

**Poster Session I**  
*Al Hamra Convention Center*  
**Sunday, February 18, 2018 18:30-20:30**

## **I.1 Impact of Exogenous Caffeine on the Physio-anatomical Characteristics in Tobacco**

**Rami Alkhatib, Batool Alkhatib, Nour Abdo**

Department of Biotechnology and Genetic Engineering, Jordan University of Science and Technology, Irbid, Jordan

## **I.2 Influence of Potassium Levels on Gladiolus Corms Production in Open Field and Intercropping Conditions**

**Farooq Abdul Sattar, Ashfaq Alam, Noor Ul Amin, Wasim Bilal, Mohammad Abdul Rauf, Khalil Ur Rahman and Roshan Ali**

Department of Arid Land Agriculture, King Abdul Aziz University, Jeddah, Kingdom of Saudi Arabia

## **I.3 Synthesis, Antiviral, Anticancer Properties of Some New Analogs of Curcumin**

**Khaled M. Cheikh, Hassan M. Faidallah, and Tariq R. Sobahi**

Department of Chemistry, King Abdulaziz University, Jeddah, Kingdom of Saudi Arabia

## **I.4 The Self-Sensitized Photo Induced Solid State Decarboxylation of N,N-Dimethylamino-luciferin Single Crystals**

**Stefan Schramm, Durga Prasad Karothu, Kyril Solntsev, Sergey P. Laptanok and Panče Naumov**

Department of Chemistry, New York University Abu Dhabi, Abu Dhabi, United Arab Emirates

## **I.5 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.6 Preparation and Characterization of Alumina NPs - UHMWPE Composites for Hard Tissue Engineering Applications**

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

Department of Chemistry, United Arab Emirates University, Al Ain, United Arab Emirates

## **I.7 Ca<sup>2+</sup>, Zn<sup>2+</sup> 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.8 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.9 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.10 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.11 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.12 Synthesis, Characterization, and Biocompatibility of Thermoplastic Polyurethanes for Medical Applications**

**Mahmoud A. Mohsin<sup>†</sup> and Balsam Q. Saeed<sup>‡</sup>**

<sup>†</sup>Department of Chemistry, University of Sharjah, Sharjah, United Arab Emirates

<sup>‡</sup>Department of Clinical Science, University of Sharjah, Sharjah, United Arab Emirates

## **I.13 Photo-catalytic Solubilization of Wastewater Sludge to Enhance Anaerobic Digestion and Biogas Production**

**Muzammil Anjum, Rajeev Kumar, Mohamed A. Barakat, Hasan A. Al-Talhi and Saleh A. Mohamed**

Department of Environment Sciences, King Abdulaziz University, Jeddah, Kingdom of Saudi Arabia

## **I.14 Activity of Gamma-Glutamyl Transferase (GGT) Enzyme as a Prognostic Tool for Heart Failures**

**Ayoub A Bazzaz<sup>†</sup>, Susan J. Ali<sup>‡</sup>, Noorhan A. Chelebi<sup>†</sup> and Abdulwadood I. Arif<sup>‡</sup>**

<sup>†</sup>Department of Basic Sciences, University of Kerkuk, Kirkuk, Iraq

<sup>‡</sup>Department of Chemistry, Faculty of Education, University of Tikrit, Iraq

## **I.15 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.16 Carbon Quantum Dots Functionalized Zirconia Based Immunosensing Platform for Ochratoxin A Detection**

**Pramod K. Gupta, Zishan H. Khan, Pratima R. Solanki**

Applied Sciences and Humanities, Jamia Millia Islamia, New Delhi, India

## **I.17 Mechanical Properties of Natural Cellulosic Yarn**

**Ahmed Belaadi and Mostefa Bouchak**

Department of Mechanical Engineering, Université 20 août 1955-Skikda, B.P.26 route El-Hadaiek Skikda-Algérie 21000 Silicates, Polymers and Nanocomposites Laboratory (SPNL), University of 08 Mai 1945, 24000 Guelma, Algeria

### **I.18 Bio-Reduction of Nano Graphene Oxide for Biomedical Application**

**K. Kavitha and R. Balagurunathan**

Department of Microbiology, Periyar University, Periyar Palkalai Nagar, Salem – 636 011, Tamil Nadu, India

### **I.19 Latest Advances of Nanomaterials in the Fabrication of Bone and Dental Cements**

**Yaser E. Greish**

Department of Chemistry, UAE University, Al Ain, UAE

### **I.20 Electrospray Fabrication of Chitosan Nanoparticles for the Treatment of Hepatocellular Carcinoma**

**Badriya M. Baig, Yaser E. Greish, Amr F. Amin**

Department of Biology, United Arab Emirates University, Al Ain, United Arab Emirates

### **I.21 Fabrication of Starch-PVA Films Incorporated with Oleoresin for Food Packaging Applications**

**Sudarshan B L, Divya K, Madhukar B S, Hemanth Kumar K, Farhath Khanum and Sanjay K R**

Department of Biotechnology, Sri Jayachamarajendra College of Engineering, Mysore, Karnataka, India

### **I.22 Solid Acid Catalyst in Esterification Reactions**

**Shagufta,<sup>†</sup> Irshad Ahmad<sup>†</sup> and Rahul Dhar<sup>‡</sup>**

<sup>†</sup>Department of Mathematics and Natural Sciences, School of Arts and Sciences

<sup>‡</sup>Department of Chemical and Petroleum Engineering, School of Engineering  
American University of Ras Al Khaimah, Ras Al Khaimah, United Arab Emirates

### **I.23 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

### **I.24 Photocatalytic Degradation of Aniline Blue Dye in an Aqueous Solution by ZnCdS Catalyst under Sunlight Radiation**

**Abdulrahman Al-Hagri, Mohammed Faisal, Mohammed Misbah Uddin, Loai Bamatraf Anas Alaidaros, Ahmad Alhamdat, Selvaraj Renga and Mohammed Meetani**

Department of Chemistry, United Arab Emirates University, Al-Ain, United Arab Emirates

### **I.25 Resources Recovery from the Scrap Tires through Catalytic Pyrolysis**

**Rashid Miandad and Ahmad Saeed**

Department of Environmental Sciences, University of Haripur, Haripur, Pakistan

### **I.26 Structural and Electronic Properties of $\text{Na}_2\text{Ti}_3\text{O}_7$ and $\text{H}_2\text{Ti}_3\text{O}_7$**

**Sara A. H. Abass and Nicola Seriani**

Department of Physics, Khartoum University, Khartoum, Sudan

### **I.27 Valorization of Bio-methane Production from Waste Activated Sludge using Newly Synthesized Visible Light $\text{Cr}_2\text{O}_3/\text{C}_3\text{N}_4$ -(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.28 Hydrogen Production via the Glycerol Steam Reforming Reaction using Nickel Supported on Alumina Catalysts: The Effect of the Addition of Basic Modifiers**

**N.D. Charisiou, K. Polychronopoulou and M. Goula**

Department of Mechanical Engineering, Khalifa University, Abu Dhabi, United Arab Emirates

### **I.29 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.30 Using Cuprous Oxide Nanomaterials for Environmental Applications**

**Asar Ahmed**

Department of Applied Chemistry, Laxminarayan Institute of Technology, Nagpur, RTM Nagpur University, Nagpur, India

### **I.31 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

### **I.32 SnO<sub>2</sub>/Au/BN Nanocomposites as Photocatalyst and its Antibacterial Effects**

**Sara AlEid, Arshia Fathima, Faheem Ahmed, Yasmin Mussa and Edreese Alsharaeh**

Department of Life Sciences, Alfaisal University Riyadh, Kingdom of Saudi Arabia

### **I.33 Impact of the Substitution of PbO by PbF<sub>2</sub> 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.34 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.35 Pressure Induced Metallization and Superconductivity in PdSe<sub>2</sub>**

**Moaz A. Elghazali, Pavel G. Naumov, Hossein Mirhosseini, Vicky Süß, Lukas Mächler, Walter Schnelle, Claudia Felser and Sergey A. Medvedev**

Solid State Chemistry, Max Planck Institute for chemical physics of solids, Dresden, Germany

### **I.36 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.37 Analysis of Defect Free Pure Cadmium Oxide (CdO) Nanoparticles**

**M. Cuba, N. Qamhieh and Saleh T. Mahmoud**

Department of Physics, United Arab Emirates University, Al-Ain, United Arab Emirates

### **I.38 Dye-Sensitized Solar Cells (DSSCs) based on TiO<sub>2</sub>/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.39 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**

Department of Physics, United Arab Emirates University, Al Ain, United Arab Emirates

### **I.40 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.41 Fabrication and Characterization of Gd<sub>2</sub>O<sub>3</sub>-HfO<sub>2</sub> based Memristor Devices for Gamma-Ray Detection**

**Maguy Abi Jaoude**,<sup>†</sup> **Lama Mahmoud**,<sup>‡</sup> **Baker Mohammad**<sup>‡</sup> and **Hamda Al Shehhi**<sup>§</sup>

<sup>†</sup>Department of Chemistry

<sup>‡</sup>Department of Electrical and Computer Engineering

<sup>§</sup>United Arab Emirates Space Agency

Khalifa University of Science and Technology, Abu Dhabi, United Arab Emirates

#### **I.42 FP-LAPW Study of the Effective Masses and Bonding Properties of Zinc-Blende Cadmium Chalcogenides**

**S.Ouendadji**

Department of Physics, Constantine University, Constantine, Algeria

#### **I.43 The Effect of Pressure and Interstitial Substitution on the Electronic Properties of Molybdenum Disulfide**

**Wadha K. AlFalasi**, **Noureddine Amrane**, **Maamar Benkraouda** and **Naser Qamhih**

Department of Physics, United Arab Emirates University, Al Ain, United Arab Emirates

#### **I.44 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.45 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.46 A Study on the Lifetime and Photostability of Chalcogen based D-A-D polymer OPVs**

**Vinila N. V.**

Department of Materials Engineering, Indian Institute of Science, Bangalore, India

### **I.47 Preliminary Investigation of Potassium doped Strontium Silicates as Electrolyte for Intermediate Temperature Solid Oxide Fuel Cells**

**Anjaneya K. C., Singh M. P. and Praveen C. R.**

Department of Materials Engineering, Indian Institute of Science, Bangalore, India

### **I.48 Effect of Fluorination on D-A-D type Hole Transporting Materials for Perovskite Solar Cells**

**G. K. Chandrashekara and Praveen. C. Ramamurthy**

Department of Materials Engineering & Center for Nanoscience and Engineering  
Indian Institute of Science, Bangalore, India

### **I.49 Photocatalytic Reduction of CO<sub>2</sub> by Employing ZnO/Ag<sub>1-x</sub>Cu<sub>x</sub>/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.50 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.51 Facile Synthesis of Nanostructured Cobalt Phosphate as an Electrode Material for High Performance Energy Storage Application**

**Navaneethan Duraisamy, Numan Arshid, K. Kavitha, K. Ramesh, S. Ramesh and Dhanaraj Gopi**

Department of Chemistry, Periyar University, Salem, India

### **I.52 Electrochromic Display Device**

**Sarfraj Mujawar, Bhushan Dhale and Sachin Pawar**

Department of Physics, Savitribai Phule Pune University, Pune, India

### **I.53 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.54 Enhanced Efficiency of Dye-Sensitized Solar Cells using Coffee as Natural Dye on TiO<sub>2</sub>/RGO Nanocomposite based Photoanode**

**Edreese H. Alsharaeh, Faheem Ahmed, A. Soliman, Joud Alsadoun, G. Bharatha, Majdi Khasawneh and K. M. Abu-Salah,**  
Department of Chemistry, Alfaisal University, Riyadh, Kingdom of Saudi Arabia

### **I.55 Synthesis and Characterization of Highly-ordered Cu Nanowires using Electrodeposition Template Method**

**Monika Nehra,<sup>†‡</sup> Deepak Kedia,<sup>‡</sup> Neeraj Dilbaghi<sup>†</sup> and Sandeep Kumar<sup>†</sup>**  
<sup>†</sup>Department of Bio and Nano Technology  
<sup>‡</sup>Department of Electronics and Communication Engineering  
Guru Jambheshwar University of Science and Technology, Hisar, India

### **I.56 Grain Size Distribution, Geochemistry and Mineralogy of Red Sea and Arabian Sea Sediments**

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

### **I.57 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,<sup>†</sup> M. A. Almeahdi,<sup>†</sup> Nadjat Rezki,<sup>†</sup> Sanaa K. Bardaweel<sup>‡</sup> and Mouslim Messali<sup>†</sup>**  
<sup>†</sup>Department of Chemistry, Faculty of Science, Taibah University, Al-Madinah Al-Munawarah 30002, Saudi Arabia  
<sup>‡</sup>Department of Pharmaceutical Sciences, Faculty of Pharmacy, University of Jordan, Amman 11942, Jordan

## **I.58 Eco-Friendly Synthesis of a New Class of Ionic Liquids with Attractive Biological Activity**

**Mousslim Messali, Nadjet Rezki and Mohamed Reda Aouad**

Department of Chemistry, Taibah University

Al-Madinah Al-Munawwarah, Kingdom of Saudi Arabia

## **I.59 Spectral and Optical Characterization of silver nanoparticles biosynthesised by *Origanum majorana* and *Calendula officinalis***

**M. El-Kemary,<sup>†</sup> M. Zahran,<sup>‡</sup> S. A. M. Khalifa,<sup>§</sup> H. R. El-Seedi<sup>†∇</sup>**

<sup>†</sup>Division of Pharmacognosy, Department of Medicinal Chemistry, Uppsala University, Uppsala, Sweden

<sup>∇</sup>Ecological Chemistry Group, Department of Chemistry, School of Chemical Science and Engineering, KTH Royal Institute of Technology, Stockholm, Sweden

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

**Rami Alkhatib, Batool Alkhatib, Nour Abdo**

Department of Biotechnology and Genetic Engineering  
Jordan University of Science and Technology  
Irbid, Jordan  
E-mail: rqalkhatib@just.edu.jo

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-d using Hoagland's solution supplemented with 0 (control), 25, 50, 100, 1,000, and 5,000  $\mu\text{M}$  caffeine. None of the investigated caffeine concentrations significantly decreased the net photosynthetic rate except in the 1,000 and 5,000  $\mu\text{M}$  caffeine-treated plants. Light microscopy of thick-sectioned roots showed that 1,000  $\mu\text{M}$  and 5,000  $\mu\text{M}$  caffeine-treated plants possessed deformed epidermal cells, reduced number of cortical cells, and deformed vascular tissues with cells exhibiting thickened xylem walls as compared with control plants. Moreover, transmission electron micrographs of roots revealed that mitochondria and the plasma membrane were affected.

## **Influence of Potassium Levels on Gladiolus Corms Production in Open Field and Intercropping Conditions**

**Farooq Abdul Sattar, Ashfaq Alam, Noor Ul Amin, Wasim Bilal,  
Mohammad Abdul Rauf, Khalil Ur Rahman and Roshan Ali**

Department of Arid Land Agriculture  
King Abdul Aziz University  
Jeddah, Kingdom of Saudi Arabia  
E-mail: farooq.aup@gmail.com

The influence of potassium levels on gladiolus corm (*Gladiolus grandiflorus*) production under two growing conditions were studied at Agriculture Research Institute, Mingora Swat. The two growing conditions (open field and intercropping) and potassium levels (0, 30, 60 and 90) were studied during the experiment. The experiment was planned in randomized complete block design having split plot arrangement with three replications. Light intensity and soil humidity were also recorded in both conditions. Data was recorded on various growth attributes, which showed that both growing conditions and potassium levels had significantly affected most of the attributes. The maximum sprouting percentage (93.7%), diameter of corms (5.3 cm), corms weight (69.9 g), number of cormels plant<sup>-1</sup> (19.0) and survival percentage (88.8%) were recorded in open field, while maximum plant height (120.2 cm) was observed in intercropping. Moreover, maximum number of leaves plant<sup>-1</sup> (6.5), plant height (120.4 cm), diameter of corms (4.3 cm), corms weight (47.9 g), number of cormels plant<sup>-1</sup> (16.9) and survival percentage (88.8%) were recorded in plots applied with 90 kg potassium ha<sup>-1</sup>. Hence, it was concluded that gladiolus could be grown in open field condition with application of potassium @ 90 kg ha<sup>-1</sup> for better growth and production of corms under the agro-climatic conditions of Swat valley.

## **Synthesis, Antiviral, Anticancer Properties of Some New Analogs of Curcumin**

**Khaled M. Cheikh, Hassan M. Faidallah, and Tariq R. Sobahi**

Department of Chemistry  
King Abdulaziz University  
jeddah, Kingdom of Saudi Arabia  
E-mail: khalidyat@hotmail.com

Cyclocondensation of dienones 4-9 with malononitrile in the presence of piperidine yielded the target 2-aminopyranopyridine-3-carbonitriles 10-14. Reaction of dienones 4, 5, 7 and 8 with malononitrile or ethyl cyanoacetate in presence of excess ammonium acetate afforded the corresponding 2-aminonaphthyridine 15-18 or 2-oxonaphthyridine derivatives 19-22 respectively in good yields. The pyrimido[4,5-b][1,6]naphthyridin-4(3H)-ones 23-26 and their 2-methyl analogs 27-30 as well as the hexahydropyrimido[4,5-b][1,6]naphthyridine-2(1H)-thiones 31-34 and the targeted tetrahydropyrimido[4,5-b][1,6]naphthyridin-4-amines 35-38 was successfully achieved from the reaction of the 2-aminonaphthyridine derivatives 15,16,17 and 18 with the appropriate reagent. The cytotoxicity and antiviral activity of some of the prepared derivatives was also investigated.

