the bilirubin. Results demonstrate that 0.3 M AC concentration results in 0.82 left over bilirubin fraction after 16 hours, while a 0.1 M AC concentration results in 0.9 bilirubin fraction after the same time interval. Moreover, observations show that chitosan coated AC shows an increase in adsorption percentage from about 25% to 96% when left for a longer period of time.
Neem Gum Modifications for Museum Conservation

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Neem is a tree that grows in tropical and semi-tropical regions. Products made from neem have been used in India for over two millennia for their medicinal properties, selectively in controlling pests in plants, and also for curing skin diseases. Further, neem trees are one of the famous and well known trees in UAE. Products from neem trees are cheap, easy to obtain and not poisonous to animals and friendly insects.

The gum was collected from locally grown neem tree, physical and chemical characterization was carried out. Physical and chemical properties of local neem gum such as color, solubility; and effects of different parameters such as temperature, acidity, organic solvent were recorded. Modified neem gum solution was applied on selected museum collections, after exposure to different environmental factors of light, heat, relative humidity, pollutants, pest and insect control used commercially. The results will be presented.
Synthesis, Characterization, and Biocompatibility of Thermoplastic Polyurethanes for Medical Applications

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Linear thermoplastic polyurethane elastomers, with a range of formulations based on soft-to-hard segment ratio were synthesized in bulk using diphenylmethane-4,4’-diisocyanate (MDI), butandiol (BD) as chain extender, and polycaprolactone diol (PCL) having varying molecular weights. The polymers, having chemical and structural variables that affect the overall properties were produced, analyzed and characterized using thermogravimetric analysis (TGA), fourier transform infrared spectroscopy (FTIR), nuclear magnetic resonance spectroscopy (NMR) and differential scanning calorimetry (DSC). Hardness and rheological properties were also examined. Biocompatibility tests were carried out on selected polyurethane samples in order to establish its suitability for a desired medical application, such as implant or hip prosthesis. The results were analyzed using both scanning electron microscopy (SEM) for the polyurethane samples and optical microscopy (OM) for the biological tissues.

The main finding was that some polyurethane samples with uniform distribution between hard and soft segments had the lowest adverse biological effect. Other samples caused severe irritation to the tissue and had noticeable surface erosion of the polymer sample. This can be traced to the polyurethane composition and the curing process used during the synthesis process.

The initial experimental results provide evidence that the properties of polyurethanes can be tailor made to be biocompatible for biomedical applications, depending on their chemical structure, extend of hard and soft segments segregation, and their chemical composition.
Machine Learning Algorithm to Quantify Images of Materials

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Images capture a detailed two-dimensional view of materials, capturing spatial variation that gives new types of information. Quantitatively extracting these new details requires significantly more complex mathematical tools, usually in the form of image-processing algorithms specialized to a specific need. Among these algorithms, boundary-detection locates the demarcation that separates two features within an image, locating the leading edge of a martensitic phase transition or the edges of a defect. Established boundary-detection algorithms fail for images with aberrations, blur, noise, low contrast or uneven illumination. I present a new locally adaptive discriminant analysis (LADA), which uses machine-learning to locate the boundaries for images with uneven illumination, even in the presence of aberrations and high noise. I will demonstrate this algorithm’s utility across materials science, using it to precisely measure the position and velocity of shock waves, and using it to identify defects in topography.

This work was done in part by Mission Support and Test Services, LLC, under Contract No. DE-NA0003624, with the U.S. Department of Energy. DOE/NV/03624--0028.
Activity of Gamma-Glutamyl Transferase (GGT) Enzyme as a Prognostic Tool for Heart Failures

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Heart failure (HF) incidence could cause further complications to other body organs, which might sometimes be fatal, and is accompanied by various biochemical alterations i.e. enzymatic changes. The objective of this study was to measure the activity of gamma glutamyl transferase (GGT) as an early diagnostic indicator for HF patients; and to isolate the iso-enzymes for the purpose of finding the Michaelis-Menten constant (Km) and the maximum velocity Vmax of each iso-enzymes which enable follow up the development of HF disease. Samples of blood serum were collected from 120 patients of both genders (70 males and 50 female, aged 30-38 years old). Partial purification of iso-enzyme GGT was performed by precipitation, gel filtration, and ion exchange of the two iso-enzyme (I and II). The purity of the enzyme was confirmed by using sodium dodecyl sulfate-polyacryl amide gel electrophoresis (SDS-PAGE) into two clear bands. The results were compared with other 80 samples of healthy volunteers whose ages ranged between 25-78 years old, used as control. There has been a significant increase (p≤0.01) in the activity of the enzyme GGT in the heart failure patient (66.9±1.7 IU/L) in comparison with control (12.07±0.60 IU/L). It is concluded that measurements of the iso-enzyme GGT could well benefit as a clear indicator criteria in prognosis of heart failure.
Encapsulation of Rosemary Essential Oil on Sodium Alginate and Sodium Alginate/Modified Bentonite Composites

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Beads of sodium alginate (SA) and alginate/modified bentonite (SA/Na-B) have been used as matrices for the encapsulation of rosemary essential oil. Encapsulation is a technique mainly used in the protection of sensitive compounds like active molecules against external conditions such as oxygen, heat, moisture and pH until their release, yet the studies about essential oils as the inner core of microbeads are limited.

The need to develop renewable source-based biopolymer materials that do not involve the use of toxic components and allow for degradation via natural processes is increasing. Polysaccharides and clays are the most promising candidates because they are made or come from naturally abundant products and are biodegradable. Alginates are polysaccharides excreted from seaweeds or synthetized by bacteria mainly used in their water soluble form, SA. Essential oils (EO) are complex mixtures of different volatile molecules like aliphatic components, terpenoids and phenols that have a high interest in food, cosmetic, sanitary and pharmaceutical industries for their antimicrobial, antioxidant and antibacterial properties. In this perspective, rosemary essential oil (REO) has been used for this work. Rosemary (Rosmarinus officinalis L) is a common dense, evergreen, aromatic shrub belonging to the mint family that grows in many parts of the world. The leaves (fresh or dried) are widely used in Mediterranean regions especially in gastronomy and traditional medicine. There are three main chemotypes of REO according to the quantity of the major component: Camphor REO, Eucalyptol REO, and Verbenone or alpha pinene REO. A CPG-mass spectroscopy analysis showed that the REO used in this work is Eucalyptol chemotype.

The present work is focused on the comparison between the characteristics of the beads obtained with SA only and SA/Na-B following the optimal conditions to avoid the loss of active compounds due the temperature. The alginate beads and composed beads were characterized by IR spectroscopy, Thermal analysis TGA. The morphology of these particles changes according to the formulation, SA beads showed a spherical and a narrower size compared to the SA/Na-B beads. The results showed that the SA/Na-B beads present a higher encapsulation efficiency owing to the large adsorption capacity of the bentonite and a slower release of the essential oil during time.
Carbon Quantum Dots Functionalized Zirconia Based Immunosensing Platform for Ochratoxin A Detection

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The limitations of zirconia nanostructures (ZrO$_2$) such as higher aggregation and absence of functional groups hinder the biosensing performance of material[1]. This problem can be overcome by modification of the nanomaterial surface with a substrate material having higher electrochemical behaviour and desired functional groups[2,3]. In this scenario, N-doped graphene quantum dots functionalized ZrO$_2$ nanoflowers (NGQDs@ZrO$_2$) were synthesized by a one-step hydrothermal method and utilized to develop an immunosensor for Ochratoxin-A (OTA). NGQDs@ZrO$_2$ was investigated using X-ray diffraction, transmission electron microscopy (TEM), UV-visible, fluorescence spectroscopy, fourier transform infrared spectroscopy, and electrochemical characterizations. Presence of NGQDs, on the surface of ZrO$_2$ (~20 nm), not only prevented aggregation but also enhanced the electrochemical behaviour due to interfacial interactions between the inorganic particles and carbon matrix[3]. Further, incorporation of NGQDs also provided favourable functional groups for immobilization of biomolecules such as antibody specific to OTA (anti-OTA) and bovine serum albumin (BSA). NGQDs@ZrO$_2$ nanoflowers were mixed with 1% Nafion solution to form stable and adhesive film on indium tin oxide (ITO) coated glass substrate using a simple drop-casting method[4]. FTIR and electrochemical studies confirmed the successful immobilization of anti-OTA and BSA on Nafion/NGQDs@ZrO$_2$/ITO electrode. The fabricated of BSA/anti-OTA/Nafion/NGQDs@ZrO$_2$/ITO immunosensor revealed improved and selective detection of OTA in the linear range of 1-15 ng mL$^{-1}$ with a sensitivity of 1.3 µA ng$^{-1}$ mL cm$^{-2}$ and LOD of 1 ng mL$^{-1}$.

Bone cements are usually used for the temporary fixation of bone fractures, while dental cements are used as temporary linings and/or fillings for teeth cavities. A wide range of bone and dental cements have been developed since the early discovery of these cements in the 20th century. The main differences between currently available cements are their compositions as well as their properties and long term performance. However, there has not been such a cement that fulfills all requirements of bone or dental filling applications. This is attributed to the superiority of natural bone and teeth structure and properties over all developed cements in the market. Therefore, nanomaterials in the form of biocompatible nanoparticles and nanofibers have been heavily investigated as fillers to the optimally recognized bone and dental cements to improve their overall performance. The current study reviews the latest advances in this regard with a special reference to biocompatible nanomaterials that have been found highly promising for a long term use in cement formulations. The study reviews the latest updates in the last 10 years with a critical comparison of the properties and potential of new cements formulations made thereafter.
Electrospray Fabrication of Chitosan Nanoparticles for the Treatment of Hepatocellular Carcinoma

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Since the emergence of nanotechnology, attention has centered upon utilizing it to its best abilities. Tackling problematic medical issues through nanotechnological approaches has seen an increasing demand among the research community, in particular oncologists as cancer remains one of the leading causes of death worldwide. Multifunctional biocompatible nanoparticles (NPs) offer a new perspective on drug delivery systems by offering solutions to the usual anti-cancer drug shortcomings such as low solubility, bioavailability and absorption. NPs may be used to directly deliver anti-cancer drugs to the tumor site in order to maximize efficiency of drug delivery.

For this study, chitosan nanoparticles were selected to be prepared using an electrospray method. Electrospray has been reported to generate reproducible polymer particles along with the ability to manipulate the particle size by changing the synthesis parameters such as working distance, flow rate, voltage and polymer concentration. Further, therapeutic agents such as metformin and vismodegib as well as a targeting agent, EpCAM monoclonal antibody, were selected as bioactive agents that are specific to target and eliminate cancer stem cells (CSCs).

In the current study, chitosan nanoparticles were prepared by an electrospray approach. Nanoparticles were characterized by infrared spectroscopy, thermogravimetric analysis and scanning electron microscopy. Currently, chitosan nanoparticles decorated with metformin, vismodegib as well as EpCAM monoclonal antibody as targeting agent are being prepared for testing in vitro with hepatic cancer stem cells. These experiments are highly expected to produce a successful system for a targeted treatment of hepatic carcinoma.
Fabrication of Starch-PVA Films Incorporated with Oleoresin for Food Packaging Applications

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Bioactive edible films were prepared by blends of starch isolated from Colocasia esculenta and polyvinyl alcohol (PVA), incorporated with Oleoresin (OL) extracted from Curcuma longa (CL). The antimicrobial, antioxidant, physicochemical, mechanical and barrier properties of the films were studied with the varied concentration of OL in contrast to glycerol as plasticizer and glutaraldehyde as a crosslinking agent. The OL (5%) incorporated films exhibited antibacterial activity in relative percent inhibition to standard rifampicin is 142 ± 13% and 118 ± 9% against E. coli a gram-negative and a gram-positive Bacillus cereus respectively. The flavonoids concentration was found to be 24.5 ± 5 µg/cm² quercetin equivalents and total polyphenols content was 62 ± 8 µg/cm² Gallic acid equivalents. DPPH inhibition capacity of the films in IC₅₀ value showed to be 0.7 ± 0.06 cm²/ml, iron chelating activity is 0.25 ± 0.03 cm²/ml, nitrate scavenging capacity is 0.075 ± 0.008 cm²/ml, and FRAP assay is 0.02 ± 0.003 cm²/ml. Fourier transform infrared spectrum and X-ray diffraction indicated the miscibility and interaction between the starch-PVA and OL, scanning electron microscopy revealed the starch-PVA as a cocontinuous phase with OL and confirmed the interaction between starch-PVA and OL. Addition of OL restrained the amount of glycerol by improved the tensile strength of the films without affecting their puncture strength in the films with lesser glycerol. Oxygen permeability was higher and water vapor values were lower when compared to the films without OL. The average thickness of the films is 0.128 mm, moisture content is 0.12% and water solubility is 0.16%. Active films and film-forming solutions were intended to evaluate the shelf life of grapes, bread, and nutrient agar cakes; and the shelf life extended up to 6, 3 and 2 days respectively. The above study described the properties of starch-PVA films modified with the addition of OL and this finds its versatile application in food packaging.
Solid Acid Catalyst in Esterification Reactions

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The recent development of an environmentally benign solid acid catalyst has been a relatively cutting-edge area of research in the synthesis of value added esters and biodiesel. Solid acid catalysts are economically viable, effective, and environmentally friendly compared to conventional homogeneous catalysts and reusability of the catalyst is another advantage of these catalysts. Great efforts have been made by scientists to replace the conventional acid catalysts with solid acid heterogeneous catalyst in various organic transformations. Various solid acid catalysts like zeolite, heteropoly acids, Amberlyst-15, Nafion-H, silica sulfuric acid, silica phosphoric acid with lower toxicity, high stability and recyclability have attracted more attention. The applicability of sulfonic acid functionalized solid acid catalysts in the well-known esterification and transesterification reactions for the synthesis of esters and biodiesel, respectively, along with their reusability aspects has been discussed in the recent literature.[1,2]

This presentation will highlight the application of sulfonic acid functionalized solid acid catalysts as an environmentally benign catalyst in the synthesis of various organic compounds having industrial and pharmaceutical applications.