## **The Self-Sensitized Photo Induced Solid State Decarboxylation of N,N-Dimethylamino-luciferin Single Crystals**

**Stefan Schramm, Durga Prasad Karothu, Kyril Solntsev, Sergey P. Laptanok and Panče Naumov**

Department of Chemistry  
New York University Abu Dhabi  
Abu Dhabi, United Arab Emirates  
E-mail: stefan.schramm@nyu.edu

N,N-Dimethylamino-luciferin is a nitrogen-analogue of Firefly-luciferin, which is a molecule that is used in many different fields of sciences ranging from fundamental photochemical studies on the bioluminescence of firefly to biomedical applications such as bioluminescence and fluorescence based tumor detection in mammalian tissues. Recently we noticed that crystals of N,N-dimethylamino-luciferin undergo a photochemical transformation when irradiated with light in the blue region of the visible spectra. This also resulted in an initial jumping of the crystals followed by a uniform and then a sequential change in the fluorescence color and intensity. We were seeking to understand this phenomenon, which to our knowledge has not been reported for amino-luciferin or luciferins in general, via a combined approach of experimental and computational investigations. The formation of carbon dioxide within the reaction indicated that a photo induced decarboxylation reaction was taking place. This hypothesis was confirmed via single-crystal X-ray diffraction of the starting material and the reaction products. Furthermore, the reaction was monitored using fluorescence, fluorescence lifetime, absorbance and infrared spectroscopy, which gave valuable insights into the kinetics of the herein presented process. Moreover, photocalorimetry was applied to record the energy profile of the reaction. Based these results and data obtained from density functional theory (DFT) and time-dependent density functional theory calculations of the molecule during its reaction in its ground state as well as at its first six excited singlet states, we suggest a mechanism for the observed photodecarboxylation of N,N-Dimethylamino-luciferin where the molecule itself acts as a sensitizer to absorb light in order to induce its own decarboxylation. Moreover, we explore the emission characteristics of the reactions product which shows high fluorescence quantum yields up to 88%.



## **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  
E-mail: [hsweidan@uaeu.ac.ae](mailto:hsweidan@uaeu.ac.ae)

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 (CO<sub>2</sub>-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 CO<sub>2</sub>-DP contained less organic material than R-DP. In addition the FTIR spectrums of S-DP and CO<sub>2</sub>-DP showed a sharp decrease in the band attributed to the 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**

Department of Chemistry  
United Arab Emirates University  
Al Ain, United Arab Emirates  
E-mail: 200935228@uaeu.ac.ae

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 ( $Al_2O_3$ ) nanoparticles as a reinforcing agent for a polymeric matrix based on ultrahigh molecular weight polyethylene (UHMWPE). Groups of Alumina nano-Particles ( $Al_2O_3$ ) 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-particles concentration on the characteristics of the produced composites. Different characterization techniques have been used. Among these 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 tissues 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.

## **Ca<sup>2+</sup>, Zn<sup>2+</sup> 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  
E-mail: 201450044@uaeu.ac.ae

Zinc polycarboxylate bone cement is one of the commercially available dental cements. It has been also investigated for bone fixation applications. However, it lacks the 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 are 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<sup>2+</sup> and Zn<sup>2+</sup> 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**

**Fatima Merza and Yaser E. Greish**

Department of Chemistry  
United Arab Emirates University  
Al Ain, United Arab Emirates  
E-mail: 201350212@uaeu.ac.ae

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 ( $\text{CaSO}_4 \cdot \frac{1}{2}\text{H}_2\text{O}$ ; 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), an improved mechanical properties of the gypsum composites was observed where 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 than 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**

**Maryam Alqaydi and Yaser E. Greish**

Department of Chemistry  
United Arab Emirates University  
Al Ain, United Arab Emirates  
E-mail: 201305003@uaeu.ac.ae

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 ( $\text{CaHPO}_4$ ) 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 compounds 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.

## **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  
E-mail: 201304592@uaeu.ac.ae

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 illustrate that a 0.3M AC concentration shows a 0.82 left over bilirubin fraction after 16 hours, while a 0.1M AC concentration demonstrate a 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**

**Ideisan I. Abu-Abdoun, Reem R. Alteneiji, Amna A. Al Hamadi**

Department of Chemistry  
University of Sharjah  
Sharjah, United Arab Emirates  
E-mail: [abuabdoun@sharjah.ac.ae](mailto:abuabdoun@sharjah.ac.ae)

Neem is a tree that grows in tropical and semi-tropical regions and 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.

Neem trees are one of the famous and well known trees in UAE, the products 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. Modified neem gum solution was applied on selected museum collections, after exposure to different environmental factors of light, heat, UV light relative humidity, pollutants, pest and insect control used commercially

## **Synthesis, Characterization, and Biocompatibility of Thermoplastic Polyurethanes for Medical Applications**

**Mahmoud A. Mohsin<sup>†</sup> and Balsam Q. Saeed<sup>‡</sup>**

<sup>†</sup>Department of Chemistry, University of Sharjah, Sharjah, United Arab Emirates

<sup>‡</sup>Department of Clinical Science, University of Sharjah, Sharjah, United Arab Emirates

E-mail: mmohsin@sharjah.ac.ae

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 provided 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.



## **Photo-catalytic Solubilization of Wastewater Sludge to Enhance Anaerobic Digestion and Biogas Production**

**Muzammil Anjum, Rajeev Kumar, Mohamed A. Barakat, Hasan A. Al-Talhi and Saleh A. Mohamed**

Department of Environment Sciences  
King Abdulaziz University  
Jeddah, Kingdom of Saudi Arabia  
E-mail: mabarakat@gmail.com

In anaerobic digestion of sludge, the major requirements are breaking the complex structure of wastewater sludge and transforming it into an available form suitable for biodegradation. This work investigated a novel ZnO-ZnS@Polyaniline visible light photocatalyst for pre-solubilization of sludge using photochemical catalysis reactor. Sequentially, this sludge was treated in a batch mode anaerobic reactor using mixed methanogenic enriched culture as an inoculum source. The results indicated that the photocatalysis of sludge has increased the sCOD content (2620 mg L<sup>-1</sup>) by 2.6 times from raw sludge within 6 h of catalytic process. Later, in anaerobic digestion the pre-solubilized sludge achieved onset of methanogenesis just after 12 days where a sharp decline in organic acids (1367 mg L<sup>-1</sup>) and reducing sugar (14 g L<sup>-1</sup>) content was observed. On the other hand, this was achieved after 20 days in un-solubilized sludge. The main reason behind this is the enhanced bioavailability of organic matter to methanogenic bacteria due to the addition of the pre-solubilization step. The biogas production was increased by 54% as compared to that in raw sludge where cumulative biogas was observed up to 1547 ml L<sup>-1</sup> sludge after 45 days. Furthermore, total organic content was degraded by 65% that is even higher by 26% as compared to the control reactor. Overall, this study determined photocatalysis as an alternative pre-solubilization step to increase the efficiency of bioenergy production and sludge processing to generate new mechanisms applicable to the real sludge treatment. Furthermore, the use of visible light (solar) is cost-effective than can improve the feasibility of anaerobic digestion of sludge to attain high net energy potential.

## **Activity of Gamma-Glutamyl Transferase (GGT) Enzyme as a Prognostic Tool for Heart Failures**

**Ayoub A Bazzaz,<sup>†</sup> Susan J. Ali,<sup>‡</sup> Noorhan A. Chelebi<sup>†</sup>  
and Abdulwadood I. Arif<sup>‡</sup>**

<sup>†</sup>Department of Basic Sciences, University of Kerkuk, Kirkuk, Iraq

<sup>‡</sup>Department of Chemistry, Faculty of Education, University of Tikrit, Iraq

E-mail: ayoubbazzaz@yahoo.co.uk

Heart failure (HF) incidence could cause further complications to other body organs, which might sometimes be fatal, 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 sera 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 ( $p \leq 0.01$ ) in the activity of the enzyme GGT in the heart failure patient ( $66.9 \pm 1.7$  IU/L) in comparison with control ( $12.07 \pm 0.60$  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**

**Doha Berraaouan, Najla Kaabouch, Samira Salhi and Abdesselam Tahani**

Department of Chemistry  
Mohamed First University  
Oujda, Morocco  
E-mail: dohaberraaouan@gmail.com

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 technic 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 would not involve the use of toxic components and would allow the degradation via a natural process 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 synthesized by bacteria mainly used in their water soluble form; Sodium Alginate (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. It exists three main chemotypes REO according to the quantity of the major component: Camphor REO, Eucalyptol REO, 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 comparing 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.

Keywords: Encapsulation, Clay composite, Sodium Alginate, Rosemary essential oil, Encapsulation Efficiency

## **Carbon Quantum Dots Functionalized Zirconia Based Immunosensing Platform for Ochratoxin A Detection**

**Pramod K. Gupta, Zishan H. Khan, Pratima R. Solanki**

Applied Sciences and Humanities  
Jamia Millia Islamia  
New Delhi, India  
E-mail: pramod5321@gmail.com

The limitations of Zirconia nanoparticles such as higher aggregation, lower ionic conductivity and absence of functional groups hinder the biosensing performance of material [1]. This problem can be overcome by modification of nanoparticles surface with material having higher electrochemical behavior and desired functional groups [2,3]. In the scenario, Carbon quantum dots functionalized Zirconia nanoparticles (CQDs@ZrO<sub>2</sub>) were synthesized by the one-step hydrothermal method and utilized to develop an immunosensor for mycotoxin detection. CQDs@ZrO<sub>2</sub> nanoparticles were investigated using X-ray diffraction, Transmission Electron microscopy (TEM), Fourier Transform Infrared spectroscopy, contact angle, and electrochemical characterizations. Presence of QDs, on the surface of nanoparticles (~20 nm), not only avoided the aggregation but also enhanced the electrochemical behavior of material due to interfacial interactions between the inorganic particles and carbon matrix [3]. Beside these, incorporation of CQDs also enhanced the hydrophilicity of the nanoparticles. Further, CQDs@ZrO<sub>2</sub> nanoparticles were mixed with chitosan to form stable, and adhesive film on ITO coated glass substrate using the spin-coating technique [4]. FTIR and electrochemical studies confirmed the successful immobilization of anti-OTA and bovine serum albumin (BSA) on Chitosan/CQDs@ZrO<sub>2</sub>/ITO electrode. The Chitosan/CQDs@ZrO<sub>2</sub> matrix facilitates a favorable environment to immobilize antibodies specific to ochratoxin A (anti-OTA) with the desired alignment. The fabricated BSA/anti-OTA/Chitosan/CQDs@ZrO<sub>2</sub>/ITO immunosensor revealed improved biosensing parameters for the selective detection of OTA.

Keywords: Zirconia, Carbon Quantum Dots, Immunosensor, Electrochemical, Ochratoxin A

- [1] Gupta P K, Tiwari S, Khan Z H and Solanki P R 2017 Amino acid functionalized ZrO<sub>2</sub> nanoparticles decorated reduced graphene oxide based immunosensor *Journal of Materials Chemistry B* 5 2019–33
- [2] Gao L, Yue W, Tao S and Fan L 2013 Novel strategy for preparation of graphene-Pd, Pt composite, and its enhanced electrocatalytic activity for alcohol oxidation *Langmuir* 29 957–64
- [3] Chen Y-L, Hu Z-A, Chang Y-Q, Wang H-W, Zhang Z-Y, Yang Y-Y and Wu H-Y 2011 Zinc oxide/reduced graphene oxide composites and electrochemical capacitance enhanced by homogeneous incorporation of reduced graphene oxide sheets in zinc oxide matrix *The Journal of Physical Chemistry C* 115 2563–71

[4] Samicho Z and Ramli A 2011 Extraction of chitosan & its film-forming properties: A review Business, Engineering and Industrial Applications (ISBEIA), 2011 IEEE Symposium on pp 576–80

## **Mechanical Properties of Natural Cellulosic Yarn**

**Ahmed Belaadi and Mostefa Bouchak**

Department of Mechanical Engineering  
Université 20 août 1955-Skikda, B.P.26 route El-Hadaiek Skikda-Algérie 21000  
Silicates, Polymers and Nanocomposites Laboratory (SPNL), University of 08 Mai 1945, 24000  
Guelma, Algeria  
E-mail: ahmedbelaadi1@yahoo.fr

In recent years, many researchers have studied the exploitation of vegetable fibres as reinforcement in composite materials. The biodegradable nature of natural fibres makes them friendly to the environment which can lead to the preservation of nature and human wellbeing. With low cost and good performance, vegetable fibres are generating an economic interest for various industries. The objective of this work is the determination of the mechanical properties of the vegetable sisal yarns, with a twist angle equal to  $13^\circ$  and a linear density of 232 tex, subjected to tensile quasi-static loading. A test program consisting of 150 samples is performed. Due to the variability of natural yarns, more than 30 samples were tested for each gauge length (GL). Five different GLs are used: 50, 100, 150, 200 and 300 mm. The acquired results are then analysed by the statistical two and three parameter Weibull distribution for different probability index and estimation by Least Square (LS) and Maximum Likelihood Estimation (ML).

## **Bio-Reduction of Nano Graphene Oxide for Biomedical Application**

**K. Kavitha and R. Balagurunathan**

Department of Microbiology  
Periyar University, Periyar Palkalai Nagar  
Salem – 636 011, Tamil Nadu, India  
E-mail: [kkavitha07@gmail.com](mailto:kkavitha07@gmail.com)

Graphene oxide reduction, in particularly, the simple, cost effective and environmental benign microbial method attracts high over the other methods. Extracellular mediated actinobacterial reduction of nano graphene oxide is focused for the high purity and productivity of the product without any toxicity. Reduction of the nano-graphene oxide (nGO) to graphene nanoparticles (nRGO) was identified by visual colour change from brown to black. Further, the reduction of nGO into nRGO was confirmed through the conventional characterization techniques such as XRD, Ramman and SEM. Further the bioactivity of biological reduced nano graphene give the superior results compare than the chemically synthesized particles. Appropriate degradation as well as HAp layer formation supports the biological synthesis and suggest for the fruitful outcome for therapeutical applications.

## **Latest Advances of Nanomaterials in the Fabrication of Bone and Dental Cements**

**Yaser E. Greish**

Department of Chemistry  
UAE University  
Al Ain, UAE  
E-mail: y.afifi@uaeu.ac.ae

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 fillings 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**

**Badriya M. Baig, Yaser E. Greish, Amr F. Amin**

Department of Biology  
United Arab Emirates University  
Al Ain, United Arab Emirates  
E-mail: 200918733@uaeu.ac.ae

Since the emergence of Nanotechnology, all the attention has centered upon utilizing it to its best abilities. Tackling problematic medical issues through nanotechnological approach has seen an increasing demand among the research community, in particular oncologists as cancer remains one of the top causes of death worldwide. Multifunctional biocompatible nanoparticles (NPs) furnish a new perspective into drug delivery system compensating the usual anti-cancer drug shortcomings such as low solubility, bioavailability and absorption. As well as, using NPs for directly delivering the anticancer drugs to the tumor site maximize the efficiency of drug delivery. The well-known chitosan nanoparticle been chosen to be fabricated via electrospray method. Electrospray has been reported to generate reproducible polymer particles along with the ability to manipulate the particle size by changing the fabrication parameters such as working distance, flow rate, voltage and polymer concentration. The generated nanoparticles are to be loaded with therapeutic agents such as metformin and vismodegib as well as targeting agent, that is EpCAM monoclonal antibody. Theses selected bioactive agents 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 that 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**

**Sudarshan B L, Divya K, Madhukar B S, Hemanth Kumar K, Farhath Khanum and Sanjay K R**

Department of Biotechnology  
Sri Jayachamarajendra College of Engineering  
Mysore, Karnataka, India  
E-mail: sudhi.bl@gmail.com

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 crosslinking agent. The OL (5%) incorporated films exhibited antibacterial activity in relative percent inhibition to standard rifampicin is  $142 \pm 13\%$  and  $118 \pm 9\%$  against *E coli* a gram negative and a gram positive *Bacillus cereus* respectively. The flavonoids concentration was found to be  $24.5 \pm 5 \mu\text{g}/\text{cm}^2$  quercetine equivalents and total polyphenols content was  $62 \pm 8 \mu\text{g}/\text{cm}^2$  Gallic acid equivalents. DPPH inhibition capacity of the films in IC50 value showed to be  $0.7 \pm 0.06 \text{ cm}^2/\text{ml}$ , iron chelating activity is  $0.25 \pm 0.03 \text{ cm}^2/\text{ml}$ , nitrate scavenging capacity is  $0.075 \pm 0.008 \text{ cm}^2/\text{ml}$ , and FRAP assay is  $0.02 \pm 0.003 \text{ cm}^2/\text{ml}$ . 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 co-continuous 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. 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**

**Shagufta<sup>†</sup>, Irshad Ahmad<sup>†</sup> and Rahul Dhar<sup>‡</sup>**

<sup>†</sup>Department of Mathematics and Natural Sciences, School of Arts and Sciences

<sup>‡</sup>Department of Chemical and Petroleum Engineering, School of Engineering  
American University of Ras Al Khaimah, Ras Al Khaimah, United Arab Emirates  
E-mail: shagufta.waseem@aurak.ac.ae

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 than conventional homogeneous catalysts and reusability of the catalyst is another advantage of these catalysts. The 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 as well as pharmaceutical applications.

[1] J. M. Fraile, E. García-Bordejé, E. Pires, L. Roldán, *Journal of Catalysis*, 2015, 324, 107-118

[2] Shagufta, I. Ahmad, R. Dhar, *Catalysis Surveys from Asia*, 2017, 21, 2, 53-69.

## **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  
E-mail: nalrawashdeh@hct.ac.ae

Nanocomposite materials based on metal nanoparticles and graphene oxide (GO) are 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 GO's ratio with respect to the ZnO nanoparticles (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 of pollutant. An optimum catalytic activity of 84% was achieved by using a nanocomposite with a percentage of 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 showed that the activity toward MB degradation was decreased to about 50% and 70% respectively, while a significant increase in the activity of MB degradation by GO/ZnO/Ag nanocomposite was achieved, 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**

**Abdulrahman Al-Hagri, Mohammed Faisal, Mohammed Misbah Uddin,  
Loai Bamatraf Anas Alaidaros, Ahmad Alhamdat,  
Selvaraj Renga and Mohammed Meetani**

Department of Chemistry  
United Arab Emirates University  
Al-Ain, United Arab Emirates  
E-mail: mmeetani@uaeu.ac.ae

The sodium salt of aniline blue dye is water soluble and it is usually used in inks and 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 interests because of unidentified environmental effects and probable damage to aquatic life. Aniline blue dye could escape intact from conventional treatment plants, and consequently gets into the environment. In this study, three zinc cadmium sulfide catalysts (ZnCdS) were prepared - namely, Zn<sub>0.2</sub>Cd<sub>0.8</sub> S, Zn<sub>0.5</sub>Cd<sub>0.5</sub>S and Zn<sub>0.8</sub>Cd<sub>0.2</sub> S - to photo catalytically degrade the 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 photo degradation of aniline blue follows first order reaction kinetic model. Effective parameters such as pH, photo catalyst dose and contact time were optimized and well investigated. Furthermore, the identification of aniline blue intermediates during photo catalytic degradation was analyzed using LC-MS/MS. The reaction pathway based on the detected intermediates is proposed.

## **Resources Recovery from the Scrap Tires through Catalytic Pyrolysis**

**Rashid Miandad and Ahmad Saeed**

Department of Environmental Sciences  
Univresity of Haripur  
Haripur, Pakistan  
E-mail: jadoon.ciit@gmail.com

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 with  $\text{Al}_2\text{O}_3$  catalyst produced maximum liquid oil (32 wt.%) followed by  $\text{Ca}(\text{OH})_2$  (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 consist of up to 93.3% of mixed aromatic compounds. The use of catalysts decreased the concentration of aromatic compounds in liquid oil down to 60.9% with  $\text{Ca}(\text{OH})_2$ , 71.0% with natural zeolite, 84.6% with  $\text{Al}_2\text{O}_3$ , except for synthetic zeolite producing 93.7% aromatic compounds. The FT-IR data revealed that the 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/cm<sup>3</sup>), 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 $\text{Na}_2\text{Ti}_3\text{O}_7$ and $\text{H}_2\text{Ti}_3\text{O}_7$**

**Sara A. H. Abass and Nicola Seriani**

Department of Physics  
Khartoum University  
Khartoum, Sudan  
E-mail: sroiatna@gmail.com

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, their 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.  $\text{H}_2\text{Ti}_3\text{O}_7$  and  $\text{Na}_2\text{Ti}_3\text{O}_7$  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 $\text{Cr}_2\text{O}_3/\text{C}_3\text{N}_4$ -(6M) Photocatalyst**

**Muzammil Anjum, Rajeev Kumar, Samia Qadeer and M. A. Barakat**

Department of Environmental Sciences  
King Abdulaziz University  
Jeddah, Kingdom of Saudi Arabia  
E-mail: muzammilanjum@gmail.com

Herein, a visible light active photocatalysts  $\text{Cr}_2\text{O}_3/\text{C}_3\text{N}_4$ -(6M) composite was prepared by high temperature calcination method and successfully 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  $\text{Cr}_2\text{O}_3$  and  $\text{C}_3\text{N}_4$  in the composites. The catalyst was initially tested for its photocatalytic activity and afterward applied for solubilization of waste activated sludge in anaerobic digestion process. The application of  $\text{Cr}_2\text{O}_3/\text{C}_3\text{N}_4$ -(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 and volatile solids (VS) content decrease by only 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 respectively in photolytic and raw sludge (control) reactors. These results can provide a useful base and reference for the multi applications of visible light  $\text{Cr}_2\text{O}_3/\text{C}_3\text{N}_4$ -(6M) photocatalyst in enhancement of degradation of toxic pollutant in wastewater and sludge stabilization with bioenergy production in practice.



## **Hydrogen Production via the Glycerol Steam Reforming Reaction using Nickel Supported on Alumina Catalysts: The Effect of the Addition of Basic Modifiers**

**N.D. Charisiou, K. Polychronopoulou and M. Goula**

Department of Mechanical Engineering  
Khalifa University  
Abu Dhabi, United Arab Emirates  
E-mail: kyriaki.polychrono@kustar.ac.ae

The need to replace petro-oil as an energy resource in the transport sector has led to the remarkable development of the biodiesel industry with production growing at almost 25% per annum between 2005 and 2015, reaching approximately 32 billion liters. This development however has also been accompanied by an increase in the production of crude glycerol, the main by-product of the transesterification process (10 wt.% of oil undergoing transesterification). Thus, there is a need to come up with innovative options for the utilization of glycerol, which will help minimize the environmental effects of biodiesel production and also help the industry become more competitive (by reducing its costs and/or add to its revenue streams), and the energetic utilization of glycerol for the production of hydrogen via steam reforming (SR) appears as one of the most promising.

For the work presented herein, a comparative investigation of the catalytic performance for H<sub>2</sub> production through the glycerol steam reforming reaction (GSR) of Ni catalysts supported on Al<sub>2</sub>O<sub>3</sub> (Ni/Al) and alumina modified either with CaO-MgO (Ni/CaMgAl) or La<sub>2</sub>O<sub>3</sub> (Ni/LaAl) was performed. It was proven that use of basic modifiers leads to lower nickel species crystallite size (higher dispersion), increases catalyst's basicity and induces a redistribution of the acid sites in terms of strength and density. It is also clear that the presence of both modifiers has an important effect on the gaseous products' distribution, leading to increased conversion to gaseous products, by favoring H<sub>2</sub> and CO<sub>2</sub> production to the detriment of CO formation and by enhancing the water gas-shift (WGS) reaction. No liquid products were produced by the modified catalyst over 600°C, i.e., a 100°C lower compared with the Ni/Al sample, as production of gaseous products is favored by non-acidic materials supported catalysts, whereas enhanced dehydration and dehydrogenation reactions lead to the production of oxygenates for catalysts with acidic supports, such as pure alumina. The stability results confirm that deactivation in long term experiments can be prevented with the addition of basic modifiers, as apart from decreasing the amount of coke deposition these can also alter the nature of deposited coke to less graphitic and more defective structures. Thus, it can be concluded that Ni supported on Al<sub>2</sub>O<sub>3</sub> modified by basic oxides results at highly selective and stable catalysts for H<sub>2</sub> production via the glycerol steam reforming reaction (GRS).

## **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  
E-mail: fayazalisabir@gmail.com

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 microfibrils of cotton cloth (CC). 2 wt% of CH solutions was used for the coating of CC strips (CC-CH), and were kept 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 borohydride 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 NaBH<sub>4</sub> with rate constant of 0.2937 min<sup>-1</sup> and 0.3804 min<sup>-1</sup>, 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<sup>-1</sup>, respectively. Beside 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.

## **Using Cuprous Oxide Nanomaterials for Environmental Applications**

**Asar Ahmed**

Department of Applied Chemistry, Laxminarayan Institute of Technology, Nagpur  
RTM Nagpur University, Nagpur  
Nagpur, India  
E-mail: ahmed.2013@iitkalumni.org

The cuprous oxide nanomaterials were synthesized by adopting a simple polyol method using SDS and Tween 80 as the surfactants. Surprisingly these nanomaterials doped with transition metal ions like Fe, Co, Ni and Mn ions were found to exhibit ferromagnetic behavior at room temperature. Their ferromagnetic behaviors were found to be dependent on the dopant concentration. It was suggested that ferromagnetic behavior could have been originated from defects formed as cation vacancies in the material. Existence of these defects has been further corroborated by photoluminescence and EPR spectra. The investigation of photocatalytic activity of the various Cu<sub>2</sub>O nanomaterials for the degradation of different organic pollutants like rhodamine B, methyl orange, methylene blue and phenol. For this, nanomaterials in their fixed amounts were mixed with the aqueous solution of the organic dye and the solution was then exposed to UV-visible or visible radiation. Methyl orange, methylene blue and phenol were found to be photocatalytically degradable in the presence of visible light while rhodamine B was found to be photocatalytically degradable only in the presence of UV-visible light. The concentrations of the organic dye after every hour were measured by the UV-visible spectroscopy.

## **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  
E-mail: yaldrees@alfaisal.edu

A recent way to treat waste water is by 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 the 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 images. Photocatalytic tests were done along with antibacterial studies which are in progress.

## **SnO<sub>2</sub>/Au/BN Nanocomposites as Photocatalyst and its Antibacterial Effects**

**Sara AlEid, Arshia Fathima, Faheem Ahmed,  
Yasmin Mussa and Edreese Alsharaeh**

Department of Life Sciences  
Alfaisal University  
Riyadh, Kingdom of Saudi Arabia  
E-mail: Saleid@alfaisal.edu

Photocatalysts play an important role in the degradation of organic pollutants. They have also shown to simultaneously inactivate bacteria. SnO<sub>2</sub> is a semiconductor, having a band gap of 3.6eV 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<sub>2</sub>/Au/BN nanocomposite was synthesized and showed enhanced photocatalytic activity compared to SnO<sub>2</sub>. Functionalized BN was shown to improve the visible light absorption for photocatalysts like TiO<sub>2</sub>. Similar behavior was observed with our nanocomposite. In this work, we synthesized SnO<sub>2</sub>/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<sub>2</sub> on Structural Properties and Luminescence of Neodymium-doped Lead Borate Glass**

**Asmaa Ratep and Ismail Kashif**

Physics  
Ain Shams University  
Cairo, Egypt

E-mail: [assmakalifa@yahoo.com](mailto:assmakalifa@yahoo.com); [ismailkashif52@yahoo.com](mailto:ismailkashif52@yahoo.com)

The rare-earth-doped glasses have a great significance for potential applications in optical devices and laser technology. The glass samples were prepared by melt quenching technique. XRD, FTIR, UV/VIS/NIR spectrophotometer and photoluminesces were used to measure the glass samples. And found the amorphous nature of glass papered, the lead oxide entre in the glass network as a former, analysis of splitting of Nd<sup>3+</sup> 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<sub>1/2</sub>, 4G<sub>11/2</sub>, 2D<sub>3//2</sub>+2G<sub>9/2</sub>+2P<sub>3/2</sub>, 4G<sub>9/2</sub>, 2K<sub>13/2</sub>+4G<sub>7/2</sub>, 4G<sub>5/2</sub>+2G<sub>7/2</sub>, 2H<sub>11/2</sub>, 4F<sub>9/2</sub>, 4S<sub>3/2</sub>+4F<sub>7/2</sub>, 4F<sub>5/2</sub>+2H<sub>9/2</sub> and 4F<sub>3/2</sub> 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<sup>3+</sup> concentrations due to the quenching effect.

## **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  
E-mail: khadija\_khanum@yahoo.com

Electrospinning of polymers has emerged out to be one of the versatile techniques to obtain 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 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

1. Bhardwaj N, Kundu SC (2010) Electrospinning: A fascinating fiber fabrication technique. *Biotechnol Adv* 28:325–347 . doi: 10.1016/j.biotechadv.2010.01.004
2. Khanum KK, Hegde S, Ramamurthy PC (2014) Fabrication of free-standing PEDOT:PSS nanofiber mats using electrospinning. In: 2014 IEEE 2nd International Conference on Emerging Electronics (ICEE). pp 1–4
3. Khanum KK, Bora PJ, Vinoy KJ, Ramamurthy PC (2016) Evaluation of electromagnetic interference shielding using Poly(3,4-ethylenedioxythiophene) Polystyrene sulfonate blend. In: 2016 3rd International Conference on Emerging Electronics (ICEE). pp 1–4

## **Pressure Induced Metallization and Superconductivity in PdSe<sub>2</sub>**

**Moaz A. Elghazali, Pavel G. Naumov, Hossein Mirhosseini, Vicky Süß, Lukas Müchler, Walter Schnelle, Claudia Felser and Sergey A. Medvedev**

Solid State Chemistry  
Max Planck Institute for chemical physics of solids  
Dresden, Germany  
E-mail: moaz.elghazali@cpfs.mpg.de

Transition Metal Dichalcogenides (TMDs) have been attracting an increasing attention among scientific community over the past few decades due to their intriguing physical properties and potential applications in electronics and optoelectronics. [1] The prosperity of (TMDs) MX<sub>2</sub> originates from their unique layered structural in which each layer is formed of a transition metal atom (M) sandwiched between two chalcogen (X: Se or S) via strong covalent bond. The layers are weakly stacked together through Van der Waals interactions leading to wide range of possible structural variations and electronic novel properties. Owing to these unique properties, external applied pressure would be a useful tool to tune such systems and in many cases inducing novel states of matter such as insulator-to-metal transition, CDW or superconductivity. [2,3] External applied pressure has proved to be clean, powerful technique that can tune compounds by altering the lattice parameters, and in turn changing the structural and electronic properties.

PdSe<sub>2</sub> can be considered as a prototypical example of TMDC due to their novel structure and electronic properties. PdSe<sub>2</sub> crystallizes at ambient pressure in an orthorhombic PdS<sub>2</sub>-type layered crystal structure, space group Pbc<sub>2</sub>a and shows a semiconducting behaviour with a sizeable indirect bandgap of ~ 0.25 eV. At high pressure, PdSe<sub>2</sub>, however, crystallizes in the pyrite- type structure. [4] Tuning structure across the boundaries of quasi-2D and 3D system would be of interest to reveal the underlying physics and search for novel states of matter.

Here, we present electrical transport measurement under pressure accompanied by Raman Spectroscopy. We also report an electronic driven insulator-to-metal transition without a structural phase transition. This electronic driven metallization at relatively low pressures has potential applications in electronics, namely in memory devices, sensors and switches. Applying further pressure drives the system into a dome-shaped pressure-induced superconductivity with maximum T<sub>c</sub> of 13.1 K.

Ab initio band structure calculations agrees with the experimental findings and even more interestingly indicate Dirac and nodal line fermions in the vicinity of Fermi energy.



## **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  
E-mail: zia.hameed@superior.edu.pk

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. In this research there is 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. In this research there is also a comparison actual data and the measured data of 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**

**M. Cuba, N. Qamhieh and Saleh T. Mahmoud**

Department of Physics  
United Arab Emirates University  
Al-Ain, United Arab Emirates  
E-mail: saleh.thaker@uaeu.ac.ae

The electroluminescence devices based on transparent metal oxide semiconductors (II-VI semiconductors) have much attention owing 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 material 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 also used to control the band gap and surface morphology by forming 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 know the presence of defects in the CdO powder sample prepared by precipitation technique. The starting materials taken for the preparation of CdO were CdCl<sub>2</sub>.H<sub>2</sub>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) spectra. 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) spectra, which was shifted towards higher values for the annealed CdO nanoparticles as compared to the as-prepared sample. The Raman spectrum showed band at 400 and 450 cm<sup>-1</sup> that corresponds 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<sub>2</sub>/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  
E-mail: naldosary@alfaisal.edu

Organic dyes and metals (Ag) have been used as sensitizers to improve the optical absorption properties of TiO<sub>2</sub> nanomaterials in the visible light region. It is a major challenge to modify titanium dioxide (TiO<sub>2</sub>) 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<sub>2</sub> 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<sub>2</sub>/h-BN/Ag nanocomposites were synthesized in situ via microwave route. 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<sub>2</sub>/h-BN/Ag with pure anatase phase of TiO<sub>2</sub>. Optical properties such as band gap were studied using Ultraviolet/Visible (UV/Vis) spectroscopy which indicated modifications of the band gap of TiO<sub>2</sub> followed the addition of h-BN. Dye-sensitized solar cells (DSSCs) were fabricated using the synthesized TiO<sub>2</sub>/h-BN/Ag nanocomposites. Results showed that a significant improvement of solar cell efficiency can be achieved using the synthesized TiO<sub>2</sub>/h-BN/Ag nanocomposites. Interestingly, functionalized h-BN has shown to enhance TiO<sub>2</sub> activity in visible light range. Moreover, thermogravimetric (TGA) analyses showed that the as synthesized TiO<sub>2</sub>/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**

**Amin Reyhan Sadek, Basem Abdel Aziz, Ibrahim Al Ghoul,  
Adel Najjar and Naser Qamhieh**

Department of Physics  
United Arab Emirates University  
Al Ain, United Arab Emirates  
E-mail: Adel.najar@uaeu.ac.ae; nqamhieh@uaeu.ac.ae

The synthesis of a perovskite based on lead halide perovskites ( $\text{CH}_3\text{NH}_3$ ) $2\text{PbI}_3$  is reported. Simple precursors such as  $\text{PbI}_3$  and  $\text{CH}_3\text{NH}_3\text{Cl}$  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. Then a stability study will be presented, which carried by measuring the absorption coefficient after exposing the perovskite to air for different time intervals. This organic–inorganic perovskites is receiving the interest of researchers due to its various optoelectronic applications.

## **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  
E-mail: ramzi.maalej@fss.usf.tn

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<sup>3+</sup> and Yb<sup>3+</sup> ions was prepared, and its optical properties were analyzed. The incorporation of Yb<sup>3+</sup> 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<sup>3+</sup>/Yb<sup>3+</sup> 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 200–300K. The significant temperature sensitivity indicates its potential as a temperature sensing probe. The maximum sensitivity was  $15 \times 10^{-4} \text{ K}^{-1}$  at 200 K.