Nanoparticles Embedded in Graphene Oxide: Toward Photochemical Applications

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Nanocomposite materials based on metal nanoparticles and graphene oxide (GO) have attracted considerable research interest because of their potential applications, including surface-enhanced Raman scattering, catalysis, sensors, biomedicine and antimicrobials. In this study, several GO/ZnO nanocomposites were synthesized via changing the ratio of GO to ZnO (6.25, 3.125, 1.25, 0.625 and 0.125%) and used as photocatalysts for degradation of organic pollutants present in water. The degradation of methylene blue (MB) was investigated as model compound. An optimum catalytic activity of 84% was achieved using a nanocomposite with 3.125% GO, exposed to irradiation of sunlight for 90 min. Furthermore, a nanocopper, nanopalladium and nanosilver particles were used as dopants to study their effects on activity of the photocatalyst. The GO/ZnO/Cu and GO/ZnO/Pd composites decreased activity toward MB degradation to approximately 50% and 70%, respectively. However, a significant increase in the activity of MB degradation was achieved using GO/ZnO/Ag, which reached 100% of MB degradation after only 30 min exposure to light irradiation.
Photocatalytic Degradation of Aniline Blue Dye in an Aqueous Solution by ZnCdS Catalyst under Sunlight Radiation

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The sodium salt of aniline blue dye is water soluble and it is usually used in inks and as a coloring agent for wool, nylon, leather, and paper. The presence of this compound and other dyes in surface water and wastewater is a serious issue and has been acquiring increasing interest because of unidentified environmental effects and probable damage to aquatic life. Aniline blue dye could escape intact from conventional treatment plants, and consequently get into the environment. In this study, three zinc cadmium sulfide catalysts (ZnCdS) were prepared, namely, Zn_{0.2}Cd_{0.8}S, Zn_{0.5}Cd_{0.5}S and Zn_{0.8}Cd_{0.2}S, to photocatalytically degrade aniline blue in aqueous solution using sunlight irradiation. Approximately 95% degradation of the dye solution was achieved in 120 min. The kinetic studies showed that photodegradation of aniline blue follows first order reaction kinetic model. Effective parameters such as pH, photocatalyst dose and contact time were optimized and well investigated. Furthermore, the identification of aniline blue intermediates during photocatalytic degradation was analyzed using LC-MS/MS. A reaction pathway is proposed based on the intermediates detected.
Resource Recovery from Scrap Tires through Catalytic Pyrolysis

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This study aims to examine the influence of various catalysts on tire waste pyrolysis oil using a small pilot-scale pyrolysis reactor with a capacity of 20 L. The catalytic pyrolysis using an Al₂O₃ catalyst produced maximum liquid oil (32 wt%) followed by Ca(OH)₂ (26 wt%), natural zeolite (22 wt%) and zeolite (H-SDUSY) (20 wt%), whereas liquid oil yield of 40% was obtained without catalyst. The GC-MS results confirmed the pyrolysis liquid oil produced without catalyst was comprised of up to 93.3% mixed aromatic compounds. The use of catalysts decreased the concentration of aromatic compounds in liquid oil down to 60.9% with Ca(OH)₂, 71.0% with natural zeolite, 84.6% with Al₂O₃. However, synthetic zeolite increased aromatic compounds, producing 93.7%. The FT-IR data revealed that a mixture of aromatic and aliphatic hydrocarbon compounds was found in all liquid oil samples. The characteristics of pyrolysis liquid oil had viscosity (1.9 cSt), density (0.9 g/cm³), pour point (-2 °C) and flash point (27 °C), similar to conventional diesel. The liquid oil had higher heating values, key feature of a fuel, in the range of 42-43.5 MJ/kg that is same to conventional diesel (42.7 MJ/kg). However, liquid oil requires post-treatments to be used as a fuel or source of energy.
Structural and Electronic Properties of Na$_2$Ti$_3$O$_7$ and H$_2$Ti$_3$O$_7$

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Hydrogen and sodium titanates have attracted interest as possible photocatalysts for energy conversion, storage and environmental remediation. Here, first-principles calculations based on density functional theory have been carried out to study their crystal and electronic structures, exfoliation behaviour and defect formation. In the hydrogen titanate, half of the hydrogen forms water in the stoichiometric compound, and the crystal cell has a lower symmetry with respect to its sodium counterpart. H$_2$Ti$_3$O$_7$ and Na$_2$Ti$_3$O$_7$ have electronic gaps of 2.96 eV and 3.13 eV, respectively. Hydrogen and sodium vacancies are the defects with the lowest formation energies, making these compounds p-type semiconductors. Oxygen vacancy formation is suppressed with respect to titanium dioxide. Finally, the two compounds have a low surface energy, promoting exfoliation of the bulk and the formation of 2D materials and nanotubes.
Valorization of Bio-methane Production from Waste Activated Sludge using Newly Synthesized Visible Light Cr$_2$O$_3$/C$_3$N$_4$-(6M) Photocatalyst

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Herein, a visible light active photocatalyst Cr$_2$O$_3$/C$_3$N$_4$-(6M) composite was prepared by a high temperature calcination method and successful applied for improvement in bio-methane production from waste activated sludge. The composite samples were characterized by XPS, XRD, SEM, EDX, UV-visible spectroscopy and particle size analysis, which clearly indicated the coexistence of both Cr$_2$O$_3$ and C$_3$N$_4$ in the composites. The catalyst was initially tested for its photocatalytic activity and afterward applied for solublization of waste activated sludge in anaerobic digestion process. The application of Cr$_2$O$_3$/C$_3$N$_4$-(6M) for photocatalytic pretreatment of sludge released the soluble substances in solution where sCOD was increased from 431 mg/L to 3666 mg/L after 6 h. Further, volatile solids (VS) content decreased by 9.1%, which indicated that the short time pretreatment could avoid the further mineralization of organic to complete degradation. Thereafter, anaerobic digestion of solubilized sludge in bioreactor was achieved 634 ml/kg VS of methane and 46% of organic matter removal efficiency (OMRE), compared with 472 ml/kg VS and 402 ml/kg VS of methane, 35 and 31% of OMRE in photolytic and raw sludge (control) reactors, respectively. These results can provide a useful base and reference for the applications of Cr$_2$O$_3$/C$_3$N$_4$-(6M) photocatalyst in enhancement of degradation of toxic pollutants in wastewater and sludge stabilization with bioenergy production in practice.
Chitosan Coated Cotton Cloth Supported Zero-Valent Nanoparticles: Simple but Economically Viable, Efficient and Easily Retrievable Catalysts

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A simple, economically viable and fast method has been utilized for the preparation of highly active metal nanoparticles (MNPs) in coating layer of chitosan (CH) over cellulose microfibers of cotton cloth (CC). 2 wt% CH solution was used for the coating of CC strips (CC-CH), and were placed in aqueous solutions of metal salts to adsorb metal ions. The CC-CH templated with metal ions were then treated with aqueous solution of sodium borohydrate to reduce the metal ions into nano zero-valent metal nanoparticles (nZV-MNPs). The CC-CH strips loaded with nZV-MNPs were characterized by XRD, XPS, ATR-FTIR, FE-SEM, EDS and TGA, which indicates the successful synthesis of nZV-MNPs by this method. The nZV-MNPs/CC-CH strips were used as an efficient catalyst for the model reduction reaction of nitrophenol and toxic organic dyes. Compared to all loaded nZV-MNPs, Fe/CC-CH showed good catalytic activity for 4-NP and Rh-B dye reduction in the presence of NaBH₄ with rate constant of 0.2937 min⁻¹ and 0.3804 min⁻¹, respectively. Moreover Fe/CC-CH has good catalytic reduction ability for MO and MB having rate constant equal to 0.1698 and 0.2802 min⁻¹, respectively. In addition to the good catalytic ability, it could be easily recoverable as compared to other available techniques. The recovery was completed by simply pulling the strip from the reaction matrix after completion of the reaction and can be used several times.
ZnO/Au/BN for Photocatalysis and its Antibacterial Effects

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A recent method for the treatment of waste water is using nanomaterials as photocatalysts to degrade toxic or harmful compounds by exposure to solar radiation. ZnO has been widely used as a photocatalyst due to its wide band gap, high photochemical stability, low cost and non-toxic nature. In this research, ZnO/Au/BN nanocomposites were synthesized using a quick and environmentally friendly microwave hydrothermal method in a CEM microwave. As ZnO has poor quantum yield, Au was used to delay the process of recombination of the photogenerated electrons and holes. Functionalized BN provided a high surface area for optimizing the photocatalytic activity of ZnO in addition to enhancing activity in visible light region. The nanocomposite was analyzed using XRD, UV-vis, FT-IR, and its morphological structure was confirmed by SEM. Photocatalytic tests were done along with antibacterial studies, which are in progress.
SnO$_2$/Au/BN Nanocomposites as Photocatalyst and its Antibacterial Effects

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Photocatalysts play an important role in the degradation of organic pollutants. They have also shown to simultaneously inactivate bacteria. SnO$_2$ is a semiconductor, having a band gap of 3.6 eV that has potential as a photocatalyst. However, the issue of electron hole recombination with photocatalysts persists. Moreover, efficient absorption in visible range is a challenge. To address these issues, SnO$_2$/Au/BN nanocomposite was synthesized and showed enhanced photocatalytic activity compared to SnO$_2$. Functionalized BN was shown to improve the visible light absorption for photocatalysts like TiO$_2$. Similar behavior was observed with our nanocomposite. In this work, we synthesized SnO$_2$/Au/BN nanocomposite via an easy, eco-friendly and one pot synthesis method. The synthesized material was characterized using XRD, IR, UV, and SEM techniques. The effects of certain synthesis parameters on size and shape have also been examined. The antibacterial study for the nanocomposites is in progress.
Impact of the Substitution of PbO by PbF$_2$ on Structural Properties and Luminescence of Neodymium-doped Lead Borate Glass

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Rare-earth-doped glasses have great significance for potential applications in optical devices and laser technology. The glass samples were prepared using a melt quenching technique. XRD, FTIR, UV/VIS/NIR spectroscopy and photoluminescence were used to measure the glass samples. The prepared glass was amorphous in nature. Results further showed that lead oxide was inserted into the glass matrix. Analysis of splitting of Nd$^{3+}$ in glasses, UV–Vis–IR spectra exhibit ten prominent bands centered at 428, 457, 471, 511, 524, 582, 624, 679, 744, 803 and 875 nm corresponding to the transitions from the ground state to $2P_{1/2}$, $4G_{11/2}$, $2D_{3/2}+2G_{9/2}$, $4G_{9/2}$, $2K_{13/2}+4G_{7/2}$, $4G_{5/2}+2G_{7/2}$, $2H_{11/2}$, $4F_{9/2}$, $4S_{3/2}+4F_{7/2}$, $4F_{5/2}+2H_{9/2}$ and $4F_{3/2}$ respectively.

The Judd–Ofelt intensity parameters $\Omega_{\lambda}$ ($\lambda=2$, 4, 6) were determined from the spectral intensities of absorption bands as $\Omega_{6}>\Omega_{4}>\Omega_{2}$ and the presence of the emission peak due to the presence of lead oxide. The emission intensity is found to decrease with the increase of Nd$^{3+}$ concentrations due to the quenching effect.
Electrospinning as a Tool in Controlling the Morphology and Porosity: A Electromagnetic Interference Shielding Perspective

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Electrospinning of polymers has emerged to be one of the most versatile techniques to obtain a wide variety of nanofibers and structures in sub-micron to nano range.[1] In this process high voltage is used between nozzle tip and collector to stretch the polymer solution in obtaining nanofibers. Electrospinning aids in generating various morphologies by tuning processing parameters like applied voltage, flow rate, tip to collector distance, needle diameter, type of collectors, process duration with much ease. Hence, it has found application in diverse areas of tissue engineering, air filtration, supercapacitors, sensors and solar devices.

In this study, nanofibers of various shaped cross sections through the electro spinning process has been shown by (i) use of various solvents (ii) solvent effect on various polymers and (iii) collector rotating speed. Morphological analysis was carried out to obtain various geometrical structures using poly (vinyl alcohol), PVA, poly (methyl methacrylate), PMMA and poly (ethylene oxide), PEO as case studies. This model was next extended to conjugated polymers (Poly(3,4-ethylenedioxythiophene) Polystyrene sulfonate, PEDOT:PSS) to obtain nanofiber mats.[2] Hence this study would be beneficial in understanding the effect of electrospinning parameters on evolving morphology employed for various applications.

Further, electrospinning of PEDOT:PSS/PVA/PEO, a ternary blend was carried out, and its electromagnetic interference (EMI) shielding properties were studied.[3] Wherein the effect of porosity in ternary blend nanofiber mat was studied for X-band (8.2-12.4 GHz) and Ku-band (12.4-18GHz). Thus demonstrating the effective shielding stability in PEDOT:PSS ternary blend.

References
Approximation Technique to Determine the Solar Cell Temperature in Mega Solar Power Plants by using Climatological Data

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The demand of solar power plants is increasing day by day in remote areas. In this research there is constructing an analytical system which detects the modules of the mega solar power plant in which any fault occur. This analytical system is used to find the solar irradiations of mega solar power plants, which are used to find the power generated and temperature of any individual cell of the Mega Solar Power Plants. This research uses a technique to find the crystalline silicon solar cell temperature, which are very commonly used in Mega Solar Power Plants. This is achieved by using the measured data of wind speed, solar irradiations, powers of the cell and atmospheric temperature. This research shows a comparison of actual and measured data of the surface of the cell temperature and measured temperature of Quaid-e-Azam mega solar power plant Pakistan.
Analysis of Defect Free Pure Cadmium Oxide (CdO) Nanoparticles

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Electroluminescence devices based on transparent metal oxide semiconductors (II-VI semiconductors) have received much attention due to their wide applications from small area telecom devices to large area displays. Among the various transparent metal oxide semiconductors, cadmium oxide (CdO) is one of the most promising materials due to the existence of a relatively small band gap (2.2 eV), high luminescence efficiency, long life time, good stability, intrinsic defect center which turns it to a low resistive material and high transmittance in the visible region. It has been widely applied in optoelectronic devices such as phototransistors, photovoltaic cell, photodiodes, gas sensors, batteries, fuel cells etc. The physical and chemical properties of semiconducting nanoparticles are sensitive to defects. Therefore, improving the crystalline nature of CdO nanoparticles will find active application in blue/green laser diodes (LDs), LEDs (white and blue) as a complementary to several other transition materials. Moreover, annealing is an important parameter which can remove the defects or impurities from the surface of the sample. It may also be used to control the band gap and surface morphology through nanostructural rearrangement. In addition to annealing, the semiconducting nanoparticle leads to enhance the visible luminescence and modify the morphological properties. Tailoring those properties will play an important role to fabricate optoelectronic micro/nano devices.

Post-preparation annealing was carried out in this work to understand the presence of defects in the CdO powder sample prepared by precipitation technique. The starting materials taken for the preparation of CdO were CdCl\(_2\)·H\(_2\)O and NaOH. Pure CdO with cubic crystal structure was obtained for the sample annealed at 600 °C as examined by X-ray diffraction. Moreover, the characteristics bands of CdO are also analyzed using Fourier transform infrared (FTIR) spectroscopy. The scanning electron microscopy (SEM) with energy dispersive X-ray analysis (EDS) confirmed the presence of CdCl defects. The particle size distribution was analyzed using Dynamic Light Scattering (DLS), which was shifted towards higher values for the annealed CdO nanoparticles as compared to the as-prepared sample. The Raman spectrum showed bands at 400 and 450 cm\(^{-1}\) that correspond to two-phonon combinations such as longitudinal optical (LO) mode and transverse optical (TO) mode at the CdO Brillouin zone. From the photoluminescence analysis, the as-prepared and annealed CdO samples exhibit blue emission when excited at 320 nm. The defect free CdO nanoparticle shows approximately 88% improvement in the emission intensity, which makes CdO nanoparticles useful in producing micro/nano optoelectronic devices.
Dye-Sensitized Solar Cells (DSSCs) based on TiO$_2$/BN/Ag Nanocomposites

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Organic dyes and metals (Ag) have been used as sensitizers to improve the optical absorption properties of TiO$_2$ nanomaterials in the visible light region. It is a major challenge to modify titanium dioxide (TiO$_2$) due to its high chemical inertness, wide bandgap, narrow light-response range and a fast recombination of electrons and holes. Graphene an excellent candidate is used to enhance the performance of TiO$_2$ nanocomposite in DSSCs. Having an alternative isostructural material that is chemically stable, and thermally conductive may hold many advantages over the carbon analogue for certain applications.

In this work, TiO$_2$/h-BN/Ag nanocomposites were synthesized \textit{in situ} via microwave. The method is facile, quick, cost effective and eco-friendly. The synthesized materials were characterized using X-ray diffraction (XRD) and Fourier transform-infrared radiation (FT-IR) spectroscopy which confirmed the formation of TiO$_2$/h-BN/Ag with pure anatase phase of TiO$_2$. Optical properties such as band gap were studied using Ultraviolet/Visible (UV/Vis) spectroscopy which indicated modifications of the band gap of TiO$_2$ followed the addition of h-BN. Dye-sensitized solar cells (DSSCs) were fabricated using the synthesized TiO$_2$/h-BN/Ag nanocomposites. Results showed that a significant improvement of solar cell efficiency can be achieved using the synthesized TiO$_2$/h-BN/Ag nanocomposites. Interestingly, functionalized h-BN has shown to enhance TiO$_2$ activity in visible light range. Moreover, thermogravimetric (TGA) analyses showed that the as synthesized TiO$_2$/h-BN/Ag nanocomposites have high thermal stability with only 2-3% weight loss 550 °C.
Synthesis and Characterization of Lead Halide Perovskite for Solar Cell Applications

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The synthesis of a perovskite based on lead halide perovskites (CH$_3$NH$_3$)$_2$PbI$_3$ is reported. Simple precursors such as PbI$_3$ and CH$_3$NH$_3$Cl are used to synthesize this material under ambient conditions. The variation in the number of solution droplets on the substrate leads to different perovskites film thicknesses. The morphology, structure, optical gap of these perovskites are investigated using SEM couples with EDX, X-ray diffraction, and UV/Vis measurements, respectively. A stability study will be presented, which was carried out by measuring the absorption coefficient after exposing the perovskite to air for different time intervals. This organic–inorganic perovskite is receiving the interest of researchers due to its various optoelectronic applications.
Efficient Temperature Sensing using Photoluminescence of Er/Yb Implanted GaN Thin Films

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The luminescence characteristics of GaN films implanted with Er at low doses were evaluated. The defect-related yellow luminescence (YL) and green luminescence (GL) bands observed under direct excitation with 488 nm were attributed to the transitions via different charge levels of the same defect. The quenching behavior of the luminescence intensity either with the temperature or concentration variation can be attributed to nonradiative energy transfer (ET) and/or charge transfer by trapping impurities. The temperature dependence of the YL band allowed us to identify the defect responsible for this emission. The best candidate for this defect was found to be a nitrogen-vacancy. A GaN sample co-doped with Er$^{3+}$ and Yb$^{3+}$ ions was prepared, and its optical properties were analyzed. The incorporation of Yb$^{3+}$ improved the PL emission intensity in the visible region. This feature results from the efficient ET processes between these two doping ions. The color coordinate analysis indicates that Er$^{3+}$/Yb$^{3+}$ co-doped GaN semiconductor emits light with color in the white-light region. To investigate the temperature sensing application of the synthesized co-doped semiconductor, the temperature-sensing performance was evaluated using the fluorescence intensity ratio technique in the temperature range 200–300 K. The significant temperature sensitivity indicates its potential as a temperature sensing probe. The maximum sensitivity was 15×10$^{-4}$ K$^{-1}$ at 200 K.

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Sensors and Actuators B: Chemical 248, 769-776
Fabrication and Characterization of Gd$_2$O$_3$-HfO$_2$ based Memristor Devices for Gamma-Ray Detection

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While the research on metal-oxide memristive devices is actively pursued in the development of next-generation in-memory computing, little work is documented on the suitability of this technology for other critical application fields [1]. Environmental sensing brings up new avenues for integrating the low power memory and distributed state storage capabilities of a detector memristor, where the actual computing reservoir is tailored to simultaneously function as an environmental signal transducer [2,3]. Sensing ionizing electromagnetic radiations, such as gamma rays, is a subject receiving close review in radiation protection and dosimetry market [4]. In this area, the use of high-Z/high-k metal-oxide materials such as hafnia (HfO$_2$) and gadolinia (Gd$_2$O$_3$) in memristive radiation detectors, is attractive considering their recognized photoelectric receptivity and increasing appreciation among solid-state metal-oxide semiconductor dosimeters [5,6]. In this work, a 2×2 mm crossbar micro-thick Ag(TE)/ Gd$_2$O$_3$ – HfO$_2$ (~50 µm)/Cu(BE) metal-insulator-metal structure (where Gd:Gd+Hf is 0, 10 and 50 at.%) is developed for the first time, via a sol-gel drop-coating method. The objective of this work is to examine the suitability of the mixed metal-oxide computing reservoir for low-power memristive switching and active gamma-ray sensing, under ambient conditions. Typically, the memristor’s switching polarity, turn-on voltage, resistance ratio, and response-current are systematically explored through I-V characterization to establish a preliminary understanding of the electrical transport properties across the device with varying Gd$^{3+}$ doping composition. Additional complementary scanning electron-microscopy/energy dispersive X-ray spectroscopy (SEM/EDS) mapping studies are conducted to assess the quality and composition of the insulator oxide layer upon fabrication and after electrical testing. A preliminary structure-to-performance comparison is established across the native and doped devices before, during and after ambient exposure to Cs-137 662 keV gamma-rays (source activity ~0.67 MBq).

References:

This work is funded by the United Arab Emirates Space Agency, Space Missions Science and Technology Directorate, project reference K08-2016-001.
FP-LAPW Study of the Effective Masses and Bonding Properties of Zinc-Blende Cadmium Chalcogenides

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We present the results of density functional calculations to study the electronic structures and the effective masses for II-VI zinc-blende wide band gap semiconductor compounds by computing the curvature of the principal band extrema at the Γ point. We also calculated the optical properties of the technologically important, using the full potential linearized augmented plane wave method within the (GGA) approximation. Our calculations were performed to evaluate the dielectric function (real and imaginary parts), and the loss function of the II–VI semiconductors. Also the refractive index and extinction coefficient are studied. Detailed comparisons are made with published experimental and theoretical data and show generally good agreement. The present results regarding the studied quantities are predictions and may serve as reference for experimental work.
The Effect of Pressure and Interstitial Substitution on the Electronic Properties of Molybenum Disulfide

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Molybdenum disulfide has some of graphene’s properties but has an edge over graphene as this new 2D nanomaterial has a band gap in its electronic structure, which is absent in graphene. The purpose of this study is to study the electronic properties of the Molybdenum Disulfide (MoS₂) material in its bulk and monolayer forms by undertaking a systematic theoretical approach. We will mainly study the band gap, the density of states and the electronic charge distribution which is considered as the most important electronic characteristics of semiconductors. In this study, the density functional theory (DFT) – implemented in WIEN2k and VASP- is used. The generalized gradient approximation (GGA), Modified Becke-Johnson and Hybrid functional approximation are used for the exchange–correlation potential. Band structure, density of states and band gap pressure coefficients are calculated. WSe₂ – MoS₂ heterostructure and the effect of impurities are covered to search for MoS₂ metallization and band gap tuning possibilities.

MoS₂, in its monolayer form, has a direct band gap (1.8 eV) in the visible range (1.6-3.1 eV) which makes it an excellent candidate for optical applications and increases the possibility of creating an electron-hole pair. The manipulation of the monolayer MoS₂ band gap can be done using substitutional impurities and induced pressure. Metallizing MoS₂ is possible by applying a positive pressure, which even widens the range of its applications.
Bioelectricity Generation from Human Feces by Microbal Fuel Cell using Graphite Electrodes

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Microbial Fuel Cell (MFC) is an emerging technique that offers wastewater treatment and simultaneous electricity generation for the increasing demand of sustainable energy and waste management. MFC generate electricity with the help of microorganism by utilizing the organic contents of the wastewater used as substrate that coincide the treatment of the wastewater. Diverse wastewaters are used in MFC as a substrate, due the rich organic content of human feces this study focuses on the use of its feasibility in electricity generation and its treatment by MFC using graphite electrodes. Dual chamber fuel cells with a high working volume of 1250 mL were fabricated. Two fuel cells were operated at batch mode with same operational condition. The fuel cells used in the experiment resulted in similar output under same operational condition. The highest voltage generated by the HFMFC (Human Feces MFC) was 560 mV, the maximum power density generated is 209168 mW/m$^2$. The HFMFC resulted in 92% COD reduction, Phospahte (P) 77% and Sulphate (S) 78%, Columbic efficiency (CE) 76%. The study shows the promising potential of human feces for electricity generation by MFC and its treatment.
Enhanced Photoelectrochemical Water Splitting on a Stainless Steel 316L Porous-nanostructured Photoanode

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The urgency to secure alternative resources for fossil fuels along with the advanced revolution in nanoscience have stimulated a significant motivation in the sector of energy to develop nanostructured materials for several electrochemical and photoelectrochemical applications. Of these applications, the hydrogen production, storage, and oxidation received exceptional attention in renewable energy plants. Actually, most of renewable plants perform efficiently under certain circumstances (e.g., the daytime for solar cells). Therefore, a storage/restoring system is required to save excess electricity from the time of plenty to the time of delay. So far, the applications of water splitting experience a lack of materials ensuring enhanced efficiency and reasonable stability. We herein propose a procedure to develop metal oxide nanostructured-based material for solar energy conversion. We herein suggest a propitious photoanode prepared by the anodization strategy for water splitting. This novel photoanode is composed of nanoporous arrays of stainless steel 316L oxide films. The anodization parameters (potential, time, temperature, electrolyte, pH, etc) were tuned to improve the catalytic properties towards visible-light-driven water splitting. The morphology, composition, and crystal structure of as-prepared photoanode were investigated using the state-of-art instrumentations as the field-emission scanning electron microscope, the energy dispersive X-ray spectrometer and the X-ray photon electron spectroscopy (XPS). The current-potential measurements were carried out in a three-electrode electrochemical cell and a scanning potentiostat was employed to measure the dark and illuminated currents.
A Study on the Lifetime and Photostability of Chalcogen based D-A-D polymer OPVs

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A power conversion efficiency of ~13% has reached for organic photovoltaic devices (OPV), as most of the research efforts have been focused on improving power conversion efficiency (PCE), so as to compete with the more developed silicon solar cells. Apart from the PCE, just as important but less considered element is material stability. Improving the stability of organic devices would greatly enhance their industrial viability. This work focuses on the stability of chalcogenide based D-A-D polymer (i) active material, and (ii) as organic photovoltaic devices. An investigation on the lifetime of the un-encapsulated devices at inert atmosphere and ambient condition has been carried out. An initial study on the OPVs shows that they are stable for more than 5000 hrs at ambient conditions. One of the main contributors of the device decay is the photo oxidation of the active layer. An analysis of the photostability of the un-encapsulated polymer and polymer fullerene blend (which forms the active layer of the OPV) exposed to ambient conditions will be presented. The photostability of the polymer on active material improves by mixing with fullerene. Since the fullerene acts as a scavenger to protect the polymer from undergoing photodegradation. A detailed study on the photodegradation of the active layer in the OPV will be presented.
Energy levels and the physiochemical properties of hole transporting materials can be finely tuned by introducing the fluorine atom in the molecule. Thus, compared to non-substituted fluorine derivatives, the fluorinated hole transporting materials generally show better device performances because of their lower HOMO levels, planar backbones, and internal dipole moments. In order to study the effect of fluorination on hole transporting materials for the efficient perovskite solar cells, we designed and synthesized a novel D-A-D type hole transporting molecule having benzo[1,2-c][1,2,5]thiadiazole (BTD) as electron acceptor unit and thiophene (Th) as a simple electron donor unit. The D-A-D molecules were synthesized by palladium(0) catalyzed Stille coupling reaction. The electrochemical band gap of synthesized compounds varies from -1.5 eV to -1.7 eV. These molecules are expected to show good hole mobility. Further, synthesized polymers expected have desired HOMO and LUMO energy levels such that it is ideal as a hole transport material (with perovskite active layer) and effective electron blocking layer. Perovskite solar cell will be fabricated using synthesized D-A-D type molecule as hole transporting material. The architecture of the perovskite device is glass/ITO/TiO₂/Perovskite/Hole Transport Material/Au. Further, device morphology will be studied using AFM, SEM, etc.
Photocatalytic Reduction of CO\textsubscript{2} by Employing ZnO/Ag_{1-x}Cu\textsubscript{x}/CdS and Related Heterostructures

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In view of the great importance of finding ways to reduce CO\textsubscript{2} by using solar energy, we have examined the advantage of employing heterostructures containing bimetallic alloys for the purpose. This choice is based on the knowledge that metals such as Pt reduce CO\textsubscript{2}, although the activity may not be considerable. Our studies with reduction of CO\textsubscript{2} by ZnO/M/CdS (M = Ag, Au, Ag\textsubscript{1-x}Au\textsubscript{x}, Ag\textsubscript{1-x}Cu\textsubscript{x}) type heterostructures in liquid phase have shown good results specially in the case of ZnO/Ag\textsubscript{1-x}Cu\textsubscript{x}/CdS reaching a CO production activity of 327.4 µmol h\textsuperscript{-1}g\textsuperscript{-1}. The heterostructures also reduce CO\textsubscript{2} in the gas-phase although the production activity is not high. Some of the heterostructures exhibit reduction of CO\textsubscript{2} even in the absence of sacrificial reagents.
Utilizing the Potential of Raw and Modified Natural Zeolite for the Process Optimization of Food Waste Composting