## **Fabrication and Characterization of Gd<sub>2</sub>O<sub>3</sub>-HfO<sub>2</sub> based Memristor Devices for Gamma-Ray Detection**

**Maguy Abi Jaoude<sup>†</sup>, Lama Mahmoud,<sup>‡</sup>  
Baker Mohammad<sup>‡</sup> and Hamda Al Shehhi<sup>§</sup>**

<sup>†</sup>Department of Chemistry

<sup>‡</sup>Department of Electrical and Computer Engineering

<sup>§</sup>United Arab Emirates Space Agency

Khalifa University of Science and Technology

Abu Dhabi, United Arab Emirates

E-mail: maguy.abijaoude@kustar.ac.ae

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<sub>2</sub>) and gadolinia (Gd<sub>2</sub>O<sub>3</sub>) in memristive radiation detectors, is attractive considering their recognized photo-electric receptivity and increasing appreciation among solid-state metal-oxide semiconductor dosimeters [5,6]. In this work, a 2 mm × 2 mm crossbar micro-thick Ag(TE)/ Gd<sub>2</sub>O<sub>3</sub> – HfO<sub>2</sub> (~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<sup>3+</sup> 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).

This work is funded by the United Arab Emirates Space Agency, Space Missions Science and Technology Directorate, project reference K08-2016-001.

[1] Zidan, M. A., Chen, A., Indiveri, G., & Lu, W. D. (2017). Journal of Electroceramics, 1-17.

- [2] Bessonov, A. A., Gartseev, I. B., & Kirikova, M. N. (2017). U.S. Patent No. 20,170,261,355. Washington, DC: U.S. Patent and Trademark Office.
- [3] Athanasiou, V., & Konkoli, Z. (2017). International Journal of Parallel, Emergent and Distributed Systems, 1-20.
- [4] Radiation Detection, Monitoring and Safety Market by Product - Global Forecast to 2021 retrieved from <http://www.marketsandmarkets.com/Market-Reports/radiation-protection-market-987.html>
- [5] Srinivasan, V. S., & Pandya, A. (2011). Thin Solid Films, 520(1), 574-577.
- [6] Kahraman, A., & Yilmaz, E. (2017). Radiation Physics and Chemistry, 139, 114-119.

## **FP-LAPW Study of the Effective Masses and Bonding Properties of Zinc-Blende Cadmium Chalcogenides**

**S.Ouendadji**

Department of Physics  
Constantine University  
Constantine, Algeria  
E-mail: ouendadji@yahoo.fr

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  $\Gamma$  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 the extinction coefficient are all 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 Molybdenum Disulfide**

**Wadha K. AlFalasi, Nouredine Amrane,  
Maamar Benkraouda and Naser Qamhieh**

Department of Physics  
United Arab Emirates University  
Al Ain, United Arab Emirates  
E-mail: w.201001502@gmail.com

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 promising Molybdenum Disulfide (MoS<sub>2</sub>) 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. WSe<sub>2</sub> – MoS<sub>2</sub> heterostructure and the effect of impurities are covered to search for MoS<sub>2</sub> metallization and band gap tuning possibilities.

MoS<sub>2</sub>, in its monolayer form, has a direct band gap (1.8eV) 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 MoS<sub>2</sub> band gap can be done using substitutional impurities and induced pressure. Metallizing MoS<sub>2</sub> is possible by applying a positive pressure, which even widens the range of its applications.

## **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  
E-mail: mhchane@yahoo.in

Microbial Fuel Cell is an emerging technique offers wastewater treatment and simultaneous electricity generation for the developing demand of the era in 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<sup>2</sup>. 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**

**Heba H. Farrag, Sayed Y. Nagy, Nageh K. Allam and Ahmad M. Mohammad**

Department of Chemistry  
Cairo University  
Cairo, Egypt  
E-mail: hhamdy@sci.cu.edu.eg

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**

**Vinila N. V.**

Department of Materials Engineering  
Indian Institute of Science  
Bangalore, India  
E-mail: vinilanv@gmail.com

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 ~5000hr 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 the 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.

## **Preliminary Investigation of Potassium doped Strontium Silicates as Electrolyte for Intermediate Temperature Solid Oxide Fuel Cells**

**Anjaneya K. C., Singh M. P. and Praveen C. R.**

Department of Materials Engineering  
Indian Institute of Science  
Bangalore, India  
E-mail: anji.kundur@rediffmail.com

Here, we synthesized.  $\text{Sr}_{1-x}\text{K}_x\text{SiO}_3-\delta$  ( $x = 0.00 - 0.20$ ) solid solutions as electrolyte materials for intermediate temperature solid oxide fuel cells. From the XRD, it is evident that  $\text{Sr}_{1-x}\text{K}_x\text{SiO}_3-\delta$  samples can be indexed to monoclinic  $c2/c$  space group (15) structure. Solid state  $^{29}\text{Si}$  NMR spectrum of  $\text{SrSiO}_3$  exhibits a sharp single peak centered at  $-83$  ppm. A broad NMR peak centered at  $\sim -89$  ppm indicates the presence of amorphous  $\text{K}_2\text{Si}_2\text{O}_5$  phase in  $\text{Sr}_{0.80}\text{K}_{0.20}\text{SiO}_3-\delta$ . FE-SEM images and WDS mapping shows the segregation of amorphous  $\text{K}_2\text{Si}_2\text{O}_5$  along the grain boundaries. TEM image of  $\text{Sr}_{0.80}\text{K}_{0.20}\text{SiO}_3-\delta$ . clearly indicates the presence of both crystalline and amorphous phases.  $\text{Sr}_{0.80}\text{K}_{0.20}\text{SiO}_3-\delta$  exhibits conductivity comparable to other electrolytes in the literature which makes it as potential electrolyte for intermediate temperature solid oxide fuel cells.

## **Effect of Fluorination on D-A-D type Hole Transporting Materials for Perovskite Solar Cells**

**G. K. Chandrashekara and Praveen. C. Ramamurthy**

Department of Materials Engineering & Center for Nanoscience and Engineering.  
Indian Institute of Science  
Bangalore, India  
E-mail: gk.chandu7486@gmail.com

Energy levels and the physiochemical properties of hole transporting materials can finely tune 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. So 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 expected 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/TiO<sub>2</sub>/Perovskite/Hole Transport Material/Au. Further, device morphology will be studied using AFM, SEM etc.

## **Photocatalytic Reduction of CO<sub>2</sub> by Employing ZnO/Ag<sub>1-x</sub>Cu<sub>x</sub>/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  
E-mail: monis@jncasr.ac.in

In view of the great importance of finding ways to reduce CO<sub>2</sub> 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<sub>2</sub>, although the activity may not be considerable. Our studies with reduction of CO<sub>2</sub> by ZnO/M/CdS (M = Ag, Au, Ag<sub>1-x</sub>Au<sub>x</sub>, Ag<sub>1-x</sub>Cu<sub>x</sub>) type heterostructures in liquid phase have shown good results specially in the case of ZnO/Ag<sub>1-x</sub>Cu<sub>x</sub>/CdS reaching a CO production activity of 327.4 μmol h<sup>-1</sup>g<sup>-1</sup>. The heterostructures also reduce CO<sub>2</sub> in the gas-phase although the production activity is not high. Some of the heterostructures exhibit reduction of CO<sub>2</sub> even in the absence of sacrificial reagents.

## **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  
E-mail: mwaqas222@gmail.com

The present study aimed to optimize the 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 compare with an un-amended control trail using an in-vessel compost bioreactor. The use of natural zeolite significantly affect 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 thermophilic 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<sub>4</sub><sup>+</sup>) and nitrate (NO<sub>3</sub><sup>-</sup>) concentration in modified natural zeolite was increased by 11.1 and 21.5 % respectively in comparison 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.



**Facile Synthesis of Nanostructured Cobalt Phosphate  
as an Electrode Material for  
High Performance Energy Storage Application**

**Navaneethan Duraisamy, Numan Arshid, K. Kavitha,  
K. Ramesh, S. Ramesh and Dhanaraj Gopi**

Department of Chemistry  
Periyar University  
Salem, India  
E-mail: naveennanoenergy@gmail.com

The nanostructured cobalt phosphates are achieved via eco-friendly technique. The cobalt phosphates with superior electrochemical performances are achieved via sonochemical method and followed by calcination. The nanostructured cobalt phosphates are significantly influenced by varying the ultrasonic time. The structural crystallinity and surface purity of as synthesized cobalt phosphates are clearly examined via X-ray diffraction and FTIR spectrum. The surface morphology revealed the shape and size of the metal phosphate with respect to sonication time. The electrochemical studies revealed the effective electrochemical utilization as well as superior specific capacity with longer cyclic life. Further, the asymmetric cell system is elucidated in detail for commercial application.

## **Electrochromic Display Device**

**Sarfraj Mujawar, Bhushan Dhale and Sachin Pawar**

Department of Physics  
Savitribai Phule Pune University  
Pune, India  
E-mail: sarfraj100@gmail.com

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<sub>3</sub>) 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<sub>3</sub> 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<sub>2</sub>O<sub>5</sub>=45 ml and WO<sub>3</sub>=5 ml, which has shown electrochemical reversibility and coloration efficiency 96% and 19cm<sup>2</sup>/C.

## **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, United Arab Emirates  
E-mail: 201350166@uaeu.ac.ae

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 foot print need to be reduced through using the recycling. The aim of this research is to recycle carbon fiber pre-preg 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 the consideration. As a result, mainly two techniques were used to handle the pre-preg waste. The first one was using the hot press. The second method was using Auto Clave 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 done for three samples 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 Auto Clave methodology in STRATA, fine shreds, not fine shreds and strips carbon fiber produces 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<sub>2</sub>/RGO Nanocomposite based Photoanode**

**Edreese H. Alsharaeh, Faheem Ahmed, A. Soliman, Joud Alsadoun, G. Bharatha, Majdi Khasawneh and K. M. Abu-Salah,**

Department of Chemistry  
Alfaisal University  
Riyadh, Kingdom of Saudi Arabia  
E-mail: ealsharaeh@alfaisal.edu

In this work, a simple, cost effective, and biofriendly methodology was reported to design sol-gel assisted TiO<sub>2</sub>/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<sub>2</sub> nanoparticles were crystallized in the tetragonal anatase phase. TEM images showed the TiO<sub>2</sub> nanoparticles are uniform and densely covered on the surface of the graphene oxide. Modification of the anatase TiO<sub>2</sub> NPs was carried out by incorporating graphene oxide (GO) to enhance the efficiency. The results showed that the TiO<sub>2</sub>/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<sub>2</sub>. 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 and also significantly, this technique could be used to a 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**

**Monika Nehra,<sup>†‡</sup> Deepak Kedia,<sup>‡</sup> Neeraj Dilbaghi<sup>†</sup> and Sandeep Kumar<sup>†</sup>**

<sup>†</sup>Department of Bio and Nano Technology

<sup>‡</sup>Department of Electronics and Communication Engineering  
Guru Jambheshwar University of Science and Technology

Hisar, India

E-mail: ssmonikanehra@gmail.com

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.

## **Grain Size Distribution, Geochemistry and Mineralogy of Red Sea and Arabian Sea Sediments**

**Jawad Majeed, Ibrahim Muhammad Ghandour and Ali Saeed Basaham**

Department of Marine Geology  
King Abdulaziz University  
Jeddah, Kingdom of Saudi Arabia  
E-mail: majeed.jawad@hotmail.com

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<sub>3</sub> 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**

**Mohamed R. Aouad,<sup>†</sup> M. A. Almehmadi,<sup>†</sup> Nadjat Rezki,<sup>†</sup>  
Sanaa K. Bardaweel<sup>‡</sup> and Mouslim Messali<sup>†</sup>**

<sup>†</sup>Department of Chemistry, Faculty of Science, Taibah University, Al-Madinah Al-Munawarah  
30002, Saudi Arabia

<sup>‡</sup>Department of Pharmaceutical Sciences, Faculty of Pharmacy, University of Jordan, Amman  
11942, Jordan

E-mail: aouadmohamedreda@yahoo.fr

Benzimidazoles are one of the most prevalent classes of pharmacologically active azoles endowed with important pharmacological properties such as anti-inflammatory,<sup>1</sup> antiviral<sup>2</sup> and antitubercular<sup>3</sup> activities. Moreover, Sulfa drugs are of particular interest as antibacterial,<sup>4</sup> anticancer,<sup>5</sup> antitubercular<sup>6</sup> and antifungal<sup>7</sup> 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.<sup>8-10</sup> 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.<sup>11</sup> 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:H<sub>2</sub>O (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**

**Mousslim Messali, Nadjat Rezki and Mohamed Reda Aouad**

Department of Chemistry  
Taibah Umiversity  
Al-Madinah Al-Munawarrah, Kingdom of Saudi Arabia  
E-mail: mouslim@mail.be

Nowadays, Considerable challenges surveys by many chemical industries have 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 several outstanding properties such as zero- vapor pressure, good chemical and thermal stability, low flammability, excellent solubility for many organic and inorganic compounds and high ionic conductivity and [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 from 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

- [1] S. Ahrens, A.Peritz, *Angew. Chem. Int. Ed.* 2009, 48, 7908–7910.
- [2] M.AM. Ibrahim, M. Messali, *Prod. Finish.* 76 (2), 14 (2011).
- [3] M. Messali, *acta Pharmaceutica*, 65 (3), 2015, 253-270.
- [4] M. Messali, *Molecules*, 2015, 20, 14936-14949.
- [5] M. Messali, M.R. Aouad, A.A. Ali, N. Rezki, Adeeb A-S Ali, T. Ben Hadda, B. Hammouti, *Medicinal Chemistry Research*, 24 (4), 2015, 1387-1395.
- [6] M. Messali, M.N. Almtiri, A. Bousskri, R. Salghi, M.R. Aouad, S.F. Alshahateet, Adeeb A-S Ali, *South African Journal of Chemistry*, 68, (2015) 219-225.



## Spectral and Optical Characterization of silver nanoparticles biosynthesised by *Origanum majorana* and *Calendula officinalis*

M. El-Kemary,<sup>†</sup> M. Zahran,<sup>‡</sup> S. A. M. Khalifa,<sup>§,⊥</sup> H. R. El-Seedi<sup>||∇</sup>

<sup>†</sup>Division of Photo- and Nanochemistry, Chemistry Department, Faculty of Science, Kafrelsheikh University, Egypt

<sup>‡</sup>Department of Chemistry, Faculty of Science, El-Menoufi a University, Egypt

<sup>§</sup>Department of Experimental Hematology, Karolinska University Hospital, Stockholm, Sweden

<sup>⊥</sup>Department of Molecular Biosciences, Stockholm University, the Wenner-Gren Institute, Stockholm

<sup>||</sup>Division of Pharmacognosy, Department of Medicinal Chemistry, Uppsala University, Uppsala, Sweden

<sup>∇</sup>Ecological Chemistry Group, Department of Chemistry, School of Chemical Science and Engineering, KTH Royal Institute of Technology, Stockholm, Sweden

E-mail: hesham.el-seedi@fkog.uu.se

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 (AgNO<sub>3</sub>) solution. Size, shape, and crystallinity of the biosynthesized AgNPs were determined by using a transmission electron microscope (TEM). Zeta potential analyzer was used to prove the stability of the metallic nanoparticles, while Fourier transform infrared spectroscopy 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 refers to 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.