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The present study aims to optimize food waste (FW) composting through the addition of natural zeolite. Raw and modified natural zeolite was applied at 10 and 15 % (w/w) of the total waste and compared with an un-amended control trial using an in-vessel compost bioreactor. The use of natural zeolite significantly affects the composting process, however the prominent results for compost stability parameters were observed for 15 % zeolite concentration. Similarly, for raw and modified natural zeolite the prominent results were recorded for modified natural zeolite. It was noticed that the rapid and long term thermophillic temperature and moisture content reduction to an optimum range was recorded for modified natural zeolite. Furthermore, on the basis of peak values the total ammonium (NH$_4^+$) and nitrate (NO$_3^-$) concentration in modified natural zeolite was increased by 11.1 and 21.5 %, respectively in comparision to raw zeolite. Compost stability for the studied parameters such as moisture contents (MC), electrical conductivity (EC), organic matters (OM), total carbon (TC), mineral nitrogen, nitrification index (NI) and germination index (GI) was achieved after 60 days of composting that was in accordance with international compost quality standards. Therefore, the present study suggested the suitability of modified natural zeolite addition at 15 % to the total waste as the best formulation for the composting of FW for achieving a value-added stable compost.
Electrochromism is the phenomenon displayed by some materials of reversibly changing colour under the application of small voltage. In order to attain maximum charge storage capacity and hence to improve coloration efficiency, electrochromic material should have xerogel like structure as well as material should have high cyclic stability in acidic electrolytes. Tungsten oxide (WO$_3$) thin films prepared by spray pyrolysis technique in our laboratory were having relatively porous and favorable structure for ion intercalation/de-intercalation. Also the WO$_3$ thin films have exhibited higher coloration efficiency, but have relatively low electrochemical stability. So in order to improve the EC performance these two materials can be combined in layered form and accordingly we have made attempts in this direction and results of layered structure are presented in this manuscript. The optimum content for the layered configuration is Nb$_2$O$_5$=45 mL and WO$_3$=5 mL, which has shown electrochemical reversibility and coloration efficiency 96% and 19 cm$^2$/C.
Prepreg Waste to Produce Sustainable Non-Structural Aerospace Elements

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The volume of the prepreg scrap is growing rapidly in the near future because of the increase in demand for carbon fiber prepreg from the aerospace industry. The carbon footprint needs to be reduced through recycling. The aim of this research is to recycle carbon fiber prepreg wastes to produce subsidiary structural elements that can be used for many non-structural applications. Pre-impregnated means that the carbon fibers are combined together with a predefined amount of resin and protected by thin polyethylene film. Our research satisfies the waste management policies aiming to minimize waste pollution. However, the waste management’s laws from the Competent Authority, an environmental agency in Abu Dhabi, is taken into consideration. As a result, two techniques were used to handle the prepreg waste. The first one was using the hot press. The second method was using autoclave in STRATA. We started in the preparation of carbon fiber samples using shredders. Three samples were obtained in different formations fine, not fine and strips. Three different techniques were used to handle the shreds samples. In the hot press methodology, the technique produces open mold products and was carried out for three grades of shredded carbon fibers with the packing polyethylene (Nylon) film. In addition, closed mold were produced by hot pressing the fine shreds in a cylindrical aluminum mold. Under the autoclave methodology in STARTA, fine shreds, coarse shreds and strips of carbon fiber produce cured carbon fiber samples. After producing the samples, a tensile test is implemented to investigate the mechanical properties of the specimen.
Enhanced Efficiency of Dye-Sensitized Solar Cells using Coffee as Natural Dye on TiO$_2$/RGO Nanocomposite based Photoanode

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In this work, a simple, cost effective, and biofriendly methodology was reported to design sol-gel assisted TiO$_2$/RGO nanocomposites used as the materials for the dye-sensitized solar cells (DSSCs) working electrode using coffee extract as a dye and carbon as a counter electrode by candle flame. The XRD and TEM results confirmed that the TiO$_2$ nanoparticles were crystallized in the tetragonal anatase phase. TEM images showed the TiO$_2$ nanoparticles are uniform and densely covered on the surface of the graphene oxide. Modification of the anatase TiO$_2$ NPs was carried out by incorporating graphene oxide (GO) to enhance the efficiency. The results showed that the TiO$_2$/RGO (2 wt%) nanocomposites electrode exhibited a power conversion efficiency (PCE) of DSSCs, with a maximum value of 4.63% compared to 2.1% of DSSCs with pure TiO$_2$. This enhancement in the performance of DSSC with RGO might be due to the improvement in dye loading, preventing the electron–hole pair recombination process and also improved the electronic conductivity for the photogenerated charge carriers. This technique may be used for large scale production using existing economical, biosafe, and highly effective DSSCs fabrication technique.
Synthesis and Characterization of Highly-ordered Cu Nanowires using Electrodeposition Template Method

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Remarkable advancement in modern material technology have facilitated the use of nanomaterials for application in diverse fields of science, engineering, and healthcare. Nanomaterials exhibit novel physical, chemical, optical, and electro-mechanical properties depending upon their size and morphology. Among different nanostructures, 1D nanowires have significant importance as electrodes in photovoltaic devices. The nanowires offer direct electrical path for rapid collection of charge carriers throughout the device structure. Here, well-aligned and highly ordered Cu nanowires have been synthesized using a simple template-assisted electrochemical deposition technique. The electrochemical deposition technique offer accurate process control for in situ growth of Cu nanowires. There are several parameters that effect the growth of nanowires inside porous alumina membrane such as pH of electrolyte solution, deposition time, temperature, and deposition voltage. By varying these parameters, the length of Cu nanowires can be controlled. This mechanism opens up new opportunities for fabrication of several metallic or semiconducting or hybrid nanowires depending upon the growth mechanism. The present work deals with investigation of optical properties, morphological studies, growth directions, and crystalline properties of as produced nanowires using different microscopic and spectroscopic techniques. The synthesized nanostructures are proposed to be utilized in solar cell applications.
An Overview of Grain Size Distribution, Geochemistry and Mineralogy of Red Sea and Arabian Sea Sediments

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Arabian Peninsula is landlocked in between Arabian Sea in east and Red Sea in west. Area is exposed to high aridity and grain size distribution is mainly controlled by seasonal wadis. Texturally, sediments in the Red Sea and Arabian Sea classified as gravel, sand and mud. Sand dominates in nearshore areas and fine fraction increases with increase in depth. The major mineralogical constituents of the surficial sediments of Red Sea are carbonate minerals (calcite and aragonite) and detrital siliciclastic minerals (quartz and feldspar). Some evaporitic deposits and trace of pyrite is also noted in the sediments depicting reducing environment at some locations. Whereas, in Arabian Sea, fine grained terrigenous sediments are enriched in Al and coarse grained sediments are comprises of carbonate material. This grain size variability in conjunction with mineralogical assemblage present in the sediments controls the distribution and abundance of major and trace elements, CaCO$_3$ and organic content. In Res Sea, sand friction is composed of carbonate material eroded from coralline terraces and terrigenous detrital material transported by seasonal wadis during monsoon and contains high concentration of Ca, Mg and Sr, whereas, trace element concentrations are positively correlated with mud, Fe, Al, Ti, Mn, Cu, Cr, Co, Ni, V and B contents. In Arabian Sea, Ca and Sr is associated with carbonate material and terrigenous association comprising Al, Fe, Mg, Ba, Mn, Zn, Cu, Cr, V, Ni and Hg.
An Eco-Friendly Microwave-Assisted Click Synthesis, Characterization and Anticancer Screening of Novel 1,2,3-Triazoles Tethering Benzimidazole and Sulfa Drug Conjugates

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Benzimidazoles are one of the most prevalent classes of pharmacologically active azoles endowed with important pharmacological properties such as anti-inflammatory, antiviral and antitubercular activities. Moreover, Sulfa drugs are of particular interest as antibacterial, anticancer, antitubercular and antifungal agents. The 1,2,3-triazole ring system has been also recognized as a fascinating scaffold for a number of chemotherapeutic agents that have exhibited remarkable medicinal potentialities. Recent advances in modern drug design aimed to introduce the 1,2,3-triazole moiety as a connecting unit to link together two or more pharmacophores for the design of novel bioactive molecules. The present study reports the click synthesis and anticancer screening of novel benzimidazole-1,2,3-triazoles appended with sulfa drug moieties under both conventional and microwave procedures.

Base-catalyzed alkylation of 2-mercaptobenzimidazole with one or two equivalents of propargyl bromide in presence of triethylamine as catalyst selectively produced the thiopropargylated benzimidazole in 93 % yield. Conversely, when the propargylation was carried out in presence of sodium bicarbonate, the S,N-bis(propargylated) benzimidazole was obtained in 89 % yield. The click 1,3-dipolar cycloaddition reaction of the mono- and/or bis(propargylated)-imidazoles with a variety of sulfadrug azides, conducted in DMSO:H2O (1:1) in presence of sodium ascorbate and copper(II) sulfate at room temperature, afforded the regioselective 1,4-disubstituted mono- and bis-1,2,3-triazoles tethered with sulfa drug-benzimidazole molecular conjugates.
Eco-Friendly Synthesis of a New Class of Ionic Liquids with Attractive Biological Activity

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Considerable interest in many chemical industries has been directed toward finding alternatives to toxic or hazardous volatile organic compounds (VOCs). For these problems ionic liquids (ILs) appear as suitable solution due to their outstanding properties, which include zero- vapor pressure, good chemical and thermal stability, low flammability, excellent solubility for many organic and inorganic compounds and high ionic conductivity [1]. The general definition of ILs are organic salts with a melting-point below 100 °C which contained organic cation, combined with various organic and inorganic anions [2]. The numerous combinations made between the cation and the anion permits the design of appropriate ILs for a particular application.

ILs have been dramatically expanding in popularity as a new generation of chemicals with potential uses in various areas in industry. Additionally, several studies have shown the very interesting biological activity of ILs against both environmental and clinically important microorganisms [3-6].

Following on our work on the synthesis of ILs, recent results concerning an efficient green method for the preparation of novel functionalized ionic liquids using ultrasound containing combined antibacterial, antifungal and antitumor Pharmacophore sites will be presented.

References
Silver nanoparticles (AgNPs) were biologically synthesized in an eco-friendly manner using aqueous leaf extracts of *Origanum majorana* and *Ambrosia maritima* plants and silver nitrate (AgNO₃) solution. Size, shape, and crystallinity of the biosynthesized AgNPs were determined by using a transmission electron microscope (TEM). Zeta potential analysis was used to demonstrate the stability of the metallic nanoparticles, while Fourier transform infrared spectroscopy (FTIR) was used to identify the bioreducing and capping agents. AgNPs were electrochemically investigated using cyclic voltammetry (CV), while the optical properties of the metallic nanoparticles were studied using UV-Vis and fluorescence spectroscopies. According to TEM images, AgNPs are spherical with an average size of 35 nm. TEM also shows the presence of mono and polycrystalline AgNPs. The value of zeta potential (−39 mV and −26.29 mV, respectively) proved the stability of AgNPs caused by capping molecules of *O. majorana* plant. CV studies showed that AgNPs were electrochemically investigated at 0.39 mV and 0.4 mV, respectively. AgNPs showed a surface plasmon resonance peak at 440 nm, while the emission peak was detected at 466 nm. These nanoparticles are promising for many industrial and medical applications.
**H$_2$S Gas Sensor based on Chitosan-WO$_3$ Hybrid Nanocomposite**

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The nanostructure tungsten oxide (WO$_3$) has been one of the most promising metal oxide-semiconductor materials that is widely used in H$_2$S gas monitoring systems. WO$_3$ nanoparticles (NPs) enhance the results of H$_2$S gas sensors because of its outstanding characteristics such as small size, simple construction, low weight, low power consumption and cost effectiveness.

Low-power and selective H$_2$S gas sensors based on tungsten oxide (WO$_3$) nanoparticles embedded in organic polymer membranes are presented in our work. WO$_3$ NPs were synthesized using the sol-gel method. Polymer solutions consisting of chitosan and ionic liquid (IL) were doped with WO$_3$ NPs. Then, the doped solutions were casted to obtain flexible membranes (200 mm in thickness). The sensors (CS-IL-WO3 NPs membranes) are under continuous testing to investigate gas sensing performance and obtain the best working conditions by measuring the electrical current response signals at different operating temperatures.

The results revealed that the best response to H$_2$S gas for all sensors was obtained at 80 ºC, yet a reasonable response was noticed at a low operating temperature of 20 ºC. As a result, the power consumed to heat up the sensor is reduced by almost 89%. The detection limit of the sensor was 10 ppm and the results showed a fast response of 20.1 ± 3.4 s. Moreover, these sensors exhibited excellent reproducibility and stability, and were identified to be selective to H$_2$S. These characteristics, these sensors were identified to be promising materials for hazardous H$_2$S gas sensing applications.
Poster Session II

Al Hamra Convention Center

Monday, February 19, 2018 18:30-20:30
II.1 Influence of Magetite Incorporated on Zinc Oxide Hybrid Nanostructures

Selvendiran Periyasamy, Allen Joseph Anthuvan and Muthukumar Muthuchamy
Department of Environmental Sciences, Bharathiar University, Coimbatore, India

II.2 Structure Evolution with Temperature of Formamidinium Halide Perovskites

Department of Materials, University of California, Santa Barbara, United States of America

II.3 Analysis of Hybrid Concrete Using Red Mud, Pet Coke Adding Fibre and Admixture

Zeeshan Ahmad, Vartika Varshney and J.P. Tegar
Department of Civil and Environmental Engineering
National Institute of Technical Teacher's Training and Research, Bhopal, India

II.4 Crystal Structure and Magnetic Properties of α’, α- and β-MnB

Nalan Kalyon, Kathrin Hofmann, Maximilian Fries, Konstantin Skokov, Michael Dürrschnabel, Hans-Joachim Kleebe, Oliver Gutfleisch, and Barbara Albert
Eduard-Zintl-Institute of Inorganic and Physical Chemistry, Technische Universität Darmstadt
Darmstadt, Germany

II.5 Nanomechanical Behavior of Indium and Silver Doped Chalcogenide Glass Systems

Abhishek Chaturvedi, G. Sreevidya Varma, S. Asokan and U. Ramamurty
Department of Materials Engineering, Indian Institute of Science, Bangalore, India

II.6 Improved Mechanical Properties through Engineering the Interface by poly (ether ether ketone) Grafted Graphene Oxide in Epoxy based Nanocomposites

Prajakta Katti, S. Kumar and Suryasarathi Bose
Department of Materials Engineering, Indian Institute of Science, Bangalore, India
II.7 Non-Toxic SPIONs-RGO-PEG Nanocomposite Synthesis, Characterization and Gene Delivery Application for Breast Cancer Theranostics

Roa Fardous, Faheem Ahmed, Edreese Alsharaeh, Abdulaziz Almalik and Ali AlHasan
Department of Chemistry, Alfaisal University, Riyadh, Kingdom of Saudi Arabia

II.8 Structural Properties of ZnO–SnO₂ Composite Nanoparticle Thin Film

Khaleed Waleed and Ali Jaseem
Department of Advanced Materials, Building Research Department, Baghdad, Iraq

II.9 Synthesis, Characterization and Utilization of Carbon Nanotubes for Wastewater Management

Sandeep Kumar,† Monika Nehra,‡ Gaurav Bhanjana† and Neeraj Dilbaghi†
and Ki Hyun Kim§
†Department of Bio and Nano Technology, Guru Jambheshwar University of Science and Technology, Hisar-Haryana, 125001, India;
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§Department of Civil & Environmental Engineering, Hanyang University, 222 Wangsimni-Ro, Seoul 04763, Republic of Korea

II.10 Ultrafast, Highly Oriented, and Stress Free ZnO Thin Film Growth by Microwave Assisted Hydrothermal Growth

Randhir Kumar and Rudra Pratap
Centre for Nano Science and Engineering, Indian Institute of Science, Bengaluru, India