**Poster Session II**  
*Al Hamra Convention Center*  
**Monday, February 19, 2018 18:30-20:30**

## **II.1 Influence of Magnetite 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**

**E. C. Schueller, D. H. Fabini, G. Laurita, C. C. Stoumpos, M. G. Kanatzidis, and R. Seshadri**  
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 $\alpha'$ -, $\alpha$ - and $\beta$ -MnB**

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

## **II.5 The Effect of Temperature and Humidity on the Fracture Behavior of a Plate Repaired by Patch**

**K. Madani, L. Rezgani, C. Ezzine, M. Mokhtari, M. Elhannani**  
Mechanical Engineering Department, Djillali Liabes University, Sidi Bel Abbes, Algeria

## **II.6 An Investigation of Partial Replacement of Cement with Metakaolin in Association with Super Plasticizer**

**Anas Shahid Multani**  
Department of Civil Engineering, Dr. A.P.J. Abdul Kalam Technical University, Lucknow, India

## **II.7 Nanomechanical Behavior of Indium and Silver Doped Chalcogenide Glass Systems**

**Abhishek Chaturvedi,<sup>†</sup> G. Sreevidya Varma,<sup>‡</sup> S. Asokan<sup>‡</sup> and U. Ramamurty<sup>†</sup>**

<sup>†</sup>Department of Materials Engineering, Indian Institute of Science, Bangalore, India

<sup>‡</sup>Department of Instrumentation and Applied Physics, IISc Bangalore, India

## **II.8 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.9 Molecular Self-assembly for Nanotechnology Applications**

**Mohammad Changez,<sup>†</sup> Hong-Joon Lee,<sup>‡</sup> Nam-goo Kang<sup>‡</sup> and Jae-Suk Lee<sup>‡</sup>**

<sup>†</sup>Department of Basic Sciences, College of Applied Sciences, A'Sharqiyah University, Ibra, Oman

<sup>‡</sup>School of Materials Sciences and Engineering, Gwangju Institute of Science and Technology, Gwangju, South Korea

## **II.10 Non-Toxic SPIONs-RGO-PEG Nanocompsite 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.11 Structural Properties of ZnO –SnO<sub>2</sub> Composite Nanoparticle Thin Film**

**Khaleed Waleed and Ali Jaseem**

Department of Advanced Materials, Building Research Department, Baghdad, Iraq

## **II.12 Elaboration and Characterization of Nanocrystalline Fe and FeNi Powders Prepared by High Energy Ball Milling Process**

**B. Naoumam, A. Djekoun, A. Chebli, A. Otmani, B. Bouzabata and J. M. Greneche**

Laboratoire de Magnétisme et de Spectroscopie des Solides Université Badji Mokhtar Faculté des sciences B. P: 12 (23000) Annaba, Algérie

Ecole Préparatoire aux Sciences et Techniques Annaba, Algérie

### **II.13 Synthesis, Characterization and Utilization of Carbon Nanotubes for Wastewater Management**

**Sandeep Kumar, Monika Nehra, Gaurav Bhanjana and Neeraj Dilbaghi**

Department of Bio and Nano Technology

Guru Jambheshwar University of Science and Technology, Hisar, Haryana-125001, India

### **II.14 Quasiclassical Molecular Dynamics Study of Chemisorption of CO(vi,ji) Molecule on Pd<sub>n</sub> Cluster**

**Refah AlKhalidi, Nada Omer, Shaffa A.Almehbad and Eman M. Algrafy**

Physics Department, Imam Abdulrahman Bin Faisal University, Dammam, Kingdom of Saudi Arabia

### **II.15 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.16 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.17 Morphological Design of Pure and Doped Nanocrystalline Ceria in the Course of Thermal Decomposition of corresponding Oxalate Precursors**

**Daniel Maslennikov,<sup>†‡</sup> Alexander Matvienko,<sup>†‡</sup> Mikhail Popov,<sup>†</sup> Evgenii Kondratenko,<sup>§</sup> Stanislav Chizhik<sup>†‡</sup> and Anatoly Sidelnikov<sup>†‡</sup>**

<sup>†</sup>Institute of Solid State Chemistry and Mechanochemistry SB RAS, Novosibirsk, Russia

<sup>‡</sup>Novosibirsk State University, Novosibirsk, Russia

<sup>§</sup>Leibniz Institute for Catalysis (LIKAT Rostock)

## **II.18 Quantification of Surface Functionalities on Graphene, Boron Nitride and Borocarbonitrides by Fluorescence Labeling**

**Manaswee Barua, M. B. Sreedhara, K. Pramoda and C. N. R. Rao**

New Chemistry Unit, Jawaharlal Nehru Centre for Advanced Scientific Research, Bangalore, India

## **II.19 Effect of Iron Oxide Nanoparticles on the Photosynthetic Parameters in Tobacco**

**Batool Alkhatib, Rami Alkhatib and Nour Abdo**

Applied Biology Department, Jordan University of Science and Technology, Irbid, Jordan

## **II.20 Covalent Functionalization of Graphene Oxide with Steroidal Diamine Dimer**

**Khaled Shwakfeh, Borhan Albiss, Edreese Alsharaeh and Sally Abadeer**

Department of Chemistry, Jordan University of Science and Technology, Irbid, Jordan

## **II.21 Absorption Dominated Electromagnetic Wave Suppressor Derived from Ferrite Doped Cross-linked Graphene Framework and Conducting Carbon Nanotubes**

**Sourav Biswas and Sujit Sankar Panja**

Department of Chemistry, National Institute of Technology Durgapur, Durgapur, India

## **II.22 Influence of High Energy Mechanical Milling on Ferroelectric and Dielectric Properties of Ca-Zr Doped BaTiO<sub>3</sub> Materials**

**A. R. Tanna and H.H.Joshi**

Department of Physics, RK University, Rajkot, India

## **II.23 Modeling of Diameter Dependent Fe and Co Ultrathin Nanowires from First-Principles Calculations**

**Shivam Kansara, Sanjeev K. Gupta, Yogesh Sonvane and Igor Lukačević**

Department of Applied Physics, Sardar Vallabhbhai National Institute of Technology, Surat, India

## **II.24 Temperature-Dependent Thermal Conductivity and Viscosity of Synthesized $\alpha$ -Alumina Nanofluids**

**Janki Shah, Mukesh Ranjan, Vipul Davariya, Sanjeev K. Gupta and Yogesh Sonvane**  
Department of Applied Physics, Sardar Vallabhbhai National Institute of Technology, Surat, India

## **II.25 Pure and Coexistence of Antiferromagnetic and Ferromagnetic Phases in Mechanically Milled $\text{CaCu}_3\text{Ti}_4\text{O}_{12}$ Quadruple Perovskite**

**P. Y. Raval, P. R. Pansara, A. R. Makadiya, N. H. Vasoya, S. N. Dolia and K. B. Modi**  
Department of Physics, Saurashtra University, Rajkot, India

## **II.26 Synthesis and Characterization of $\text{CuInSe}_2$ Thin Films for Photoelectrochemical Application**

**Sachin Pawar, Sarfraj Mujawar, Bhushan Dhale and Navnath Chavan**  
Department of Physics, Shivaji University, Kolhapur, Kolhapur, India  
Shri Vijaysinha Yadav Arts & Science College Peth Vadgaon, Peth Vadgaon, India

## **II.27 Optical Properties of Gold Nanoparticles Synthesized using Pulse Laser Ablation**

**Hana Alluhaybi, S. K. Ghoshal, W. N. Wan Shamsuri, O. A. Yassin, B. O. Alsobhi, A. A. Salim and G. Krishnan**  
Department of Physics, Taibah University, Al-Madinah Al-Monwarah, Kingdom of Saudi Arabia

## **II.28 UAE Sand into Paper**

**Sidra Siraj Ahmed, Rukshana Mangattu Veetil, Nour Shehadeh Hussein Abdel Rahman and Ali Al Marzouqi**  
Department of Chemical Engineering, United Arab Emirates University, Al Ain, UAE

## **II.29 The Effect of La Dopants on the Phase Stability and Opto-Magnetic Properties of $\text{ZnFe}_{2-x}\text{La}_x\text{O}_4$ Nanopowders**

**Fathalla Hamed and Tholkappian Ramachandran**  
Department of Physics, United Arab Emirates University, Al Ain, UAE

### **II.30 Flow Chemistry Process for Continuous Synthesis of Silver Nanowires**

**Kam Sheng Lau, Chin Hua Chia, Soon Wei Chook, Hanisah Syed Sulaiman, and Sarani Zakaria**

School of Applied Physics, Universiti Kebangsaan Malaysia, Bangi, Malaysia

### **II.31 Magnetic Alloy-MWNT Wool-ball-like Heterostructures as Efficient Electromagnetic Wave Suppressors in Soft Nanocomposites**

**Aishwarya Menon, Giridhar Madras and Suryasarathi Bose**

Department of Materials Engineering, Indian Institute of Science, Bangalore, India

### **II.32 Au Coated ZnO Nanospheres and RGO Nanocomposites for Nanomed Application**

**Mariyah Almanasif, Arshia Fathima, Faheem Ahmed, Roa Fardous, Ali Alhasan and Edreese H. Alsharaeh**

Department of Chemistry, Alfaisal University, Riyadh, Kingdom of Saudi Arabia

### **II.33 Synthesis and Characterization of AC/V<sub>2</sub>O<sub>5</sub>/Bi<sub>2</sub>O<sub>3</sub> Nano-Bimetallic Composite Catalyst for Catalytic Ozonation of Bisphenol A**

**P. Hariprasad, C. U. Aniz, P. Selvendiran, C. H Hanish Mohammed and M. Muthukumar**

Department of Environmental Sciences, Bharathiar University, Coimbatore, India

### **II.34 Semiconductor Titania Nanostructures as Photoactive Catalysts for Effective Water Microbial Purification**

**Walaa A. Abbas, Alaa Y. Faid, Mohamed Ramadan, Ahmed M. Abdellah, Amged Ouf, Nadine Moustafa and Nageh K. Allam**

Department of Physics, The American University in Cairo (AUC), Cairo, Egypt

### **II.35 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***



**M. K. Hema, C. S. Karthik, P. Mallu and N. K. Lokanath**  
Department of Physics, University of Mysore, Mysuru, India

### **II.36 Sensitive 3-chlorophenol Sensor Development based on Facile Er<sub>2</sub>O<sub>3</sub>/CuO Nanomaterials for Environmental Safety**

**Tahir Ali Sheikh, Abdullah M. Asiri, Mohammed M. Rahman and Hadi M. Marwani**  
Department of Chemistry, King Abdulaziz University, Jeddah, Kingdom of Saudi Arabia

### **II.37 Applications of Spinel Ferrite Nanoparticles for Selective Gas Sensors**

**Ahmad I. Ayesh and Mohammad Abu Haija**  
Department of Math., Stat. and Physics, Qatar University, Doha, Qatar

### **II.38 H<sub>2</sub>S Gas Sensor based on Chitosan-WO<sub>3</sub> Hybrid Nanocomposite**

**Fajr I. M. Ali, Falah Awwad, Yaser E. Greish and Saleh T. Mahmoud**  
Department of Physics, United Arab Emirates University, Al Ain, UAE

### **II.39 Selective Adsorption of H<sub>2</sub> Molecule on N-doped ZnO Nano-ribbons: *Ab-initio* Investigation**

**Alaa Shaheen, Wael Othman, Younes Aitladi, Sultan Atatri, Yahya Abdelhadi, Golibjon Berdiyrov and Nacir Tit**  
Department of Physics, United Arab Emirates University, Al Ain, UAE

### **II.40 Au coated SPIONS ( $\gamma$ Fe<sub>3</sub>O<sub>4</sub>) Quantum Dots and RGO composites for Cancer Therapy via Hyperthermia**

**Ghyoudh Alarwan, Yara Alkurdi, Kholoud Almashjari, Arshia Fathima, Roa Fardous, Faheem Ahmed, Edreese Alsharaeh and Ali Hasan**  
Department of Chemistry, Alfaisal University, Riyadh, Kingdom of Saudi Arabia

### **II.41 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**

**Ahmed M. Soliman,<sup>†</sup> Ehab Soltan,<sup>‡</sup> Dalal Alshamsi,<sup>‡</sup> Ahmed A. Murad<sup>†</sup> and Ala Aldahan<sup>‡</sup>**

<sup>†</sup>Department of Chemistry, United Arab Emirates University, Al-Ain, United Arab Emirates

<sup>‡</sup>Geology Department, United Arab Emirates University, Al-Ain, United Arab Emirates

## **II.42 Fabrication of Self-Cleaning Gypsum Composite Paints**

**Aya Al Sadik and Yaser E. Greish**

Department of Chemistry, United Arab Emirates University, Al Ain, United Arab Emirates

## **II.43 Conjugated Molecule based Sensor Designed for Selective Detection of Lithium Ion in Water**

**Ashwini N. Mallya, Mithrabinda P. and Praveen C. Ramamurthy**

Department of Materials Engineering, Indian Institute of Science, Bangalore - 560012, India

## **II.44 Development of Piezo-MEMS Process Flow with PZT Thin Films**

**Sudhanshu Tiwari, Ajay Dangi and Rudra Pratap**

Centre for Nano Science and Engineering, Indian Institute of Science, Bangalore, India

## **II.45 Analysis of Diesel Soot on Paper based Analytical Sensors using SERS Studies**

**Naidu Dhanpal Jayram, Vikram S Raghavan and G. Mohan Rao**

Department of Instrumentation and Applied Physics, Indian Institute of science, Bangalore, India

## **II.46 Development of Phenylhydrazone based Solveto-chromic Receptor for Selective and “Naked Eye” Detection of Fluoride Ion**

**H. Nagarajaiah, Amit G. Anil and Praveen C. Ramamurthy**

Department of Materials Engineering, Indian Institute of Science, Bangalore, India

## **II.47 Simultaneous Detection of Heavy Metal Ions using Modified Carbon Paste Electrode with Reduce Graphene Oxide-SnO<sub>2</sub>-Polyaniline**

**Ramakrishnan Shanmugam, Nandita S. and Praveen C. Ramamurthy**

Department of Materials Engineering, Indian Institute of Science, Bangalore, India

## **II.48 Construction of a Potentiometric Biosensor for the Detection of Glucose using Green Synthesized Silver Nanohybrids and Polypyrrole**

**Santhosh A. S.**<sup>†</sup> **Sandeep S.**<sup>†</sup> **Kumara Swamy N.**<sup>†</sup> **Suresh G. S.**<sup>‡</sup> **Melo J. S.**<sup>§</sup>

<sup>†</sup>Department of Chemistry, Sri Jayachamarajendra College of Engineering, Mysuru, India

<sup>‡</sup>Department of Chemistry and Research Centre, NMKRV College for Women, Jayanagar, Bangalore, India

<sup>§</sup>Nuclear Agriculture and Biotechnology Division, Bhabha Atomic Research Centre, Mumbai, India

## **II.49 Fabrication of Catechol Biosensor using Graphene Nano-ribbons Decorated Biosynthesized Silver Nanoparticles and its Application in Detection of Catechol in Green Tea Samples**

**Sandeep S.**<sup>†</sup> **Santhosh A. S.**<sup>†</sup> **Kumara Swamy N.**<sup>†</sup> **Suresh G. S.**<sup>‡</sup> **and Melo J. S.**<sup>‡</sup>

<sup>†</sup>Department of Chemistry, Sri Jayachamarajendra College of Engineering, Mysuru, India

<sup>‡</sup>Department of Chemistry and Research Centre, NMKRV College for Women, Jayanagar, Bangalore, India

<sup>§</sup>Nuclear Agriculture and Biotechnology Division, Bhabha Atomic Research Centre, Mumbai, India

## **II.50 Fabrication of 2,4-Dinitrophenol based on Nd-doped ZnO Nanorods**

**Abdul Wahid,** **Abdullah M. Asiri** and **Mohammed M. Rahman**

Center of Excellence for Advanced Material Research (CEAMR)

King Abdulaziz University, Jeddah, Kingdom of Saudi Arabia

## **II.51 3D Spongy Graphene-Modified Screen-Printed Sensors for the Voltammetric Determination of the Narcotic Drug Codeine**

**Dalia M. El-Gendy,** **Mona A. Mohamed,** **Nashaat Ahmed,** **Craig E. Banks** and **Nageh K. Allam**

Department of Chemistry, National Research Centre, Dokki, Giza, Egypt

The American University in Cairo, New Cairo 11835, Egypt

## **II.52 Embroidered Conductive Threads on E-Textiles for Wearable Smart Applications**

**Eman M. Swielam,** **Samiea M. Eltopshy,** **Sania K Sobhy,** **Z. M. Abdel-Megied** and **Ahmad Labeeb**

Department of Textile industry, National Research Center, Cairo, Egypt

## **II.53 Near Surface Nitrogen Delta Doping in Diamond**

**Maneesh Chandran**

Departments of Physics & Nanotehnology, SRM University, Kattankulathur, Chennai, India

## **II.54 Graphene Membrane for Desalination of Seawater**

**Dezairi Aouatif, Rochd Sanaa, Mizani Sofia, Moulrif Rachida and Lahlou Souad**

Department of Physics, Hassan II University, Casablanca, Morroco

## **II.55 Molecular Dynamics Simulation of Aluminosilicate Glasses**

**Mohamed Zekri, Andreas Erlebach and Ramzi Maalej**

Department of Physics, Sfax University, Sfax, Tunisia

## **II.56 Defect Chemistry and Oxygen Vacancy Migration in Gd-doped CeO<sub>2</sub>: Hybrid Functional Study**

**Xiaoping Han, Nouredine Amrane and Maamar Benkraouda**

Department of Physics, United Arab Emirates University, Al Ain, United Arab Emirates

## **II.57 Newly Discovered Topological Insulator Sr<sub>3</sub>SnO for Spintronics, Optical and Electronic Properties**

**Rasha W. Adnan Moh'd, Juwayni Lucman, Faris Mahmoud Safieh, Nouredine Amrane and Maamar Benkraouda**

Department of Physics, United Arab Emirates University, Al-Ain, United Arab Emirates

## **II.58 Thermal Decomposition Synthesis of Cobalt-Oxide Nanocrystals**

**N. K. Lokanath and M. K. Hema**

Department of Physics, University of Mysore, Mysuru, India

## **II.59 Defects and Persistent Conductivity in Strontium Tintanate Single Crystals**

**Marianne C. Tarun and Matthew D. McCluskey**

Department of Physics and Astronomy, Washington State University, Pullman, Washington,  
USA

## **Influence of Magnetite Incorporated on Zinc Oxide Hybrid Nanostructures**

**Selvendiran Periyasamy, Allen Joseph Anthuvan  
and Muthukumar Muthuchamy**

Department of Environmental Sciences  
Bharathiar University  
Coimbatore, India  
E-mail: selvendiranpelectrochem@gmail.com

The present work demonstrates the preparation of magnetite ( $\text{Fe}_3\text{O}_4$ ) incorporated Zinc oxide (ZnO) nanostructures by a simple co-precipitation assisted reflux condensation method. The X-ray diffraction, Field emission scanning electron microscopy (FE-SEM), Trans-mission 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  $\text{Fe}_3\text{O}_4$  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

**E. C. Schueller, D. H. Fabini, G. Laurita, C. C. Stoumpos,  
M. G. Kanatzidis, and R. Seshadri**

Department of Materials  
University of California, Santa Barbara  
Santa Barbara, United States of America  
E-mail: schueller@umail.ucsb.edu

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.<sup>1</sup> 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  $P4/mbm$  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.<sup>2</sup> Finally,  $FAPbBr_3$  displays unusual pseudo-cubic behavior in the tetragonal regime, similar to that seen in  $FAPbI_3$ .<sup>3</sup>

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

### References:

- 1) D. H. Fabini, J. G. Labram, A. J. Lehner, J. S. Bechtel, H. A. Evans, A. Van der Ven, F. Wudl, M. L. Chabinyc, R. Seshadri, *Inorg. Chem.* 56 (2017) 11–25.
- 2) G. Laurita, D. H. Fabini, C. C. Stoumpos, M. G. Kanatzidis, R. Seshadri, *Chem. Sci.* 8 (2017) 5628–5635.

3) D. H. Fabini, C. C. Stoumpos, G. Laurita, A. Kaltzoglou, A. G. Kontos, P. Falaras, M. G. Kanatzidis, R. Seshadri, *Angew. Chem. Int. Ed.* 55 (2016) 15392–15396.



## **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  
E-mail: zeeshanahmad09@hotmail.com

Conventional concrete has been used for civil construction for many years, which eminently exploits the natural or virgin materials which is in scarcity. Erstwhile several researches have 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 the 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 CO<sub>2</sub>. 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 & 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 study 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.

Keywords: Concrete, Red Mud, Petroleum coke, Fibre, Admixture, Cement, Sand.

References:

- [1] MahinSha O B, Remya C P, Red mud Concrete, International Research Journal of Engineering and Technology, Volume: 03 Issue: 04, April-2016
- [2] Kirankumar M S, Raghavendra Naik, Experimental Study on Utilization of Red Mud and Quarry Dust in Cement Mortar and Concrete, International Journal of Civil and Structural Engineering Research, Volume: 04, Issue: 01, PP: (324-330), April 2016 - September 2016
- [3] Daniel Vêras Ribeiro, João António Labrinchab, Marcio Raymundo Morellia, Potential Use of Natural Red Mud as Pozzolona for Portland cement, Materials Research, Volume: 14, Issue: 01, PP: (60-66), 2011.

## Crystal Structure and Magnetic Properties of $\alpha'$ -, $\alpha$ - and $\beta$ -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  
E-mail: kalyon@ac.chemie.tu-darmstadt.de

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:

[1] M. Fries, Z. Gercsi, S. Ener, K.P. Skokov, O. Gutfleisch, Acta Mater. 2016, 113, 213-220. [2] S. Ma, K. Bao, Q. Tao, P. Zhu, T. Ma, B. Liu, Y. Liu, T. Cui, Sci. Rep. 2017, 7, 43759. [3] G. Papesch, H. Nowotny, F. Benesovsky, Monatsh. Chem. 1973, 104, 933-942. [4] I. Smid, P. Rogl, F. Weitzer, Proc. 12th Int. Plansee Sem. 1985. [5] R. Kiessling, Acta Chem. Scand. 1950, 4, 146-159.

## **The Effect of Temperature and Humidity on the Fracture Behavior of a Plate Repaired by Patch**

**K. Madani, L. Rezgani, C. Ezzine, M. Mokhtari, M. Elhannani**

Mechanical Engineering Department  
Djillali Liabes University  
Sidi Bel Abbes, Algeria  
E-mail: koumad10@yahoo.fr

The effect of temperature and humidity on the mechanical behavior of the adhesive has been studied. The adhesive samples were immersed in distilled water at various temperatures. The tensile properties of the adhesive were inventoried and used in a numerical study to analyze the breaking behavior of a damaged patch-repaired plate. The results obtained illustrate the variation of the mechanical behavior as a function of the immersion time and the temperature. The presence of water in the adhesive decreases its tensile strength and modulus of elasticity but also increases the ductility of the material. These changes in mechanical properties are greater as the percentage of water absorbed increases. The temperature will increase the amount of water absorbed, increase the kinetics of degradation with the immersion time and will directly affect the values of the stress intensity factor at the head of the crack.

## **An Investigation of Partial Replacement of Cement with Metakaolin in Association with Super Plasticizer**

**Anas Shahid Multani**

Department of Civil Engineering  
Dr. A.P.J. Abdul Kalam Technical University  
Lucknow, India  
E-mail: anasmultani90@gmail.com

These day's natural issues are increasingly noteworthy. The modern region creates loads of waste materials and CO<sub>2</sub>, respectably. A champion among the best approaches to take care of these issues is the usage of these waste materials. Metakaolin is non conventional materials obtained from the calcinations of kaolin clay. Metakaolin seems to be a auspicious additional cementitious material for superior cement. Properties of cement with metakaolin are for the most part favoured added substances in superior cement. A conceivable lower cost, because of huge accessibility in our nation itself might be points of interest to metakaolin use in making superior concrete. The metakaolin consolidations increment the quality of the concrete specimens. In this work, the impact of various contents of Metakaolin included to concrete containing super plasticizer its compressive quality strength and workability has been contemplated. Samples with 0%, 5%, 10%, 15%, 20% and 25% content of metakaolin replacing the cement have been evaluated for M30 grade. The outcomes have been contrasted and those for the control test and practicality of adding metakaolin to concrete has been examined. It was watched that up to 15% of concrete can be supplanted with metakaolin blended with superplasticizer. 15% substitution is the ideal rate at which expanded quality of test sample is seen from the base sample test.

## **Nanomechanical Behavior of Indium and Silver Doped Chalcogenide Glass Systems**

**Abhishek Chaturvedi,<sup>†</sup> G. Sreevidya Varma,<sup>‡</sup>  
S. Asokan<sup>‡</sup> and U. Ramamurty<sup>†</sup>**

<sup>†</sup>Department of Materials Engineering, Indian Institute of Science, Bangalore, India

<sup>‡</sup>Department of Instrumentation and Applied Physics, IISc Bangalore, India

E-mail: abhishekc@iisc.ac.in

Connections between the local structure (floppy, rigid or intermediate) and mechanical properties in ternary (Ge-Te-In) and quaternary (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**

**Prajakta Katti, S. Kumar and Suryasarathi Bose**

Department of Materials Engineering  
Indian Institute of Science  
Bangalore, India  
E-mail: prajaktakatti@gmail.com

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.

## **Molecular Self-assembly for Nanotechnology Applications**

**Mohammad Changez,<sup>†</sup> Hong-Joon Lee,<sup>‡</sup> Nam-goo Kang<sup>‡</sup> and Jae-Suk Lee<sup>‡</sup>**

<sup>†</sup>Department of Basic Sciences, College of Applied Sciences, A'Sharqiyah University, Ibra,  
Oman

<sup>‡</sup>School of Materials Sciences and Engineering, Gwangju Institute of Science and Technology,  
Gwangju, South Korea  
E-mail: mchangej@asu.edu.om

Three-dimensional (3D) molecular-level ordering is an important and challenging objective of current research in materials chemistry and physics. It can improve the efficiency of systems or generate entirely new types of systems containing functionalities that were previously unattainable. Self-assembly is emerging as an elegant and powerful approach to fabricating nanostructured materials. However, controlling the precise arrangement of molecules on the molecular scale is most demanding because of the difficulty in making such small structures.[1] To keep up with the pace of development of our civilization, we need more compact, faster, and efficient devices for our daily use. These goals require the design of systems with atomic- or molecular-level precision at a reasonable cost.

For semi conducting polymers, the difficulty is in controlling the precise arrangement of polymers with both facile and low-cost processes at once, which is the advantage and core principle of using certain polymer materials over others. Crosslinked polymers are widely used in various devices due to their high mechanical strength or solvent resistance during device fabrication. Unlike typical research on crosslinked polymers, our group has used controlled crosslinking techniques for precisely ordering polymers. We reported molecular ordering in poly(2-vinylpyridine) (P2VP) and PANI through self-recognition and organization during the chemical reaction of P2VP and a cross-linker.[1,3] Recently, we also achieved the molecular level ordered in conjugated polymers using zinc salt, finally producing a crosslinked structure.[10] Since the crosslinking of molecules under specific conditions is able to effectively suppress the directional freedom of polymers, inhibiting chain entanglements, molecular ordering by crosslinking may be a solution to resolving the inherent morphological limitations of resulting conducting polymers.

### References :

1. Mohammad Changez, et al. Molecular-Level Ordering of Poly(2-vinylpyridine), *Adv. Materials*, 24, 3253-3257(2012).
2. Hong-Joon Lee, Sang-Ook Hur, Min-Kyoon Ahn, Mohammad Changez, and Jae-Suk Lee, In *Situ Formation of Molecular-scale Ordered Polyaniline Film by Zinc Coordination*, *Nano Scale* 2017, DOI: 10.1039/c7nr01060e.

**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  
E-mail: rfardous@kacst.edu.sa

Abstract



## **Structural Properties of ZnO –SnO<sub>2</sub> Composite Nanoparticle Thin Film**

**Khaleed Waleed and Ali Jaseem**

Department of Advanced Materials  
Building Research Department  
Baghdad, Iraq  
E-mail: kaliedbuildingresearch@gmail.com

Attached below is a brief description of the research, which is the study of the( structural properties of the (Zno -Sno2) composite nano particles preparation by thermal chemical spraying) with different deposition conditions ratio mixture , angle spraying and temperature substrate

Thin film samples prepared by using the thermal chemical spraying machine, the structure properties Are verified X-ray diffraction machine, sensitivity for gases and steams using a sensitivity system. The samples were exposed to methanol and ethanol and the results oobtaining hexagonal crystallization membranes with directional (002) for ( zno , zno:sno2 )samples except( Sno2 )as the results showed obtaining nanoscale structures at the rate from to (2.4) to (46 )nm.

allergic measurements showed high sensitivity at the base temperature of 450 ° C with a 45 ° angle of spray and at a ( zno 50%:sno2 50%) percentage mixture.

The most effective factor in the improvement of sensitivity properties is the increase in the percentage of Sno2 mixing and this is evident through the results.

## **Elaboration and Characterization of Nanocrystalline Fe and FeNi Powders Prepared by High Energy Ball Milling Process**

**B. Naoumam, A. Djekoun, A. Chebli, A. Otmani,  
B. Bouzabata and J. M. Greneche**

Laboratoire de Magnétisme et de Spectroscopie des Solides Université Badji Mokhtar Faculté  
des sciences B. P: 12 (23000) ANNABA -Algérie  
Ecole Préparatoire aux Sciences et Techniques Annaba – Algérie  
Annaba, Algeria  
E-mail: n\_boudinar@yahoo.fr

In order to study the structural, morphological and magnetic behaviour of Fe<sub>50</sub>Ni<sub>50</sub> alloys and pure Fe powders prepared by mechanical alloying, X-ray Diffraction, Scanning electron microscopy, Mössbauer spectroscopy and vibrating sample magnetometer techniques have been employed. All the alloys were prepared until a 24 h however for Fe powders were going to 32 h of milling. X-ray diffraction for pure Fe showed that all samples exhibit bcc-type reflections. A rapid decrease in crystallite size and a slight increase in lattice parameter with increasing milling times were observed. In the case of Fe<sub>50</sub>Ni<sub>50</sub> alloys X-ray diffraction and Mössbauer spectroscopy proved that during mechanical alloying process the Fe-Ni solid solution with FCC lattice was formed. Their crystallite size was reduced to 22 nm after 24 h of milling. Morphological studies revealed that with the elongation of the milling time, mixed powders become fine totally and the distribution of powders becomes uniform. The magnetic properties of the synthesized samples were investigated by using vibrating sample magnetometer at room temperature. The effect of milling time on saturation magnetization (M<sub>s</sub>) and the coercivity (H<sub>c</sub>) of all the samples are discussed.

## **Synthesis, Characterization and Utilization of Carbon Nanotubes for Wastewater Management**

**Sandeep Kumar, Monika Nehra, Gaurav Bhanjana and Neeraj Dilbaghi**

Department of Bio and Nano Technology  
Guru Jambheshwar University of Science and Technology  
Hisar, Haryana-125001, India  
E-mail: ksandeep36@yahoo.com

Nanomaterials have astonishing future due to their excellent physiochemical, mechanical, and opto-electronic properties. The nanomaterials have been proposed to be utilized in 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.

## **Quasiclassical Molecular Dynamics Study of Chemisorption of CO(v<sub>i</sub>,j<sub>i</sub>) Molecule on Pd<sub>n</sub> Cluster**

**Refah AlKhaldi, Nada Omer, Shaffa A.Almehbad and Eman M. Algrafy**

Physics Department  
Imam Abdulrahman Bin Faisal University  
Dammam, Kingdom of Saudi Arabia  
E-mail: refa\_sa\_6@hotmail.com

The CO molecule is highly toxic for both humans and animals and the atmosphere receives an enormous amount of CO per year (1.09 billion tons in 2000). In this way, carbon monoxide (CO) dissociation is an essential step in the minimization of this pollutant. In this work the reactive channel of the Pd<sub>n</sub>(T)+Co(v<sub>j</sub>) dissociation collision system will be studied via quasiclassical molecular dynamics simulations. The Pd cluster potential energy is described using an embedded-atom potential, and LEPS (London-Eyring-Polanyi-Sato) potential energy function will be used to model the interaction between the molecule and the cluster. Dissociative chemisorption probabilities are computed as functions of the impact parameter and the collision energy which are used to evaluate the reaction cross sections and reaction rate. Effects of both initial rovibrational states of the molecule and temperature of the cluster on the reactive channel was analyzed. The reaction cross section strong dependence on cluster size was also be investigated.

## **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  
E-mail: randhir@iisc.ac.in

There are several methods reported for the growth of ZnO nanostructure 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 ( $> 500^{\circ}\text{C}$ ) 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 2.43deg. 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 110deg 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**

**Nagaraju Sykam, Naidu Dhanpal Jayram and G. Mohan Rao**

Department of Instrumentation and Applied Physics  
Indian Institute of Science Bengaluru  
Bangalore, India  
E-mail: nagarajusykam4@gmail.com

The vast increase in global population coupled with rapid pace of industrialization in the present world 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 in about 1 min. As prepared EG shows excellent 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 ( $\pm 10.2$ ), 222.32 ( $\pm 8.6$ ), 151.51 ( $\pm 9.2$ ) and 196.08 ( $\pm 5.4$ ) 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 5 cycles 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 ( $\pm 5.4$ ) 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**

**Daniel Maslennikov,<sup>† ‡</sup> Alexander Matvienko,<sup>† ‡</sup> Mikhail Popov,<sup>†</sup>  
Evgenii Kondratenko,<sup>§</sup> Stanislav Chizhik<sup>† ‡</sup> and Anatoly Sidelnikov<sup>† ‡</sup>**

<sup>†</sup>Institute of Solid State Chemistry and Mechanochemistry SB RAS, Novosibirsk, Russia

<sup>‡</sup>Novosibirsk State University, Novosibirsk, Russia

<sup>§</sup>Leibniz Institute for Catalysis (LIKAT Rostock)

E-mail: daniel@solid.nsc.ru

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  $\text{Ce}_2(\text{C}_2\text{O}_4)_3 \cdot 10\text{H}_2\text{O}$  and mixed oxalates  $\text{Ce}_{2-x}\text{M}_x(\text{C}_2\text{O}_4)_3 \cdot 10\text{H}_2\text{O}$ , where  $\text{M}=\text{Gd}$  and  $\text{Sm}$ . Various methods have been found for growing the precursors' crystals of different size (from  $\mu\text{m}$ -size up to  $\text{mm}$ -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  $S_{\text{BET}}$  values of 140–150  $\text{m}^2/\text{g}$ . 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-H<sub>2</sub> method. In addition, ceria doped with 10% Gd (10CGO), which was obtained from  $\text{Ce}_{1.8}\text{Gd}_{0.2}(\text{C}_2\text{O}_4)_3 \cdot 10\text{H}_2\text{O}$ , has been used to produce thin layer (ca. 10-20  $\mu\text{m}$ ) 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. It has been also demonstrated that the microtubular SOFCs with 10CGO as electrolyte have high thermal shock resistance and an adequate performance for practical applications.

**Acknowledgements**

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**

**Manaswee Barua, M. B. Sreedhara, K. Pramoda and C. N. R. Rao**

New Chemistry Unit  
Jawaharlal Nehru Centre for Advanced Scientific Research  
Bangalore, India  
E-mail: manaswee@jncasr.ac.in

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<sup>9</sup> groups/cm<sup>2</sup>. 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**

**Batool Alkhatib, Rami Alkhatib and Nour Abdo**

Applied Biology Department  
Jordan University of Science and Technology  
Irbid, Jordan  
E-mail: batoolkhtib@yahoo.com

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.

## **Covalent Functionalization of Graphene Oxide with Steroidal Diamine Dimer**

**Khaled Shwakfeh, Borhan Albiss, Edreese Alsharaeh and Sally Abadeer**

Department of Chemistry  
Jordan university of science and technology  
Irbid, Jordan  
E-mail: maiasharbn@yahoo.com

The functionalization of pristine graphene sheets with organic functional groups has been developed for several purposes. The main purpose is the dispersion of graphene sheets in organic solvents that is a crucial move toward the formation of nanocomposite materials with graphene. In this work, graphene oxide sheets (GO) will be activated using thionyl dichloride (SOCl<sub>2</sub>) to obtain a graphene derivative that contained acyl chloride groups. These acyl chloride groups will be reacted with the amine groups of steroidal diamine to form amide groups that anchored steroidal diamine dimer nanofibers onto the graphene oxide sheets. Several steroidal diamine dimers will be used and compared with typical diamine. These nanocomposites will be characterized using atomic force microscopy (AFM) images, UV-vis spectra, scanning electron microscopy (SEM), Fourier transform infrared (FT-IR) spectra and XRD.

# **Absorption Dominated Electromagnetic Wave Suppressor Derived from Ferrite Doped Cross-linked Graphene Framework and Conducting Carbon Nanotubes**

**Sourav Biswas and Sujit Sankar Panja**

Department of Chemistry  
National Institute of Technology Durgapur  
Durgapur, India  
E-mail: sourav.biswas210@gmail.com

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<sub>2</sub> doped MWCNTs and Fe<sub>3</sub>O<sub>4</sub> 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<sub>2</sub> 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.