II.11 A Novel Microwave Exfoliated Graphite: Synthesis and its Multifunctional Applications

Nagaraju Sykam, Naidu Dhanpal Jayram and G. Mohan Rao
Department of Instrumentation and Applied Physics, Indian Institute of Science Bengaluru
Bangalore, India
II.12 Morphological Design of Pure and Doped Nanocrystalline Ceria in the Course of Thermal Decomposition of corresponding Oxalate Precursors

Daniel Maslennikov,†‡ Alexander Matvienko,†‡ Mikhail Popov,† Evgenii Kondratenko,§ Stanislav Chizhik‡§ and Anatoly Sidelnikov†
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Influence of Magnetite Incorporated on Zinc Oxide Hybrid Nanostructures

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The present work demonstrates the preparation of magnetite (Fe$_3$O$_4$) incorporated zinc oxide (ZnO) nanostructures by a simple co-precipitation assisted reflux condensation method. X-ray diffraction, field emission scanning electron microscopy (FE-SEM), transmission electron microscopy (TEM), energy-dispersive X-ray spectroscopy (EDS), thermo gravimetric analysis (TGA) and UV-Vis DRS were applied for the characterization of structural, morphological, compositional, thermal and optical properties of the resultant samples. FESEM images reveals the hybrid structure with ZnO as matrix and Fe$_3$O$_4$ as filler. The nanostructures can be magnetically retrieved using a commercial magnet and can be reused in the visible light catalytic degradation. Therefore, the obtained hybrid nanostructure exhibit great potential in environmental applications.
Structure Evolution with Temperature of Formamidinium Halide Perovskites


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Hybrid organic-inorganic perovskites with the formula $ABX_3$, where $A$ is formamidinium (FA$^+$) or methylammonium (MA$^+$), $B$ is Sn$^{2+}$ or Pb$^{2+}$, and $X$ is Br$^-$ or I$^-$ have shown promise as high performance, low cost photovoltaic materials. Facile room-temperature solution-based synthesis techniques can be used to make perovskite solar cells with efficiencies comparable to that of commercial silicon solar cells.¹ While the MA variants have been extensively characterized, detailed structural analysis of FA containing compounds has been limited. Here, we present the structural evolution with temperature of FAPbBr$_3$ and FASnI$_3$, along with our previous work on FAPbI$_3$.

X-ray scattering studies on synchrotron X-ray powder diffraction data reveal phase transitions in both FAPbBr$_3$ and FASnI$_3$ upon cooling from 300 K to 100 K. Both distort from cubic $Pm-3m$ to tetragonal $P4/mmbm$ to orthorhombic $Pnma$. The presence of these phase transitions is confirmed via calorimetry. FAPbBr$_3$ and FASnI$_3$ both have high coefficients of volumetric thermal expansion, with FASnI$_3$ reaching $219 \times 10^{-6}$ K$^{-1}$ at 225 K, which is among the highest recorded value for any extended inorganic crystalline solid. This is something that should be taken into consideration when incorporating these materials into devices. Elevated B site atomic displacement parameters (ADPs) and highly anisotropic halide ADPs suggest dynamic motion is occurring in the inorganic sublattice of these perovskites due to the flexibility of the inorganic network and dynamic lone pair stereochemical activity on the B site, as has been observed previously.² Finally, FAPbBr$_3$ displays unusual pseudo-cubic behavior in the tetragonal regime, similar to that seen in FAPbI$_3$.³

This work was supported by the U.S. Department of Energy, Office of Science, Basic Energy Sciences under award number DE-SC-0012541.

References:
Analysis of Hybrid Concrete Using Red Mud, Pet Coke Adding Fibre and Admixture

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Conventional concrete has been used for civil construction for many years, which eminently exploits natural or virgin materials which are becoming scarce. Erstwhile research has been carried out to ameliorate concrete by using industrial by-products as waste products like fly ash, red mud, petroleum coke, silica fumes, etc. in conventional concrete and research results manifested to be significant. In India, more than 20 million tonnes of red mud are produced annually, which is dumped on land or in the oceans near alumina refineries and creating environmental problems. Pet coke is a solid by-product from oil refineries. It has over 90% carbon and producing a high amount of CO₂. Hence, industrial wastes are still a catch twenty-two situation for the environment and their effective utilization and disposal.

In view of exploring more improved quality concrete, may be hybrid in nature, an experimental investigation and analysis has been carried out by taking cementitious behavior of the red mud and low density of petroleum coke, these materials are taken into account as partial replacement of cement and sand in concrete with use of Fibre (Recron) as a secondary reinforcing material and fix percentage of Accelerating Admixture to attain early strength, early setting in concrete. The results of this experimental research, are proven at the optimum percentage of red mud, pet coke using a fixed percentage of fibre and admixture. The strength of M25 concrete is achieved almost at the cost of the M20. The outcome of this research will be efficacious for developing concrete of ameliorating properties, which will avoid brittle and instantaneous failures in concrete as well. The study has also justified the use of combination of waste materials with admixtures lead to sustainability by curtailing the problem of disposal of these wastes.

References:
Crystal Structure and Magnetic Properties of $\alpha'$-, $\alpha$- and $\beta$-MnB

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The investigation of ferromagnetic compounds has been the subject of many fundamental as well as technological studies. They form an important class of materials that are used in various applications such as magnetic recording, magnetic refrigeration as well as spintronics. Manganese monoboride recently regained interest as an inexpensive ferromagnetic material.[1,2] Not much is known about the different modifications of manganese monoboride.[1-5] We obtained single crystals of $\alpha$- and $\beta$-MnB and almost phase-pure powders of $\alpha'$-, $\alpha$- and $\beta$-MnB. Results of structural and magnetic investigations are presented. $\alpha$-MnB crystallizes with a CrB-type structure, and $\beta$-MnB with a FeB-type structure. $\alpha'$ MnB represents a defect-dominated low-temperature variant of the CrB-type structure, as shown by powder X-ray diffraction and transmission electron microscopy. All of the modifications are ferromagnetic, and the magnetic anisotropy of $\alpha$-MnB will be discussed for the first time.

References:
Nanomechanical Behavior of Indium and Silver Doped Chalcogenide Glass Systems

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Connections between the local structure (floppy, rigid or intermediate) and mechanical properties in ternary (Ge-Te-In) and quarternary (Ge-Te-In-Ag) chalcogenide glasses, which are of significant interests in optical, infrared, solar, electrical, and phase change memory devices, are sought through nanoindentation studies. The effects of the chemical composition within the glass formation window, homogenization, and the structural state on the mechanical properties are investigated. Nanoindentation was complemented with other characterization techniques such as micro-Raman spectroscopy, temperature modulated differential scanning calorimetry (mDSC), UV/visible spectrophotometry so as to obtain information into the local structures. Results show a direct influence of the local structure of these glasses, in spite of its amorphous nature, on the mechanical property variations. Furthermore, these results assist in the identification of optimum compositions for optimum mechanical performance.
**Improved Mechanical Properties through Engineering the Interface by poly (ether ether ketone) Grafted Graphene Oxide in Epoxy based Nanocomposites**

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In this work, hydroxylated HPEEK [poly (ether ether ketone)] was covalently grafted on to graphene oxide (GO) sheets and methodically characterized using FTIR, TEM and XPS. The epoxy composites with GO and HPEEK grafted graphene oxide (HPEEK-g-GO) were prepared using mechanical stirring coupled with a bath sonicator to improve the dispersion and were subsequently cured at 80 °C and 180 °C. With the addition of only a small amount (0.5 wt%) of HPEEK-g-GO, an impressive 42% increase in storage modulus, 65% enhancement in hardness and 31% increase in fracture toughness was observed with respect to the control epoxy sample. In addition, significant enhancement in tensile strength by 7 % was realized in epoxy composites containing 0.5 wt % of HPEEK-g-GO. This improvement in structural properties was attributed to reinforcement by HPEEK-g-GO having sound interface with epoxy. The epoxy composites containing HPEEK-g-GO also showed improvement in glass transition temperature along with the thermal stability up to 300 °C.
Non-Toxic SPIONs-RGO-PEG Nanocomposite Synthesis, Characterization and Gene Delivery Application for Breast Cancer Theranostics

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Abstract
Structural Properties of Zno –SnO₂ Composite Nanoparticle Thin Film

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The study of the structural properties of the ZnO-SnO₂ composite nanoparticles prepared by thermal chemical spraying will be discussed. The preparation method was studied by varying the ratio of the mixture, spray angle and temperature of the substrate. Film samples were prepared using the thermal chemical spraying machine, and the structure properties were verified using X-ray diffraction and sensitivity for gases and steams using a sensitivity system. The samples were exposed to methanol and ethanol and the results obtaining hexagonal crystallization membranes with directional (002) for ZnO and ZnO:SnO₂ samples. Results showed nanoscale structures ranging from to 2.4 to 46 nm. High sensitivity was observed at the base temperature of 450 °C with a 45° angle of spray and at a 50/50 ZnO/SnO₂ mixture. The most effective factor form improving sensitivity properties is increases the percentage of SnO₂, which is evident through the results.
Nanomaterials have an astonishing future due to their excellent physiochemical, mechanical, and opto-electronic properties. Nanomaterials have been proposed to be utilized in a variety of healthcare and environmental applications owing to their exotic features. Among different nanomaterials, carbon nanotubes (CNTs) have attracted considerable attention of researchers due to their novel properties such as large surface area, light mass density, chemical inertness, porous structure, and ease of surface modification. Present work deals with synthesis of CNTs using chemical vapour deposition method with controlled size and morphology. The high resolution microscopic techniques like FESEM, HRTEM and AFM were used to view the morphology and topography of prepared nanotubes. The as synthesized CNTs have been purified by different methods prior to their use in wastewater management. XRD and Raman spectroscopy were also employed to characterize the synthesized nanotubes. The purified CNTs have been used as adsorbent material for removal of dyes and heavy metals. Different process parameters like contact time, pH, adsorbent and adsorbate dosages have been considered and optimized in the present work. Atomic absorption spectroscopy and inductively coupled plasma mass spectroscopy techniques were used to study the heavy metal contents at different stages of experiments. Further, CNTs based sensor was also investigated for quantification of heavy metals. The toxicity of CNTs have also been evaluated in different environments. The results indicate that CNTs have huge potential towards pollutant (heavy metals/dyes) management in wastewater applications.
Ultrafast, Highly Oriented, and Stress Free ZnO Thin Film Growth by Microwave Assisted Hydrothermal Growth

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There are several methods reported for the growth of ZnO nanostructures such as chemical vapor deposition (CVD), electrochemical deposition (ED), vapor-liquid-solid (VLS) growth, metal-organic chemical vapor deposition (MOCVD) etc. All the aforementioned methods require high temperatures, >500 °C, and sophisticated equipment. In contrast, a regular hydrothermal method is a low-temperature method requiring cheaper equipment, but it takes a longer time, 4 to 6 hrs compared to few minutes, for the required growth. The microwave assisted hydrothermal method is an ultra-fast technique that can produce various ZnO hierarchical nanostructures with different shapes. Several studies have been reported on ZnO microstructures growth via microwave-assisted hydrothermal methods for different applications. However, a reproducible growth of thin film essential for device application is still missing. We have achieved highly orientated (002) ZnO thin film. The FWHM of rocking curve is 2.43 deg. We can grow good quality films of thickness up to 10 microns within 40 minutes, which is very fast in comparison to other deposition processes. The growth process temperature is 110 deg so the film is stress-free. The Silicon on insulator (SOI) wafer compatible process (because of low temperature) is suitable for getting a starting material stack for any kind of piezoelectric sensors.
A Novel Microwave Exfoliated Graphite: Synthesis and its Multifunctional Applications

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The vast increase in global population coupled with rapid pace of industrialization in the presentworld causes severe adverse effects to the environment, especially water resources. Low cost, easy production, recycling and environmental friendly material is required to solve the current environmental problems. Here, we report a simple low cost one compound based rapid and efficient production of exfoliated graphite (EG) prepared inabout 1min. As prepared EG showsexcellent electromagnetic interference (EMI) shielding properties; sorption performance of various dyes, organic solvents, oils and heavy metal ions. The maximum adsorption capacity reaches a value of 384.6 (±10.2), 222.32 (±8.6), 151.51 (±9.2) and 196.08 (±5.4) mg/g for malachite green (MG), methylene blue (MB), rhodamine 6g (Rh6g) and congo red (CR) dyes at equilibrium under aqueous solutions. The filtration of dye solutions with excellent recycling up to 5cycles was investigated. It absorbs 40-120 g/g of various chemical solvents and oils. It shows excellent adsorption of more than 80% of various heavy metal ions in aqueous solutions at equilibrium. The total electromagnetic interference (EMI) shielding effectiveness (SET) of -84 (±5.4) dB was observed for EG samples in the Ku-band region (12-18 GHz). This is the highest reported SET value for any material under these conditions till today.
Morphological Design of Pure and Doped Nanocrystalline Ceria in the Course of Thermal Decomposition of corresponding Oxalate Precursors

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Nowadays materials based on cerium dioxide are widely used in various areas of the high-tech industry: from precision polishing of glass optics and the production of high-strength ceramics prior to their use as three-way catalysts in automotive engines and applications in medicine as biomimetics. Due to a wide range of practical applications of these compounds, it is worthwhile to develop a method for obtaining these oxides with the possibility of controlling their texture parameters (particles size, porosity etc.). To solve this problem, a traditional preparative method of solid-state chemistry is well suited – the method of thermal decomposition of a precursor, which has many features and advantages in comparison with other methods. The main advantages include the environmental friendliness of the method and the possibility of obtaining products in the form of pseudomorphs. Since in this case the pseudomorph is a porous formation consisting of nanoparticles of a product and retaining shape and size of crystals, this method allows one to obtain porous granulate of nanoparticles, the size of which is set at the stage of synthesis and growth of precursor crystals. In this work as the initial precursors we used Ce₂(C₂O₄)₃·10H₂O and mixed oxalates Ce₂₋ₓMₓ(C₂O₄)₃·10H₂O, where M=Gd and Sm. Various methods have been found for growing the precursors’ crystals of different size (from µm-size up to mm-size) and habitus (2 types). The factors that influence the texture characteristics of the final oxides during the thermal decomposition of selected precursors have been determined. In addition, it has been shown that there is a direct relationship of structural transformations during the dehydration reaction with the observed morphological changes. As a result of thermal decomposition, nanocrystalline ceria was obtained with a particle size ranging from 5-6 nm that was confirmed by XRD and TEM. The specific surface area measurements were also made, which provided S_{BET} values of 140–150 m²/g. The oxidative ability of cerium oxides obtained by thermal decomposition of pure cerium oxalate decahydrate under different external conditions has been investigated by the TPR-H₂ method. In addition, ceria doped with 10% Gd (10CGO), which was obtained from Ce₁.₈Gd₀.₂(C₂O₄)₃·10H₂O, has been used to produce thin layer (ca. 10–20 µm) of solid electrolyte for microtubular SOFC using a spin-coating technique. It has been shown that this electrolyte possesses high oxygen conductivity at temperatures even lower than 500 °C.

The reported study was funded by RFBR and Government of the Novosibirsk region according to the research project №17-48-543264.
Quantification of Surface Functionalities on Graphene, Boron Nitride and Borocarbonitrides by Fluorescence Labeling

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Considering the important role played by surface functionalities on the properties of 2D materials, we have carried out a careful investigation to obtain quantitative estimates of the functionalities on graphene, boron nitride and borocarbonitrides. We have found the surface concentrations of carbonyl, carboxylic and hydroxyl groups on graphene surface. These concentrations are much higher in the case of graphene oxide. We however do not observe any carbonyl groups on reduced graphene oxide. In the case of boron nitride, the surface consists of amine groups apart from hydroxyl groups. Borocarbonitrides contain domains of graphene, BCN and boron nitride and contains all the above mentioned groups. The quantitative estimation is done by chemical labeling using fluorescent probes, wherein fluorescence labeling of surface species (FLOSS), helps to detect and quantify the surface functional groups as low as $10^9$ groups/cm$^2$. Supercapacitor performance and oxygen reduction reactivity of the borocarbonitrides have been measured along with their surface areas to illustrate the likely importance of surface functionalities.
Effect of Iron Oxide Nanoparticles on the Photosynthetic Parameters in Tobacco

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Nanoparticles are reported to act both as an inducer or inhibitor to plant growth in various species. The aim of this study was to examine the effect of different concentrations and sizes of iron oxide nanoparticles on tobacco (Nicotiana tabacum). A hydroponic experiment was carried out in a growth chamber for 14-d using Hoagland’s solution supplemented with 0 (control), 3, 10, and 30 mg/L using different sizes (5, 10, and 20 nm) iron oxide. For the photosynthetic parameters, the photosynthetic rate, stomatal conductance, and transpiration rate were drastically declined in tobacco-treated plants with size 5 iron oxide nanoparticles in all concentrations as compared to control plants. Moreover, the leaf area also reduced significantly in those plants. This suggests that stomatal conductance, and transpiration rate might be the main limiting factors in the photosynthetic rate drop causing seedling retardation. For other sizes of iron oxide nanoparticles, no significant changes were observed. In conclusion, the size and concentration of the nanoparticles have their toxicity impacts on plant development.
Absorption Dominated Electromagnetic Wave Suppressor Derived from Ferrite Doped Cross-linked Graphene Framework and Conducting Carbon Nanotubes

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Functional nanomaterial embedded lightweight polymer composites have drawn considerable attention in wide ranges of industrial applications. In addition to telecommunication and aerospace utilities, microwave absorption materials must be equipped with fascinating properties that ensure excellent performance—from mechanical features to functionalities. Although conducting polymer composites containing magnetic nanofillers have been utilized widely, however, choosing the fillers from the library of nanoparticles and their effective dispersion inside the matrix may limit their usage in terms of performance, stability and durability.

For breaking such bottleneck, herein three key properties (like reasonably high conductivity with high dielectric loss and magnetic permeability) were targeted using $\alpha$-MnO$_2$ doped MWCNTs and Fe$_3$O$_4$ doped graphene oxide (GO) sheets to design soft functional nanocomposites using bi-component blends of PC (polycarbonate) and PVDF (polyvinylidene fluoride). All hybrid structures were thoroughly characterized by SEM, TEM, TGA, FTIR, Raman, XRD. The doping of $\alpha$-MnO$_2$ onto MWCNTs ensured intrinsic wave impedance matching besides providing conducting pathways and the ferrite doped cross-linked GO facilitated in enhanced attenuation of the incoming EM radiation. This unique combination of magneto-dielectric coupling led to significantly high electromagnetic shielding efficiency (SE) of $-37$ dB at 18 GHz dominated by absorption-driven shielding. Besides the high dielectric and magnetic loss with good charge carrying capacity also ensure the higher attenuation constant of the materials. Consequently, when external electromagnetic field encounters with the designed material, it guides EM waves to come across a variety of microscopic boundary owing to the inclusions that constitute the heterostructure. Therefore, we observe that by the synergetic contribution of both dielectric and magnetic components, shielding mechanism can be altered from reflection-driven towards absorption-dominated process by dissipation of heat energy throughout the surface of the substrates. The promising results from the composites further motivated us to rationally stack individual composites into a multilayer architecture following an absorption-multiple reflection-absorption pathway. This resulted in an impressive SE of $-57$ dB for a thin shield of 0.9 mm thickness. Such high SE indicates > 99.999% attenuation of the incoming EM radiation, together with improvement in structural properties validates the potential of these materials in terms of applications in cost-effective and tuneable solutions.
Nanomaterials and their Potential Applications

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For the first time in the history of science and technology, a revolution has occurred, based on the recently developed ability to measure and manipulate matter on the nanometer scale in a skillful manner. This technology would directly benefit a common man when it comes to commercial use. Until then there is an immediate need to convert this science with proper technology.

We have discovered and explored a new bio-safe and bio-compatible route for the synthesis of oxide nanomaterials using water as solvent as well as source of oxygen. The use of water as a reagent is particularly attractive because it is safe, inexpensive, environmentally benign and bestowed with many virtues especially under supercritical conditions. The simple and straightforward route is based on simple reaction of water and metal powder at relatively low temperature. Since water is regarded as a benign solvent and non toxic, the product (nanostructures) could be used safely for biomedical and other applications. The structural and surface morphology has been ascertained by versatile equipment. In addition, the method is simple, straightforward, fast, economical, environmentally benign, involves green chemistry, which can make it suitable for scale large production. The prospects of the process are bright and promising. There are number of applications which shall be discussed during the presentation.
Modeling of Diameter Dependent Fe and Co Ultrathin Nanowires from First-Principles Calculations

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We present electronic, magnetic, thermoelectric and optical properties of ferromagnetic metal nanowires (NWs) made of iron (Fe) and cobalt (Co) atoms using a first principles approach. Each property has been investigated as a function of atomic arrangement and nanowire diameter. Magnetic anisotropy is predicted originating from the spin-orbit coupling. Significant delocalization of electronic charge density is found in Fe nanowires with the increase in nanowire diameter, while charge distribution anisotropy manifests in all studied nanowire configurations. Thermoelectric properties exhibit strong coupling to the nanowire configuration and diameter. Thermal conductivity shows large divergence from the bulk iron and cobalt. Optical properties show strongest increase for nanowires with large diameters. The theoretical modeling of configuration and diameter dependent nanowire properties serves as a cornerstone for future utilization of nanowire films in a variety of applications.
Temperature-Dependent Thermal Conductivity and Viscosity of Synthesized α-Alumina Nanofluids

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In the present work, we focused on the thermal conductivity and viscosity of the synthesis as well as characterize metal oxide α-Al₂O₃ nanoparticles suspended in distilled water (DW): ethylene glycol (EG) (60:40) ratio based stable colloidal nanofluid. The band gap of the α-Al₂O₃ with and without surfactant is 4.42eV and 4.59eV, respectively. The results show that polyvinyl alcohol (PVA) surfactant having smaller crystalline size (~23 nm) then without surfactant has large (~36 nm). The synthesized nanofluids have good stability after 15 days of synthesis which is characterized by zeta potential analyzer. Thermal conductivity and viscosity are measured for 0.1 wt. % and 0.5 wt. % concentration of alumina for with and without surfactant. The concentration of particles and added surfactant are responsible for stable fluid, increased thermal conductivity and viscosity of nanofluid with respect to temperature. Therefore, the novel combinations of characterized properties of α-Al₂O₃ nanofluid proven the best thermally stable heat transfer fluid compare to conventional cooling fluids.
Pure and Coexistence of Antiferromagnetic and Ferromagnetic Phases in Mechanically Milled CaCu$_3$Ti$_4$O$_{12}$ Quadruple Perovskite

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The consequences of high energy mechanical milling on magnetic ordering of polycrystalline CaCu$_3$Ti$_4$O$_{12}$ cubic perovskite have been investigated by means of X-ray powder diffraction (300 K), dc magnetization in field – cooled and zero – field cooled modes (H = 100 Oe and 1000 Oe, T = 5 - 300 K) and M – H loop (T = 5 K and 300 K, Hmax = 70 kOe) characteristics. The un-milled and 16 hrs milled samples show pure antiferromagnetic and ferromagnetic ordering, respectively, while 1 hr and 6 hrs milled samples demonstrate the coexistence of both the phases, well supported by the signature of M – H loops. The ball-milling induced stress that curtails hybridization of empty Ti-3d orbitals with Cu-3d and O-2p orbitals found responsible for observed transitions in the magnetic ordering.
**Synthesis and Characterization of CuInSe$_2$ Thin Films for Photoelectrochemical Application**

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The copper indium diselenide (CuInSe$_2$) thin films were prepared on stainless steel substrate using electrodeposition technique with three electrode system at room temperature. Ternary compounds were co-deposited on stainless steel substrate and FTO substrate with 4 mM CuSO$_4$, 5 mM In$_2$(SO$_4$)$_3$, 40 mM SeO$_2$ and 1 M K$_2$SO$_4$ as an additional electrolyte with pH 1.4. The films of CuInSe$_2$ were studied by cyclic voltammetry (CV) for the measurement of reduction potential. CuInSe$_2$ thin films were characterized by X-ray diffraction (XRD), scanning electron microscopy (SEM) with energy dispersive X-ray spectrum (EDS) for structural, morphological and compositional studies and discussed. The results show that the CuInSe$_2$ crystal was formed. XRD revealed that the films are crystalline in nature. The surface morphology of CuInSe$_2$ thin film is more homogeneous and contains cauliflower like particles through the examination of the SEM Images and XRD Pattern. Samples were further tested for their photoelectrochemical properties.
Pulse Laser Ablation in Liquid Assisted Growth of Gold Nanoparticles: Evaluation of Structural and Optical Traits

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Pulse laser ablation in liquid is attracting great interest for fabrication of nanoparticles due to its simplicity, versatility and free impurity contaminations. Gold nanoparticles were synthesized by pulse laser ablation in deionized water using Q-switched Nd:YAG laser (fundamental wavelength 1064 nm, pulse duration 8 ns). The purpose of the present project is to investigate the dependence of the structural and optical properties of gold nanoparticles on the laser fluence and the repetition rate. The optical properties and band gap energy of the prepared gold nanoparticles were determined using the UV-Vis absorption. The size of the nanoparticles ranges from 7 to 24 nm from TEM analysis. UV-Vis spectroscopy showed surface plasmon resonance (SPR) peaks at the range from 521 to 523 nm.
UAE Sand into Paper

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The first use of paper dates to 2\textsuperscript{nd} Century (BC). Paper may be used to represent value such as money, or to store information and has been a vital necessity globally. Paper is derived from wood by pressing together the moist fibers of cellulose pulp and drying them into flexible sheets. The consumption of paper worldwide has increased by 400\% in the past 40 years leading to a rise in deforestation and global warming. Additionally, water and air pollution are major drawbacks of the paper industry. Due to the afore mentioned detrimental effects of manufacturing paper from wood, an alternative material is being considered which is not only sustainable but also present in abundance in UAE, sand. The aim of this project is to mainly use a local sustainable source; sand with a common polymer such as high-density polyethylene and create a paper that would have a number of advantages over traditional paper made from wood pulp. The major composition of this paper is expected to consist of 80\% sand and the remaining being a photo-degradable polymer. Key experiments include to determine the optimum type and composition of the sand and polymer mixture in order to obtain a good quality paper. The possibility of bleaching the sand is also being tried, to obtain a sheet with a color similar to the ordinary paper. Various sheet preparation techniques are also being investigated. The paper is expected to be insect, grease and water resistant and have a high tear resistivity due to latex like texture. This approach will not only save trees and reduce water consumption, but boost the economy of the country since paper could then be created using a local natural resource and at the same time this innovative idea would contribute to the UAE’s 2021 vision of a more sustainable future.
The Effect of La Dopants on the Phase Stability and Opto-Magnetic Properties of ZnFe$_{2-x}$La$_x$O$_4$ Nanopowders

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ZnFe$_{2-x}$La$_x$O$_4$ ($x=0, 0.25, 0.5$ and $1$) nanopowders were synthesized via fuel assisted combustion method. The crystal structure, morphology, and elemental composition of the synthesized nanopowders were characterized by XRD, SEM, and EDS. The optical and magnetic properties were determined from UV-Vis spectroscopic and VSM studies. The crystal structure of the synthesized nanopowders varied from spinel to perovskite with increasing La concentration. The crystallite size was found to decrease from 42.32 to 23.32 nm as the concentration of La was increased. The morphology of obtained nanopowders displayed spongy porous network structure like. The optical band gaps were determined to range from 2.08 to 2.51 eV. The synthesized nanopowders were found to display different magnetic hysteresis loops.
Flow Chemistry Process for Continuous Synthesis of Silver Nanowires

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One dimensional silver nanowires (AgNWs) with high aspect ratios and crystallinity have been receiving wide attention owing to their excellent plasmonic, optical and chemical properties, as well as high electric and thermal conductivities. These properties make AgNWs a suitable candidate in various applications, such as catalysis, transparent conductive films, sterilization, and surface enhanced Raman spectroscopy. Polyol method is among the most widely used processes in synthesizing AgNWs. However, most of the synthesis of AgNWs was performed using batch reactor system. Continuous flow chemistry has received increased interest in the synthetic organic chemistry community over the past decades due to many advantages derived from its small size and flow nature. In this study, AgNWs were produced using polyol method with the aid of a flow chemistry reactor. Biphasic segmented flow was created throughout the reaction using two immiscible liquids to create high internal mixing and minimize diffusion. Effect of parameters, such as temperature of reactor heater, flow rate, concentration of NaCl and molecular weight of PVP, on the diameter and length of the nanowires was investigated.
Magnetic Alloy-MWNT Wool-ball-like Heterostructures as Efficient Electromagnetic Wave Suppressors in Soft Nanocomposites

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Iron-nickel (FeNi) alloy particles were coated with multiwall nanotubes (MWNTs) using a simple ball milling technique at various alloy to MWNT ratios. These hybrid particles, with wool-ball-like heterostructure, were then dispersed in PVDF/TPU blends to develop flexible composite materials that can shield electromagnetic (EM) radiations. These alloy particles coated with MWNT localise mostly in the TPU phase of the binary blends. The shielding effectiveness (SE) measurements obtained from the scattering parameters reveal that for a particular ratio of FeNi/MWNT (3:1), the SE was the highest (-35.7 dB) among the different composites studied here and manifested in improved microwave absorption in the blends. The absorption driven shielding is due to various polarization in the shield, thereby increasing the dielectric loss. It was observed that these MWNT wrapped magnetic alloy particles shielded the incoming EM radiations more effectively as compared to only MWNTs or only alloy particles. The soft nanocomposites designed here absorb up to 95% of the incoming EM radiations. The lowest skin depth and highest specific EMI attained was 1.4 mm and -11.89 dB cm$^3$g$^{-1}$ respectively for composites containing FeNi/MWNT- 3:1.
Au Coated ZnO Nanospheres and RGO Nanomcomposites for Nanomed Application