## **Influence of High Energy Mechanical Milling on Ferroelectric and Dielectric Properties of Ca-Zr Doped BaTiO<sub>3</sub> Materials**

**A. R. Tanna and H.H.Joshi**

Department of Physics  
RK University  
Rajkot, India  
E-mail: ashishrtanna@gmail.com

The ferroelectric material with general formula  $\text{Ca}_x\text{Ba}_{1-x}\text{Zr}_x\text{Ti}_{1-x}\text{O}_3$  ( $x=0.0$  &  $0.1$ ) is synthesized by solid state reaction. The ceramic powders of these prepared samples are milled in a planetary ball mill in air, with tungsten carbide vial and 150 tungsten carbide balls of diameter 10 mm for different hours (12 hrs, 18 hrs and 30 hrs). The powder X-ray diffractometry is employed to confirm the single phase tetragonal (P4mm) perovskite structure to all the specimens. Morphology and crystallite size have been studied by means of scanning electron microscopy for the ferroelectric samples. The polarization versus electric field (PE) hysteresis loops of ferroelectric specimens for different milling hours are carried using PE hysteresis loop tracer and the dielectric measurements are recorded in the frequency range 100Hz - 1MHz at room temperature using impedance analyzer. The properties of ferroelectric materials depended on the size of crystallites. The high energy ball milling is one of the great techniques to control the particle size of the prepared samples. The PE hysteresis loop recorded at room temperature gives the values of polarization, coercivity and remanence. The shape of PE loop drastically changes after the ball milling process and the PE hysteresis parameters are found to change. The polarization decreases and simultaneously the coercivity and remanence increase with ball milling time up to 18 hours and they are found to decrease for the 30 hour milled samples. The dielectric constant is measured for pristine BaTiO<sub>3</sub> i.e. 2200 at 100 Hz and 412 at 1 kHz frequency. The value of dielectric constant decreases with ball milling time. Similarly, the dielectric constant for Ca<sub>0.1</sub>Ba<sub>0.9</sub>Zr<sub>0.1</sub>Ti<sub>0.9</sub>O<sub>3</sub> ferroelectric specimen is 1650 at 100 Hz and 442 at 1 kHz frequency. Both the present ferroelectric specimens show universal dielectric response with frequency variation. It is to be noted that for Ca<sub>0.1</sub>Ba<sub>0.9</sub>Zr<sub>0.1</sub>Ti<sub>0.9</sub>O<sub>3</sub>, the dielectric constant initially decreases with ball milling time and thereafter it increases with further milling.

## **Modeling of Diameter Dependent Fe and Co Ultrathin Nanowires from First-Principles Calculations**

**Shivam Kansara, Sanjeev K. Gupta, Yogesh Sonvane and Igor Lukačević**

Department of Applied Physics  
Sardar Vallabhbhai National Institute of Technology  
Surat, India  
E-mail: sidkans23@gmail.com

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 $\alpha$ -Alumina Nanofluids**

**Janki Shah, Mukesh Ranjan, Vipul Davariya,  
Sanjeev K. Gupta and Yogesh Sonvane**

Department of Applied Physics  
Sardar Vallabhbhai National Institute of Technology  
Surat, India  
E-mail: janki.1311@gmail.com

In the present work, we focused on the thermal conductivity and viscosity of the synthesis as well as characterize metal oxide  $\alpha$ -Al<sub>2</sub>O<sub>3</sub> nanoparticles suspended in distilled water (DW): ethylene glycol (EG) (60:40) ratio based stable colloidal nanofluid. The band gap of the  $\alpha$ -Al<sub>2</sub>O<sub>3</sub> 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) than 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  $\alpha$ -Al<sub>2</sub>O<sub>3</sub> 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 $\text{CaCu}_3\text{Ti}_4\text{O}_{12}$ Quadruple Perovskite**

**P. Y. Raval, P. R. Pansara, A. R. Makadiya, N. H. Vasoya,  
S. N. Dolia and K. B. Modi**

Department of Physics  
Saurashtra University  
Rajkot, India  
E-mail: pooja.raval21@gmail.com

The consequences of high energy mechanical milling on magnetic ordering of polycrystalline  $\text{CaCu}_3\text{Ti}_4\text{O}_{12}$  cubic perovskite have been investigated by means of X-ray powder diffractometry (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,  $H_{\text{max}} = 70$  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<sub>2</sub> Thin Films for Photoelectrochemical Application**

**Sachin Pawar, Sarfraj Mujawar, Bhushan Dhale and Navnath Chavan**

Department of Physics, Shivaji University, Kolhapur, Kolhapur, India  
Shri Vijaysinha Yadav Arts & Science College Peth Vadgaon, Peth Vadgaon, India  
E-mail: asachinpawar@gmail.com

The copper indium diselenide (CuInSe<sub>2</sub>) thin film were prepared on the 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 4mM CuSO<sub>4</sub>, 5mM In<sub>2</sub>(SO<sub>4</sub>)<sub>3</sub>, 40mM SeO<sub>2</sub> and 1M K<sub>2</sub>SO<sub>4</sub> as an additional electrolyte with pH 1.4. The film of CuInSe<sub>2</sub> were studied by cyclic voltammetry (CV) for the measurement of reduction potential. CuInSe<sub>2</sub> 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<sub>2</sub> crystal was grown. XRD revealed that the films are crystalline in nature. The surface morphology of CuInSe<sub>2</sub> 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.

## **Optical Properties of Gold Nanoparticles Synthesized using Pulse Laser Ablation**

**Hana Alluhaybi, S. K. Ghoshal, W. N. Wan Shamsuri, O. A. Yassin,  
B. O. Alsobhi, A. A. Salim and G. Krishnan**

Department of Physics  
Taibah University  
Al-Madinah Al-Monwarah, Kingdom of Saudi Arabia  
E-mail: haalluhaibi@gmail.com

Pulse laser ablation in liquid method attracts great interest for fabricating nanoparticles due to its simplicity, versatility and free impurity contaminations. Gold nanoparticles were synthesized by pulse laser ablation in deionized water using Q-switch Nd:YAG laser (fundamental wavelength 1064 nm, pulse duration 8 ns). The purpose of the present work is to investigate the dependence of the structural and optical properties of gold nanoparticles on the laser energy and the repetition rate. The optical properties of the prepared gold nanoparticles were determined using the UV-Vis spectroscopy. UV-Vis absorption showed surface plasmon resonance (SPR) peak in the range from 521 to 523 nm. By analysing the TEM results the size of the prepared nanoparticles is found to be in the range from 7 to 24 nm.

## **UAE Sand into Paper**

**Sidra Siraj Ahmed, Rukshana Mangattu Veetil,  
Nour Shehadeh Hussein Abdel Rahman and Ali Al Marzouqi**

Department of Chemical Engineering  
United Arab Emirates University  
Alain-Abu Dhabi, United Arab Emirates  
E-mail: 201150428@uaeu.ac.ae

The first use of paper dates to 2nd Century (BC). Be it used to represent value such as money, or to store information, paper 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 $\text{ZnFe}_{2-x}\text{La}_x\text{O}_4$ Nanopowders**

**Fathalla Hamed and Tholkappiyan Ramachandran**

Department of Physics  
United Arab Emirates University  
AlAin, United Arab Emirates  
E-mail: fhamed@uaeu.ac.ae

$\text{ZnFe}_{2-x}\text{La}_x\text{O}_4$  ( $x=0, 0.25, 0.5$  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**

**Kam Sheng Lau, Chin Hua Chia, Soon Wei Chook,  
Hanisah Syed Sulaiman, and Sarani Zakaria**

School of Applied Physics  
Universiti Kebangsaan Malaysia  
Bangi, Malaysia  
E-mail: kamsheng94@outlook.com

One dimensional (1D) 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**

**Aishwarya Menon, Giridhar Madras and Suryasarathi Bose**

Department of Materials engineering  
Indian Institute of Science  
Bangalore, India  
E-mail: aishuvmenon20@gmail.com

FeNi (iron-nickel) alloy particles were coated with MWNTs using 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<sup>3</sup> g<sup>-1</sup> respectively for composites containing FeNi/MWNT- 3:1.

## **Au Coated ZnO Nanospheres and RGO Nanomcomposites for Nanomed Application**

**Mariyah Almanasif, Arshia Fathima, Faheem Ahmed,  
Roa Fardous, Ali Alhasan and Edreese H. Alsharaeh**

Department of Chemistry  
Alfaisal University  
Riyadh, Kingdom of Saudi Arabia  
E-mail: malmanasif@alfaisal.edu

According to WHO, 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 AC/V<sub>2</sub>O<sub>5</sub>/Bi<sub>2</sub>O<sub>3</sub> Nano-Bimetallic Composite Catalyst for Catalytic Ozonation of Bisphenol A**

**P. Hariprasad, C. U. Aniz, P. Selvendiran,  
C. H Hanish Mohammed and M. Muthukumar**

Department of Environmental Sciences  
Bharathiar University  
Coimbatore, India  
E-mail: [hariamc@gmail.com](mailto:hariamc@gmail.com)

Bimetallic nanomaterials/Metaloxides have received significant concern 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 various fields, specifically in catalytic field. Activated carbon based of AC/V<sub>2</sub>O<sub>5</sub>/ Bi<sub>2</sub>O<sub>3</sub> Nano-Bimetallic Composite Catalyst 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 catalytic ozonation has achieved a maximum TOC removal of 68 % where the non catalytic ozonation has achieved only 36% of TOC removal.



## **Semiconductor Titania Nanostructures as Photoactive Catalysts for Effective Water Microbial Purification**

**Walaa A. Abbas, Alaa Y. Faid, Mohamed Ramadan, Ahmed M. Abdellah, Amged Ouf, Nadine Moustafa and Nageh K. Allam**

Department of Physics  
The American University in Cairo (AUC)  
Cairo, Egypt  
E-mail: [walaa.biotech09@gmail.com](mailto:walaa.biotech09@gmail.com)

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, TiO<sub>2</sub> 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 synthesized-TiO<sub>2</sub> 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 TiO<sub>2</sub>. These factors were examined and analysed in this research work and they include the aspect ratio, crystalline phase, surface hydroxyls, physicochemical properties of TiO<sub>2</sub> 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***

**M. K. Hema, C. S. Karthik, P. Mallu and N. K. Lokanath**

Department of Physics  
University of Mysore  
Mysuru, India  
E-mail: hemamk38@gmail.com

Synthesis of nanoparticles using different synthetic strategies can lead to the 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 Benzoylacetate 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 500oC 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.

Key words: Copper complexes, Copper Oxide Nanoparticles, antimicrobial agent.

## **Sensitive 3-chlorophenol Sensor Development based on Facile Er<sub>2</sub>O<sub>3</sub>/CuO Nanomaterials for Environmental Safety**

**Tahir Ali Sheikh, Abdullah M. Asiri,  
Mohammed M. Rahman and Hadi M. Marwani**

Department of Chemistry  
King Abdulaziz University  
Jeddah, Kingdom of Saudi Arabia  
E-mail: tahirgcu786@gmail.com

Low-dimensional calcined (500.0 °C) Erbium oxide-Copper oxide (Er<sub>2</sub>O<sub>3</sub>/CuO) doped nanomaterial were synthesized in alkaline pH using the wet-chemical method. The optical, structural and morphological properties of Er<sub>2</sub>O<sub>3</sub>/CuO nanomaterial were characterized in details using FT-IR, PL, XRD, UV/vis. XPS and TEM analysis. In addition to these FESEM equipped with EDS analysis was also carried out in order to find the morphology and composition of the synthesized nanomaterial and it was found in the form of nanoblocks. A thin-layer of Er<sub>2</sub>O<sub>3</sub>/CuO nanoblocks (NBs) was fabricated on to the glassy carbon electrode (GCE) with conducting nafion binders for the development of selective and sensitive 3-chlorophenol (3-CP) sensor. Electrochemical responses along with higher sensitivity, large dynamic range, lower detection limit, limit of detection and long-term stability towards 3-CP were found by electrochemical I-V approach. The calibration curve was found linear over a wide linear dynamic range (LDR) of 3-CP concentration (0.1 nM ~ 10.0 mM). Limit of detection (LOD) and sensitivity from the slope of the calibration plot were calculated as 0.09 nM and 10.5485 μA mM<sup>-1</sup> cm<sup>-2</sup> respectively, in addition to limit of quantification (0.3 nM). It is an organized route for developing the chemical sensor based on very low-dimensional Er<sub>2</sub>O<sub>3</sub>/CuO NBs/GCE using electrochemical oxidation phenomena. As far as we know, this report is the initial reports on highly sensitive 3-CP sensor based on the Er<sub>2</sub>O<sub>3</sub>/CuO NBs/Nafion/GCE. This method could be a pioneer developer in 3-CP sensor development using codoped nano-structural materials in the simple I-V method for the important sensor applications for environmental safety.

**Key words:** Er<sub>2</sub>O<sub>3</sub>/CuO nanomaterials; Green synthesis; 3-chlorophenol; I-V method; electrochemical sensor; Sensitivity; Environmental safety

## **Applications of Spinel Ferrite Nanoparticles for Selective Gas Sensors**

**Ahmad I. Ayesh and Mohammad Abu Haija**

Department of Math., Stat. and Physics  
Qatar University  
Doha, Qatar  
E-mail: ayesh@qu.edu.qa

This work reports on sensitive and selective gas sensors based on copper ferrite ( $\text{CuFe}_2\text{O}_4$ ) nanoparticles. The nanoparticles were produced different methods including: colloid microwave assisted hydrothermal method, and co-precipitation method. Those methods enable a precise control of nanoparticle size, The produced nanoparticles were annealed at different temperatures. Structural analysis were carried out using x-ray diffraction (XRD) and transmission electron microscopy (TEM), and they revealed that the as-prepared nanoparticle exhibit cubic structure. The nanoparticles undergo crystal structure transformation to tetragonal structure upon annealing. Furthermore, the nanoparticle were found to grow in size upon annealing. The tetrahedral and octahedral absorption bands which are characteristic of the spinel ferrite were determined using Fourier Transform Infra-Red Spectroscopy (FTIR) measurements. Gas sensors were fabricate by pressing the produced nanoparticle powder into disks. The sensor device was produced utilizing capacitor structure, with the top electrode stainless steel of grid structure. The produced sensors were characterized to be sensitive to both  $\text{H}_2\text{S}$  and  $\text{H}_2$  gases, with greater sensitivity to  $\text{H}_2\text{S}$  at low temperatures, where these sensors could detect  $\text{H}_2\text{S}$  concentrations of 10 ppm at 80 °C. The low optimal operation temperature reveals the low power requirements for sensor operation. Thus, those sensors exhibit the potential to be used for industrial applications, especially for the petrochemical industry.

## **H<sub>2</sub>S Gas Sensor based on Chitosan-WO<sub>3</sub> Hybrid Nanocomposite**

**Fajr I. M. Ali, Falah Awwad, Yaser E. Greish and Saleh T. Mahmoud**

Department of Physics  
United Arab Emirates University  
Al-ain, United Arab Emirates  
E-mail: 201670363@uaeu.ac.ae

The nanostructure tungsten oxide (WO<sub>3</sub>) has been one of the most promising metal oxide-semiconductor materials that is widely used in H<sub>2</sub>S gas monitoring systems. WO<sub>3</sub> nanoparticles (NPs) enhance the results of H<sub>2</sub>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<sub>2</sub>S gas sensors based on tungsten oxide (WO<sub>3</sub>) nanoparticles embedded in organic polymer membranes are presented in our work. WO<sub>3</sub> NPs were synthesized using the sol-gel method. Polymer solutions consisting of chitosan and ionic liquid (IL) were doped with WO<sub>3</sub> NPs. Then, the doped solutions were casted to obtain flexible membranes (200 mm in thickness). The sensors (CS-IL-WO<sub>3</sub> NPs membranes) is under continues testing to investigate their gas sensing performance and obtain the best working conditions by measuring the electrical current response signals at different operating temperatures.

The result revealed that the best response to H<sub>2</sub>S gas for all sensors was obtained at 80C, yet a reasonable response was noticed at a low operating temperature of 20 C. 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  $20.1 \pm 3.4$  s. Moreover, these sensors exhibited excellent reproducibility and stability, and were identified to be selective to H<sub>2</sub>S. These characteristics, these sensors were identified to be promising materials for hazardous H<sub>2</sub>S gas sensing applications.