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According to the World Health Organization, cancer is the second leading cause of death with 8.8 million deaths worldwide. Cancer is currently treated by chemotherapy, radiation and surgery. However, most of these treatments affect normal cells thereby having serious side effects. To address this, nanomaterials have been used to deliver drugs effectively and shown to be anticancer agents with minimal side effects. Metal oxide nanoparticles such as zinc oxide (ZnO) have been developed for targeted drug delivery. In particular, ZnO nanoparticles have exhibited cancer cell selectivity. With low toxicity against normal cells and biodegradability, ZnO nanoparticles can be effectively used as anti-cancer agents/drugs. In this work, gold coated ZnO nanospheres and RGO nanocomposites were fabricated by an eco-friendly and one-step hydrothermal method. The synthesized nanocomposites were studied using X-ray diffraction (XRD), Ultraviolet/Visible (UV/Vis) spectroscopy, Fourier transform infrared spectroscopy (FT-IR) and Scanning electron microscope (SEM). The nanocomposites were tested for cytotoxicity against healthy cells. Future studies will include cytotoxicity studies against cancer cells.
Synthesis and Characterization of $\text{AC/V}_2\text{O}_5/\text{Bi}_2\text{O}_3$ Nano-Bimetallic Composite Catalyst for Catalytic Ozonation of Bisphenol A

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Bimetallic nanomaterials and metaloxides have received significant interest from international researchers in current years because their new physical and chemical properties resulting from synergistic effects between the two metals are highly desirable for specific technological applications in varies fields, specifically catalysis. Activated carbon based of $\text{AC/V}_2\text{O}_5/\text{Bi}_2\text{O}_3$ nanobimetallic composite catalysts were synthesized and characterized by XRD, FESEM, EDX, Raman spectroscopy, BET, FTIR and DLS particle size analyses. The synthesized bimetallic catalysts were then used for the catalyst for heterogeneous catalytic ozonation of BPA. The results thus obtained showed that catalytical ozonation has achieved a maximum TOC removal of 68 % where the non catalytical ozonation has achieved only 36% of TOC removal.
Semiconductor Titania Nanostructures as Photoactive Catalysts for Effective Water Microbial Purification

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Significant enhancement in the performance of antibacterial bioactive materials in water purification has historically been achieved through the use of optimized nanostructured systems. This research work includes dependance of the antibacterial performance of titania on its morphology and the method of synthesis. In this regard, TiO₂ with different morphologies, including nanoparticles (NPs), nanofibers (NFs) and nanotubes (NTs) were synthesized using different techniques and their antimicrobial properties were studied. Upon UV irradiation, hydrothermally synthetized-TiO₂ NTs showed the highest efficiency among the other architectures in deactivating E. coli (~90%). Several factors play a significant role in determining the antibacterial activity of TiO₂. These factors were examined and analysed in this research work and they include the aspect ratio, crystalline phase, surface hydroxyls, physicochemical properties of TiO₂ as well as experimental conditions.
Synthesis of Copper Oxide Nanoparticles by Thermal Decomposition from (Z)-3-hydroxy-1-phenylbut-2-en-1-one Copper (II) Complex as an Excellent Antimicrobial Agent Against methicillin-Resistant Staphylococcus aureus

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Synthesis of nanoparticles using different synthetic strategies can lead to new applications exploiting the novel physical, electronic and optical properties. In this work, a straightforward approach to copper oxide nanoparticles (CuONps) by thermal decomposition of copper benzoylacetonate copper(II) complex (BCC) as precursor is employed and method is advantageous in its versatility, low cost and eco-friendly. The X-ray structural analysis of the BCC indicates that, coordination environment around the BCC exhibits distorted square-planar geometry with cis-isomer favored structure. The (Z)-3-hydroxy-1-phenylbut-2-en-1-one free ligand and all its copper complexes were characterized by SEM, EDX, MS and TGA. Thermal Gravimetric Analysis (TGA) is a key to select the temperature larger than 500 °C were appropriate to obtain the desired CuONps in good yield with good crystallinity. The formation of CuONps was evidenced by the P-XRD, DLS and SEM. The antibacterial activity was evaluated and studied model showed both metal complex and CuONps potent on methicillin-resistant Staphylococcus aureus (MRSA) validated by inhibition of electron transport chain. The formation of membrane pore/damage by CMC and CuONps leads to changes in the bioelectrochemistry of the MRSA was assessed and mechanism involved in membrane damage was confirmed by SEM. We are currently exploring the use of other metal complexes as precursor for preparation of wide variety of nanostructured metal oxides.
Substitution of aliovalent N\(^{3-}\) and F\(^{-}\) anions in place of O\(^{2-}\) in ZnO brings about major changes in the electronic structure and properties, the composition, even with 10 atomic percent or less of the two anions, rendering the material yellow colored with a much smaller band gap. We have examined the variation of band gap of ZnO with progressive substitution of N and F and more importantly prepared Zn\(_2\)NF which is the composition one obtains ultimately upon complete replacement of O\(^{2-}\) ions. In this article, we present the results of a first complete study of the crystal and electronic structures as well as of properties of a stable metal nitride fluoride, Zn\(_2\)NF. This material occurs in two crystal forms, tetragonal and orthorhombic, both with a band gap much smaller than that of ZnO. Electronic structures of Zn\(_2\)NF as well as ZnO\(_{0.2}\)N\(_{0.5}\)F\(_{0.3}\) investigated by first-principles calculations show that the valence bands of these are dominated by the N (2p) states lying at the top. Interestingly, the latter is a p-type material, a property that has been anticipated for long time. The calculations predict conduction and valence band edges in Zn2NF to be favorable for water splitting. Zn\(_2\)NF does indeed exhibit good visible-light-induced hydrogen evolution activity unlike ZnO. The present study demonstrates how aliovalent anion substitution can be employed for tuning band gaps of materials. Cosubstitution of N\(^{3+}\) and F\(^{-}\) anions in place of O\(^{2-}\) in CdO brings the significant changes in electronic structure and properties. In this study, we have observed Cd\(_2\)NF has isostructural with ‘ideal’ cubic structure of CdO. Structure refinement was carried out by ‘FullProf Suite’ for the obtained PXRD pattern found no ordering of N/F atoms in Cd\(_2\)NF structure. The photocatalytic activity has been carried out by visible light induced water-splitting reactions and observed four times higher hydrogen generation than bulk CdO.

References
Impact of Exogenous Caffeine on the Physio-anatomical Characteristics in Tobacco

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Caffeine, a purine alkaloid, is reported to act both as an inducer or inhibitor to plant growth in various species. The aim of this study was to examine the effect of exogenous caffeine on tobacco, Nicotiana tabacum, plants, a plant that does not naturally synthesise caffeine. A hydroponic experiment was carried out in a growth chamber for 14 days using Hoagland’s solution supplemented with 0 (control), 25, 50, 100, 1,000, and 5,000 µM caffeine. None of the investigated caffeine concentrations significantly decreased the net photosynthetic rate except in the 1,000 and 5,000 µM caffeine-treated plants. Light microscopy of thick-sectioned roots showed that 1,000 µM and 5,000 µM caffeine-treated plants possessed deformed epidermal cells, reduced number of cortical cells, and deformed vascular tissues with cells exhibiting thickeneded xylem walls as compared with control plants. Moreover, transmission electron micrographs of roots revealed that mitochondria and the plasma membrane were affected.
Selective Adsorption of H$_2$ Molecule on N-doped ZnO Nano-ribbons: *Ab-initio* Investigation

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Density functional theory combined with the non-equilibrium Green’s function formalism is used to study the adsorption and gas-sensing properties of H$_2$ gas molecule on pristine and doped ZnO nano-ribbons (NRs). Substitutional doping of oxygen site with C, N and F have been tested versus adsorption of H$_2$ molecule and other molecules (e.g., N$_2$, O$_2$, H$_2$O, H$_2$S). The results of relaxation show chemisorption to occur only on C- and N-doped samples. While all these molecules exhibit chemisorption on C-doped ZnO-NR, only H$_2$ and O$_2$ molecules are chemisorbed on N-doped ZnO-NRs. The chemisorption of O$_2$ is associated with the breaking of one $\pi$-bond and thus the desorption is possible. Whereas, the chemisorption of H$_2$ is associated with a complete dissociation and introduce donor states into the gap (i.e., it plays a role of n-type dopant) and consequently enhancing the conductivity. These characteristics made N-doped ZnO-NRs have high sensitivity and selectivity towards the detection of H$_2$ gas. Furthermore, the calculated IV-curves have paved the way for estimating the sensitivity and consolidating our results. Since the change of conductance is one of the main outputs of sensors, our findings will be useful in developing Hydrogen-based solid-state sensors.
Au coated SPIONS ($\gamma$ Fe$_3$O$_4$) Quantum Dots and RGO composites for Cancer Therapy via Hyperthermia

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Superparamagnetic iron oxide nanoparticles (SPIONs) involves a fundamental technology class within the emerging field of Nano-medicine, and have been extensively researched for cancer therapy. In this study, magnetic nanoparticles in the quantum dots range were prepared. This is due to the high surface area to volume ratio required for effective hyperthermia therapy, drug loading and targeted delivery. SPIONs were synthesized via the chemical co-precipitation method using ammonium hydroxide as the precipitating agent. Gold coating of SPIONs was done in addition to preparing composites with RGO to enhance their properties for cancer therapy. The size of the magnetic nanoparticles was controlled to quantum dot range by varying the reaction temperature, amounts of ammonia, time, temperature and solvent. Biocompatibility was improved by using PEG. Their size and morphology were characterized by XRD, SEM, IR and UV. The nanocomposites were evaluated for their hyperthermia effect and cytotoxicity.
New Material for Removal of Uranium from Waste Water using Sludge Generated from Refinery Wastewater Treatment Processes: Dynamic Adsorption Studies and Effect of gamma-Irradiation

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Adsorbents prepared from low cost precursors have been used for purification of wastewater. Sludge, which is generated from wastewater treatment processes, shows high selectivity for adsorption of uranium from different effluents. Uranium was removed from wastewater using activated sludge AS (after treatment and activation) by batch and dynamic adsorption processes. The dynamic adsorption processes were carried out using column technique and the dynamic adsorption capacity was found to be 38 mg U/g sludge. The exhausted column was regenerated using 1 M HNO₃. The Effect of gamma irradiation on activated sludge was studied to control its stability for removal of uranium from nuclear effluent which contains high doses of gamma radiation. The results show that AS is stable towards gamma irradiation doses up to 10 M Gy. The adsorption capacity slightly increases with gamma irradiation up to 4 M Gy then decreases. The Electron Spin Resonance ESR studies of the irradiated AS samples shows the formation of phosphate radicals during gamma-irradiation.
Fabrication of Self-Cleaning Gypsum Composite Paints

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Gypsum (CaSO₄·2H₂O) is a known structural material, especially for the finishing and decoration of concrete surfaces. Gypsum is formed through the hydration of Plaster of Paris with a setting time of up to 12 minutes and considerable mechanical properties such as compressive strength and hardness. After setting, gypsum has a degree of hydrophilicity and porosity. These two surface properties make gypsum finishing more susceptible to being affected by pollutants such as dyes. Adsorption of dyes onto gypsum surfaces causes its coloration, hence affects its short and long term durability. In the current study, gypsum composites containing TiO₂ nanoparticles (< 20 nm), as a filler, have been fabricated. TiO₂ NPs are characterized by high surface area and photocatalytic activity. The effect of adding TiO₂ NPs at weight percentages up to 20% on the composition, surface properties, and mechanical properties has been studied. Results showed the variation of the setting time of the gypsum-based composites with the addition of TiO₂ NPs. This was observed via the increased demand of water of hydration and workability with increasing the TiO₂ NPs content. Despite these findings, no signs for chemical interaction between TiO₂ NPs and gypsum were observed. These composites are under investigation for their ability to self-clean upon the exposure to organic pollutants. The kinetics of self-cleaning through the photocatalytic degradation of the pollutants by TiO₂ NPs are being studied.
Conjugated Molecule based Sensor Designed for Selective Detection of Lithium Ion in Water

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Alkali metal ions such as lithium, sodium and potassium are important chemical species present in biological fluids – extracellular and intracellular of human body. Lithium salts have been used in medical treatment. The acceptable range of lithium ion concentration in body is 0.5-1.2 mM. The extracellular fluids generally has a high concentration of sodium and low concentration of potassium while intracellular fluid is high in potassium and low in sodium. It is important to selectively identify these ions. Generally, analytical methods such as atomic absorption spectrometry, inductively coupled plasma mass spectrometry (ICP-MS), potentiometric methods have been used to study the concentration of the ions. In the present study, a conjugated molecule is designed. The molecule is designed such that it can selectively interact with lithium. A simple method such as chemiresistor, has been used to detect the ions in water. A chemiresitive sensor is fabricated with the conjugated molecule as sensing element and tested as a proof of concept. The sensor is tested for selectivity for lithium ion. The sensor is tested for 0.2 mM to 23 mM. The interference studies are also carried out. The present study shows that, when an organic molecule is suitably designed for detection of ion can exhibit selectivity to that specific ion.
We report the development of a standard MEMS fabrication process applicable to different types of sensors and actuators working on the principle of piezoelectricity. Our process is specifically useful for the researcher interested in fabricating structures out of lead zirconate titanate (PZT). This process can be used to develop different types of devices such as inertial sensors, acoustic sensors (microphone, speaker) and energy harvesters on a single substrate. We utilize a silicon on insulator (SOI) substrate with 10 um device layer thickness with a material stack SiO₂/Ti/Pt/PZT. Different growth mechanisms used are, thermal oxidation for SiO₂, D.C. magnetron sputtering for Ti/Pt and sol-gel method for PZT. PZT thin films with 650 nm to 1 um thicknesses have been obtained by this route. Realization of any device with this material stack requires etching of different layers up to device layer of SOI followed by etching of device layer and handle in Deep Reactive Ion Etching (DRIE) and release by etching of buried oxide. The first challenge is the development of material stack, specifically getting a device grade film of PZT. Beyond material development and optimisation of various deposition and etching steps a key challenge addressed in this work is avoidance of exposure of PZT and metal layers to contamination-sensitive reactive ion etching (RIE) equipment during topside SiO₂ and Si etching steps by using a thin ALD deposited Al₂O₃ film for capping. The final process involves five masks and 15 different fabrication steps to realize multiple devices. Successful characterization of piezoelectric thin film and initial devices is also presented. The suggested process flow allows us to fabricate a variety of MEMS devices in an academic foundry where dedicated equipment may not be there for processing of PZT thin film.
Analysis of Diesel Soot on Paper based Analytical Sensors using SERS Studies

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Carbon based pollutants are considered a real threat to the environment, which can cause several adverse effects to humans, specifically emission of soot. It is essential to investigate the structure and composition of soot to understand its influence on environment and health [1]. Over the past decade, soot is monitored using complex procedures and expensive techniques [2]. In the present work we have made an attempt to deposit soot on paper based strips and characterize. Paper based analytical sensors (PASs) are receiving attention in various fields, ranging from pH strips to biosensors. Soot was directly collected from exhaust of a diesel engine on three different paper strips (whatman paper, glassy sheet, tissue paper) for a duration of 10 s. The strips were analyzed without any further modification using Raman spectroscopy. A simple casing was fabricated consisting of plastic strip holder with a shutter to collect the soot samples directly from the exhaust of diesel based motor vehicles. Raman spectra data are not enough to determine the trace elements present in diesel soot. To overcome this, Surface enhanced Raman scattering (SERS) has been employed for the first time to amplify the traces of soot using silver nanoparticles. Raman spectral analysis of G band at 1578 and D band at 1370 cm\(^{-1}\) give rise to several bands (G, D1, D2, D3, and D4) at \(~1580, 1350, 1500, 1620, \) and 1200 cm\(^{-1}\), respectively due to Lorentzian fitting curve. However, the strong enhancement of Raman signal produced by SERS allowed for observation of the second harmonic of D and G bands on silver interaction (carbon-metal interface), especially at 2715 cm\(^{-1}\) shows graphitic peak without curve fitting. Amplification in the signal using SERS reveals information such as the quality of diesel engine, presence of phosphorous and sulphur in soot, and quality of lubricant additives. Among the three PASs samples, [Sw, Sg, St] sample Sg (glassy sheet) shows enhanced intensity due to maximum interaction of silver Nps with the soot present in the surface of the Sg. The overall studies confirms that paper based analytical sensors can replace conventional sensors for monitoring soot level in engines. It could also help in development of diesel engine filters for optimization of diesel exhaust.

References:
**Development of Phenylhydrazone based Solvatochromic Receptor for Selective and “Naked Eye” Detection of Fluoride Ion**

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Chemosensors are important role due to their applications in various fields, such as chemistry, biology, medicine and environmental studies.[1] The most challenging task for analytical chemists is to recognize some anions due to the complexity of their small charge to radius ratios, geometries and heavy solvation. Generally, recognition of various anions is based on deprotonation, hydrogen bonding interaction, anion–π interaction, chemical reactions etc.[2] Among a variety of biologically important anions, fluoride is of particular interest due to its role in dental care and treatment for osteoporosis.[3] Even though a number of receptors have been developed for the recognition of fluoride ions,[3] there is a lack of reports on selective sensing via visible color change.

We have developed, a simple, cost effective phenylhydrazone based receptor (2-((2-(2,4-dinitrophenyl)hydrazono)methyl)-6-(hydroxymethyl)-4-methylphenol) for the selective sensing of fluoride ion among various others ions such as, Cl⁻, Br⁻, I⁻, OAc⁻, CN⁻, PO₄³⁻, H₂PO₄⁻ in solution of THF/acetonitrile and its solvatochromic behavior has been described. The addition of fluoride, DMF and DMSO are found to promote deprotonation of receptor. The color change from yellow (λmax = 392 nm) to dark red (λmax = 500 nm) was observed upon addition of F⁻ ion in THF/acetonitrile solution of receptor due the formation of deprotonated species. The binding stoichiometry between F⁻ and receptor was calculated using Job’s plot, it was found to be 1:1 ratio. Receptor shows ratiometric responses to fluoride ions in the presence of other anions, which allows fluoride ion detection even at the nanomolar level, accurately up to 8 nM. Hence, it can be useful as a convenient colorimetric and ratiometric probe for analyzing the fluoride ion in THF/acetonitrile.

References:
Simultaneous Detection of Heavy Metal Ions using Modified Carbon Paste Electrode with Reduce Graphene Oxide-SnO$_2$-Polyaniline

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The reduced graphene oxide-SnO$_2$/PANi (PGS) composite was synthesized and the obtained composite is embedded with carbon paste electrode to detect heavy metals ions lead (Pb$^{2+}$) and cadmium (Cd$^{2+}$). Graphene oxide is synthesized by improved Hummer’s method and the reduced graphene oxide-SnO$_2$ (RGS) is prepared by hydrothermal method. The SnO$_2$ decorated RGO polyaniline nanocomposites (PGS) is prepared by the in-situ polymerization using RGS and aniline monomer. The PGS nanocomposites are characterized by scanning electron microscopy (SEM), Raman spectroscopy, X-Ray diffraction (XRD) and Fourier transform infrared spectroscopy (FTIR). The morphological analysis showed the fibrous structure of PANi with SnO$_2$ particles decorated over RGO. The XRD analysis showed the prominent peaks of SnO$_2$, PANi and a peak shifts is observed due to the graphene-PANi interaction. FT-IR spectrum confirms the presence of PANi in PGS composites. The Raman analysis showed the visible shift in D and G peaks, also the corresponding peak of PANi and SnO$_2$ were prominent, which confirms the presence of PANi and metal oxide in the nanocomposite. We have prepared modified carbon paste electrode with PANi-RGO-SnO$_2$ using graphite (90%): PGS (10%) and 100 µL of paraffin oil. Square wave anodic stripping voltammetry (SWASV) is performed for electrochemical characterization of the modified electrode. The PGS-modified carbon modified electrode showed high electrocatalytic activity towards the oxidation of lead (Pb$^{2+}$) and cadmium (Cd$^{2+}$) in 0.1 M acetate buffer solution (pH 5.0) in square wave anodic stripping voltammetry studies. In terms of application, square wave anodic stripping voltammetry (SWASV) is performed for individual detection of lead (Pb$^{2+}$) and cadmium (Cd$^{2+}$) in the presence of Ag/AgCl electrode and PGS modified carbon paste electrode. Under optimal conditions, simultaneous detection of metal ion showed good linear relationship with the concentration range of 10–70 µM for lead ($R^2$=0.98) and for cadmium ($R^2$=0.97) and individual low detection limit of 0.001 µM is observed for lead (Pb$^{2+}$) and 0.001µM for cadmium (Cd$^{2+}$).
Construction of a Potentiometric Biosensor for the Detection of Glucose using Green Synthesized Silver Nanohybrids and Polypyrrole

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For the present work, we have synthesised silver nanohybrids (AgNHs) using cassia occidentals plant leaf extract and successfully fabricated them onto the polypyrrole modified graphite electrode (Gr/PPy). The resulting composite matrix is later used for the immobilization of glucose oxidase (GOx) enzyme. The synergistic effect of the materials employed in the nano composites showed excellent electro catalytic activity towards the detection of glucose. Further, it is used for the determination of glucose in the concentration range of 0.2-29 mM with a detection limit of 55.3 µM. In addition, the response of biosensor is found to be uninfluenced by some possible interferents.
Fabrication of Catechol Biosensor using Graphene Nano-ribbons Decorated Biosynthesized Silver Nanoparticles and its Application in Detection of Catechol in Green Tea Samples

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The present research reports the development of a highly sensitive and selective electrochemical biosensor for catechol fabricated by immobilizing crude polyphenol oxidase (PPO) enzyme on biosynthesized silver nanoparticles (AgNPs) decorated graphene nano ribbons (GrNRs) modified composite graphite electrode (Gr). Modification of Gr electrode at each step is confirmed by cyclic voltammetry (CV) and Electrochemical impedance (EIS) techniques. Under the optimized conditions the Gr/GrNRs/AgNPs/PPO modified electrode showed higher electrocatalytic activity towards the detection of catechol, which indicates excellent electron transfer efficiency of the nano-composite. The PPO based catechol sensor exhibits a wide linear detection range with the low detection limit. Furthermore, the Gr/GrNRs/AgNPs/PPO modified electrode showed superior selectivity towards the catechol detection in presence of common interfering species. In addition, the developed electrode is successfully applied for the determination of catechol in different green tea samples.
Fabrication of 2,4-Dinitrophenol based on Nd-doped ZnO Nanorods

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Neodymium doped zinc oxide nanorods (Nd/ZnO NRs) were prepared by facile wet chemical process in alkaline medium for the detection of 2,4-Dinitrophenol (2,4-DNP) in environmental samples. Nd/ZnO NRs were characterized by UV/Vis., FTIR, SEM, XEDS, XPS and XRD techniques. Nd/ZnO NRs were deposited on glassy carbon electrode (GCE) with the help of conducting binders i.e. 5% Nafion. The aforementioned NRs have several advantages like good sensitivity, lower limit of detection, reliability, reproducibility, ease of integration, range, long-term stability, and selectivity. The calibration plot was linear over large concentration range of 1.0 pM - 0.01 mM. The sensitivity value and detection limit for the chemical sensor was calculated as 28.48101 nAnM^{-1}cm^{2} and 0.33 pM respectively. Finally, the chemical sensor is useful for detection of toxic and hazardous environmental pollutants and can be used effectively on to protect green environment.
This research was conducted to apply the embroidering technique of fabricating electro-textiles. This technique has its own advantages which make embroidery more functional and plays a role as commercial conductive threads. Three types of conductive threads, based on the composition of the filaments, are compared. Microstructure properties of conductive yarns were characterized by energy dispersive X-ray (EDX) analysis and scanning electron microscopy (SEM). Embroidery process has been carried out by using a computerized embroidery machine. Fabrication specifications and embroidery parameters such as stitch type, stitch length and number of embroidered conductive threads have been analyzed and evaluated. The effects of embroidery parameters on embroidered yarn resistance are compared. The best result with respect to conductivity and coating uniformity was obtained when using 1\textsuperscript{st} and 2\textsuperscript{nd} types of coated yarn with outer metallization layers as silver and nickel in straight stitch type with 3 lines of thread with 5 mm due to its low value of resistance (R) 0.83 $\Omega$. The highest value was 10.66 $\Omega$ in the 3\textsuperscript{rd} type of silver conductive yarn in zigzag stitch type with 1 line of thread with 7 mm stitch length. The prepared intelligent textiles or e-textile can find possible applications in military and medical applications for continuous and long-term monitoring of patients in a hospital environment.
Graphene Membrane for Desalination of Seawater

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Access to drinking water and resource management are expected to be major challenges in the coming decades. In a social and industrial purpose, it seems therefore vital for some people, particularly, in remote areas to develop new facilities for drinking water production. Reverse osmosis important among the desalination methods. It is based on the principle of vapor migration of water through a hydrophobic microporous membrane by a pressure difference between a heated solution and the air in a cold channel (the condensation channel). We are studying the use of a membrane of graphene with carbon pores in the reverse osmosis.
Defect Chemistry and Oxygen Vacancy Migration in Gd-doped CeO$_2$: Hybrid Functional Study

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Oxygen vacancy formation and migration in rare-earth-doped CeO$_2$ has attracted considerable attention due to its wide application as a highly promising material for solving the environmental and energy issues. The formation and migration of oxygen vacancy in Gd-doped CeO$_2$, along with the electronic properties, has been investigated using hybrid functional method. It is found that a slight Gd substitution cannot change the insulating character of CeO$_2$, just inducing the adjustment of covalency and hardly changing its ionicity. The increased concentration of Gd substitution will make hole states in valence band of CeO$_2$, which can be compensated by the donor states brought by oxygen vacancy. The detailed analyses show that in Gd-doped CeO$_2$ the atomic arrangement with Gd-Gd pairs is more realistic than that with isolated Gd atoms, and that the Gd ions are apt to form Gd-VO-Gd cluster. The energetics of oxygen vacancy in different concentrations of Gd doping is examined, and effort has also been made to elaborate the oxygen vacancy migration in Gd-doped CeO$_2$ by means of the climbing-image nudged elastic band (c-NEB) method and molecular dynamics (MD) simulation. The results show that Gd doping effectively lowers the formation energy and migration barrier of O vacancy, beneficial for enhancing the functionality of CeO$_2$-based materials and devices. The fundamental understanding of the positive effect of Gd doping on the migration of O vacancy has been presented in detail.
Newly Discovered Topological Insulator Sr$_3$SnO for Spintronics, Optical and Electronic Properties

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A theoretical study of the electronic and optical properties of dilute magnetic semiconductor Sr$_3$SnO is presented, using the full potential linearized augmented plane wave method. In this approach, Sr$_3$SnO properties will be calculated by means of first-principles density-functional total-energy calculation using the all-electron full potential linear augmented plane-wave method (FP-LAPW). The Perdew–Burke–Ernzerhof (GGA08) generalized gradient approximation is used for the total energy calculations, while the Modified Becke–Johnson (MBJ) is used for electronic structure calculations since this functional was designed to reproduce as well as possible the exact exchange correlation potential rather than the total energy, and as a result gives significantly improved results such as band gap and electronic structure. This gives us a unique opportunity to test the accuracies of the potentials employed and the calculation schemes on nanoclusters. The results will be compared with other theoretical calculations and experimental measurements.
Thermal Decomposition Synthesis of Cobalt-Oxide Nanocrystals

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Varying synthesis conditions makes it possible to create metal nanoparticles with different morphologies such as spheres, ellipsoids, nanorods, nanostructures, nanoplates, prisms, cubes, and nanoparticles with shells. In the present investigation, a thermal decomposition approach is used to prepare CoO nanocrystals (CoONcs) with different morphologies using benzoylacetonate cobalt complex as precursor. Crystals of benzoylacetonate cobalt complex exhibit perfect octahedral geometry with trans-isomer favored structure. The formation of CoO nanocrystals with different morphologies were confirmed from various characterization techniques like SEM, EDX, P-XRD, DLS and TGA. Thermal behavior of the precursor showed a considerable weight loss at 500 °C by an exothermic reaction with a maximum weight loss. The synthesis temperature was varied to obtain different morphologies of CoONcs. SEM results revealed that the morphology of synthesized CoONcs at 1000 °C forms nano-flower shape, 900 °C as nanohybrids, 800 °C as nano-chain, and 700 °C as nano-cube structures. The shape of a nanocrystal enables control its properties, which enhances the applications. This novel material CoONcs is expected to produce various semiconductor nanocrystals with potential applications in the fields of materials science, sensors and photovoltaic cells.
Defects and Persistent Conductivity in Strontium Titanate Single Crystals

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Strontium titanate (SrTiO$_3$) is a complex oxide with unique structural and dielectric properties. It is often used as a substrate for oxide thin films such as high-temperature superconductors. It can be doped to tune it from insulating to semiconducting, metallic, and even superconducting. In our previous work, we showed that hydrogen impurities form a defect complex that contains two hydrogen atoms. We tentatively attributed this defect to a passivated strontium vacancy. In order to create titanium vacancies, bulk single crystal SrTiO$_3$ samples were annealed at 1200 °C in an evacuated ampoule with SrO powder. After exposing these samples to sub-bandgap light (>2.9 eV) at room temperature, the free-electron concentration increases significantly. This enhanced conductivity persists in the dark for several days, at room temperature, with essentially no decay. We attribute this persistent photoconductivity (PPC) to the excitation of an electron from a vacancy into the conduction band, with a low recapture rate. These observations suggest the important role of defects in determining the electrical properties of oxides and may be a potential step towards novel applications.