## **Selective Adsorption of H<sub>2</sub> Molecule on N-doped ZnO Nano-ribbons: *Ab-initio* Investigation**

**Alaa Shaheen, Wael Othman, Younes Aitladi, Sultan Atatri,  
Yahya Abdelhadi, Golibjon Berdiyrov and Nacir Tit**

Physics Department  
United Arab Emirates University  
Al-Ain, United Arab Emirates  
E-mail: [ntit@uaeu.ac.ae](mailto:ntit@uaeu.ac.ae)

Density functional theory combined with the non-equilibrium Green's function formalism is used to study the adsorption and gas-sensing properties of H<sub>2</sub> 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<sub>2</sub> molecule and other molecules (e.g., N<sub>2</sub>, O<sub>2</sub>, H<sub>2</sub>O, H<sub>2</sub>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<sub>2</sub> and O<sub>2</sub> molecules are chemisorbed on N-doped ZnO-NRs. The chemisorption of O<sub>2</sub> is associated with the breaking of one  $\pi$ -bond and thus the desorption is possible. Whereas, the chemisorption of H<sub>2</sub> 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<sub>2</sub> 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<sub>3</sub>O<sub>4</sub>) Quantum Dots and RGO composites for Cancer Therapy via Hyperthermia**

**Ghyoudh Alarwan, Yara Alkurdi, Kholoud Almashjari, Arshia Fathima, Roa Fardous, Faheem Ahmed, Edreese Alsharaeh and Ali Hasan**

Department of Chemistry  
Alfaisal University

Riyadh, Kingdom of Saudi Arabia

E-mail: Galarwan@alfaisal.edu; yaraalkurdi@alfaisal.edu; kaalmashjari@alfaisal.edu

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**

**Ahmed M. Soliman, Ehab Soltan, Dalal Alshamsi,  
Ahmed A. Murad and Ala Aldahan**

Ahmed Soliman"Department of Chemistry" Dalal Alshamsi, Ahmed A. Murad, Ala Aldahan"Geology Department  
United Arab Emirates University  
Al-Ain, United Arab Emirates  
E-mail: a.soliman@uaeu.ac.ae

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 1M HNO<sub>3</sub>. 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**

**Aya Al Sadik and Yaser E. Greish**

Department of Chemistry  
United Arab Emirates University  
Al Ain, United Arab Emirates  
E-mail: 201350337@uaeu.ac.ae

Gypsum ( $\text{CaSO}_4 \cdot 2\text{H}_2\text{O}$ ) is a known structural material, especially for the finishing and decoration of concrete surfaces. Gypsum is formed through the hydration of Plaster of Paris ( $\text{CaSO}_4 \cdot \frac{1}{2}\text{H}_2\text{O}$ ) 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  $\text{TiO}_2$  nanoparticles ( $< 20$  nm), as a filler, have been fabricated.  $\text{TiO}_2$  NPs are characterized by high surface area and photocatalytic activity. The effect of adding  $\text{TiO}_2$  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  $\text{TiO}_2$  NPs. This was observed via the increased demand of water of hydration and workability with increasing the  $\text{TiO}_2$  NPs content. Despite these findings, no signs for chemical interaction between  $\text{TiO}_2$  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  $\text{TiO}_2$  NPs are being studied.

## **Conjugated Molecule based Sensor Designed for Selective Detection of Lithium Ion in Water**

**Ashwini N. Mallya, Mithrabinda P. and Praveen C. Ramamurthy**

Department of Materials Engineering  
Indian Institute of Science  
Bangalore - 560012, India  
E-mail: ashumallya@gmail.com

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 chemiresistive 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.

## **Development of Piezo-MEMS Process Flow with PZT Thin Films**

**Sudhanshu Tiwari, Ajay Dangi and Rudra Pratap**

Centre for Nano Science and Engineering  
Indian Institute of Science  
Bangalore, India  
E-mail: sudhanshut@iisc.ac.in

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 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  $\mu\text{m}$  device layer thickness with a material stack  $\text{SiO}_2/\text{Ti}/\text{Pt}/\text{PZT}$ . Different growth mechanisms used are, thermal oxidation for  $\text{SiO}_2$ , D.C. magnetron sputtering for  $\text{Ti}/\text{Pt}$  and sol-gel method for PZT. PZT thin films with 650 nm to 1  $\mu\text{m}$  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  $\text{SiO}_2$  and Si etching steps by using a thin ALD deposited  $\text{Al}_2\text{O}_3$  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**

**Naidu Dhanpal Jayram, Vikram S Raghavan and G. Mohan Rao**

Department of Instrumentation and Applied Physics  
Indian Institute of science  
Bangalore, India  
E-mail: dhanpal.dj@gmail.com

Carbon based pollutants are considered as a real threat to environment, which can cause several adverse effects to human beings, specifically due to emission of Soot. It is essential to investigate the structural 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 characterized. Paper based analytical sensors (PASs) are getting large attention in various fields, ranging from pH strips to biosensors. Soot was directly collected from exhaust of diesel engine on three different paper strips (whatman paper, Glassy sheet, Tissue paper) for duration of 10 s and was analyzed without any further modification using Raman spectroscopy. A simple casing was fabricated consisting of plastic strip holder with 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  $\text{cm}^{-1}$  give rise to several bands (G, D1, D2, D3, and D4) at about 1580, 1350, 1500, 1620, and 1200  $\text{cm}^{-1}$  respectively due to Lorentzian fitting curve. However the strong enhancement of Raman signal produced by SERS enabled to find out second harmonic of D and G bands on silver interaction (carbon-metal interface), especially Peak at 2715  $\text{cm}^{-1}$  shows graphitic peak without peak fitting curve. Amplification in the signal using SERS technique reveals information's such quality of diesel engine, presence of phosphorous and sulphur in soot, 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 helps in development of diesel engine filters for optimization of diesel exhaust.

- 1) L. Tian, D. Ghosh, W.Chen, S.Pradhan, X. Chang and S.Chen, Nanosized Carbon Particles From Natural Gas Soot, Chem. Mater., 2803–2809, 21, 2009
- 2) T. Catelani, G. Pratesi and Matteo Zoppi, Raman Characterization of Ambient Airborne Soot and Associated Mineral Phases, Aerosol Science and Technology, 13–21,48, 2014

## Development of Phenylhydrazone based Solvetochromic Receptor for Selective and “Naked Eye” Detection of Fluoride Ion

**H. Nagarajaiah, Amit G. Anil and Praveen C. Ramamurthy**

Department of Materials Engineering  
Indian Institute of Science  
Bangalore, India  
E-mail: nagarajh6@gmail.com

Chemosensors play an important role due to their applications in various fields, such as chemistry, biology, medicine and environmental studies.<sup>1</sup> The most challenging task for the analytical chemists is to recognize some anions due to the complexity of their small charge to radius ratios, geometries and heavy solvation. Generally, recognizing of various anions is based on deprotonation, hydrogen bonding interaction, anion- $\pi$  interaction, chemical reactions etc.<sup>2</sup> Among variety of biologically important anions, fluoride is of particular interest due to its role in dental care and treatment for osteoporosis.<sup>3a</sup> Even though number of receptors has been developed for the recognition of fluoride ions,<sup>3b</sup> 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,  $\text{Cl}^-$ ,  $\text{Br}^-$ ,  $\text{I}^-$ ,  $\text{OAc}^-$ ,  $\text{CN}^-$ ,  $\text{PO}_4^{3-}$ ,  $\text{H}_2\text{PO}_4^-$  in solution of THF/acetonitrile and its solvetochromic behavior has been described. The addition of fluoride, DMF and DMSO are found to promote deprotonation of receptor. The color changes from yellow ( $\lambda_{\text{max}} = 392 \text{ nm}$ ) to dark red ( $\lambda_{\text{max}} = 500 \text{ nm}$ ) was observed upon addition of  $\text{F}^-$  ion in THF/acetonitrile solution of receptor due the formation of deprotonated species. The binding stoichiometry between  $\text{F}^-$  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:

1. (a) Wright A. T.; Anslyn, E. V. *Chem. Soc. Rev.* 2006, 35, 14–28; (b) Yoon, J.; Kim, S. K.; Singh N. J.; Kim, K. S. *Chem. Soc. Rev.* 2006, 35, 355–360; (c) Gunnlaugsson, T.; Glynn, M.; Tocci, G. M.; Kruger P. E.; Pfeffer, F. M. *Coord. Chem. Rev.* 2006, 250, 3094–3117.
2. (a) Suksai, C.; Tuntulani, T. *Chem. Soc. Rev.* 2003, 32, 192–202; (b) Beer P. D.; Gale, P. A. *Angew. Chem., Int. Ed.* 2001, 40, 486–516.
3. (a) Dreisbuch, R. H. *Handbook of Poisoning*; Lange Medical Publishers: Los Altos, CA, 1980; (b) Zhou, Y.; Zang, J. F.; Yoon, J. *Chem. Rev.* 2014, 114, 5511–5571.

## **Simultaneous Detection of Heavy Metal Ions using Modified Carbon Paste Electrode with Reduce Graphene Oxide-SnO<sub>2</sub>-Polyaniline**

**Ramakrishnan Shanmugam, Nandita S. and Praveen C. Ramamurthy**

Department of Materials Engineering  
Indian Institute of Science  
Bangalore, India  
E-mail: rammtech09@gmail.com

The reduced graphene oxide-SnO<sub>2</sub>/PANi (PGS) composite was synthesized and the obtained composite is embedded with carbon paste electrode to detect heavy metals ions lead (Pb<sup>2+</sup>) and cadmium (Cd<sup>2+</sup>). Graphene oxide is synthesized by improved Hummer's method and the reduced graphene oxide-SnO<sub>2</sub> (RGS) is prepared by hydrothermal method. The SnO<sub>2</sub> 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<sub>2</sub> particles decorated over RGO. The XRD analysis showed the prominent peaks of SnO<sub>2</sub>, 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<sub>2</sub> 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<sub>2</sub> using graphite (90%): PGS (10%) and 100 $\mu$ L 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<sup>2+</sup>) and cadmium (Cd<sup>2+</sup>) 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<sup>2+</sup>) and cadmium (Cd<sup>2+</sup>) 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 $\mu$ M - 70 $\mu$ M for lead (R<sup>2</sup>=0.98) and for cadmium (R<sup>2</sup>=0.97) and individual low detection limit of 0.001 $\mu$ M is observed for lead (Pb<sup>2+</sup>) and 0.001 $\mu$ M for cadmium (Cd<sup>2+</sup>).

## **Construction of a Potentiometric Biosensor for the Detection of Glucose using Green Synthesized Silver Nanohybrids and Polypyrrole**

**Santhosh A. S.,<sup>†</sup> Sandeep S.,<sup>†</sup> Kumara Swamy N.,<sup>†</sup> Suresh G. S.,<sup>‡</sup> Melo J, S.<sup>§</sup>**

<sup>†</sup>Department of Chemistry, Sri Jayachamarajendra College of Engineering, Mysuru, India

<sup>‡</sup>Department of Chemistry and Research Centre, NMKRV College for Women, Jayanagar, Bangalore, India

<sup>§</sup>Nuclear Agriculture and Biotechnology Division, Bhabha Atomic Research Centre, Mumbai, India

E-mail: santhu41100@gmail.com

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 0.2-29mM with a detection limit of 55.3  $\mu$ M. 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**

**Sandeep S.,<sup>†</sup> Santhosh A. S.,<sup>†</sup> Kumara Swamy N.,<sup>†</sup>  
Suresh G. S.<sup>‡</sup> and Melo J. S.<sup>‡</sup>**

<sup>†</sup>Department of Chemistry, Sri Jayachamarajendra College of Engineering, Mysuru, India

<sup>‡</sup>Department of Chemistry and Research Centre, NMKRV College for Women, Jayanagar, Bangalore, India

<sup>§</sup>Nuclear Agriculture and Biotechnology Division, Bhabha Atomic Research Centre, Mumbai, India

E-mail: sandeep12chem@gmail.com

The present paper report 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 indicate the 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**

**Abdul Wahid, Abdullah M. Asiri and Mohammed M. Rahman**

bCenter of Excellence for Advanced Material Research (CEAMR)  
King Abdulaziz University  
Jeddah, Kingdom of Saudi Arabia  
E-mail: abdul\_wahid24@yahoo.com

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  $28.48101 \text{ nA} \cdot \text{m}^{-2}$  and 0.33 pM respectively. Finally, the chemical sensor was friendly for the detection of toxic and hazardous environmental pollutants and can be used effectively on main scale for protecting green environment.

## **3D Spongy Graphene-Modified Screen-Printed Sensors for the Voltammetric Determination of the Narcotic Drug Codeine**

**Dalia M. El-Gendy, Mona A. Mohamed,  
Nashaat Ahmed, Craig E. Banks and Nageh K. Allam**

Department of Chemistry  
National Research Centre, Dokki, Giza, Egypt  
The American University in Cairo, New Cairo 11835, Egypt  
E-mail: [dalia\\_elgendy2015@aucegypt.edu](mailto:dalia_elgendy2015@aucegypt.edu)

Adenine-functionalized spongy graphene (FSG) composite, fabricated via a facile and green synthetic method, has been explored as a potential electrocatalyst toward the electroanalytical sensing of codeine phosphate (COD). The synthesized composite is characterized using Fourier transform infrared spectroscopy (FTIR), Raman spectroscopy, X-ray powder diffraction, UV-vis absorption spectroscopy, scanning electron microscopy, high resolution transmission electron microscopy (HRTEM), and thermogravimetric analysis. The FSG was electrically wired via modification upon screen-printed (macro electrode) sensors, which behave as a hybrid electrode material for the sensitive and selective codeine phosphate (COD) determination in the presence of paracetamol (PAR) and caffeine (CAF). The FSG- modified sensor showed an excellent electrocatalytic response towards the sensing of COD with a wide linear response range of  $2.0 \times 10^{-8}$ - $2.0 \times 10^{-4}$ M and a detection limit (LOD) of  $5.8 \times 10^{-9}$ M, indicating its potential for the sensing of COD in clinical samples and pharmaceutical formulations.

## **Embroidered Conductive Threads on E-Textiles for Wearable Smart Applications**

**Eman M. Swielam, Samiea M. Eltopshy, Sania K Sobhy,  
Z. M. Abdel-Megied and Ahmad Labeeb**

Department of Textile industry  
National Research Center  
Cairo, Egypt  
E-mail: emanswielam@gmail.com

The research was conducted to apply the embroidering technique of fabricating electro-textiles. This technique has its own advantages which make embroidery more functional and play roles 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 done by using the computerized embroidery machine. Fabrication specifications and embroidery parameters such as different, 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 1st and 2nd 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)  $0.83 \Omega$ , while the highest value was  $10.66 \Omega$  in the 3rd 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 application in, military, medical applications: continuous and long-term monitoring of patients in a hospital environment.

## Near Surface Nitrogen Delta Doping in Diamond

**Maneesh Chandran**

Departments of Physics & Nanotehnology  
SRM University, Kattankulathur  
Chennai, India  
E-mail: maneeshcn@gmail.com

The negatively charged nitrogen vacancy centers ( $NV^-$ ) is one of the most significant color centers in diamond due to their spin dependent fluorescence and exceptionally long coherence times. One of the key challenges for  $NV^-$  based magnetometry application is to create an ensemble of  $NV^-$  centers in the near surface region. Recently, we reported an innovative delta doping technique to fabricate an ensemble of  $NV^-$  centers at shallow depths in (100) diamond [1]. This method produces a nitrogen delta doped layer with a concentration of  $\sim 1.8 \times 10^{20}$  atoms $\cdot$ cm $^{-3}$  with abrupt interfaces. To the best of our knowledge, this is the thinnest nitrogen delta doping profile with abrupt interfaces in single a crystal diamond reported to date. Herein, we report an in-depth secondary ion mass spectroscopy (SIMS) analysis of nitrogen delta doped layer in diamond. The SIMS profile of the delta layer exhibits a positive concentration gradient of 1.9 nm/decade and a negative gradient of 4.2 nm/decade with a full width at half maximum (FWHM) of 7.5 nm. The broadening of the nitrogen profile (FWHM=7.5 nm) is partly attributed to the diffusion of nitrogen as well as to the depth resolution of SIMS measurements (ion mixing and surface roughness effects). Nitrogen delta doping in polycrystalline diamond revealed the diffusion of nitrogen through grain boundaries as well as the influence of surface roughness on the broadening of SIMS profile. An in-depth SIMS analysis of the nitrogen delta doped layer in diamond will be presented.

[1] M. Chandran et. al., Appl. Phys. Lett. 109, 221602 (2016).

## **Graphene Membrane for Desalination of Seawater**

**Dezairi Aouatif, Rochd Sanaa, Mizani Sofia,**  
**Moultif Rachida and Lahlou Souad**

Department of Physics  
Hassan II University  
Casablanca, Morocco  
E-mail: dezairi.a@hotmail.com

Access to drinking water and resource management are major challenges of the coming decades. In a social and industrial purpose, it seems therefore vital for some people, particularly, in remote site to develop new facilities for drinking water production.

Reverse osmosis is 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.

## **Molecular Dynamics Simulation of Aluminosilicate Glasses**

**Mohamed Zekri, Andreas Erlebach and Ramzi Maalej**

Department of Physics  
Sfax University  
Sfax, Tunisia  
E-mail: zekrimohamed1991@gmail.com

The molecular dynamics (MD) computer simulation technique has been used to study the structure of Barium (Ba) and Magnesium (Mg) aluminosilicate glasses (AS). The structural features of the simulated glasses are analyzed using Radial Distribution Function (RDF) and Pair Distribution Functions (PDF). With changing Ba to Mg, the environments of Mg or Ba ions alter from binding to non-bridging oxygen to bonding to the bridging oxygen associated with tetrahedral Al.

## **Defect Chemistry and Oxygen Vacancy Migration in Gd-doped CeO<sub>2</sub>: Hybrid Functional Study**

**Xiaoping Han, Nouredine Amrane and Maamar Benkraouda**

Department of Physics  
United Arab Emirates University  
Al Ain, United Arab Emirates  
E-mail: x.han@uaeu.ac.ae

Oxygen vacancy formation and migration in rare-earth-doped CeO<sub>2</sub> has attracted considerable attention due to its wide application as a highly promising material for solving the environmental and energy issues. At the present work, the formation and migration of oxygen vacancy in Gd-doped CeO<sub>2</sub>, 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<sub>2</sub>, 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<sub>2</sub>, which can be compensated by the donor states brought by oxygen vacancy. The detailed analyses show that in Gd-doped CeO<sub>2</sub> 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<sub>2</sub> 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<sub>2</sub>-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 $\text{Sr}_3\text{SnO}$ for Spintronics, Optical and Electronic Properties**

**Rasha W. Adnan Moh'd, Juwayni Lucman, Faris Mahmoud Safieh,  
Noureddine Amrane and Maamar Benkraouda**

Department of Physics  
United Arab Emirates University  
Al-Ain, United Arab Emirates  
E-mail: namrane@uaeu.ac.ae

A theoretical study of the electronic and optical properties of dilute magnetic semiconductor  $\text{Sr}_3\text{SnO}$  is presented, using the full potential linearized augmented plane wave method.

In this approach,  $\text{Sr}_3\text{SnO}$  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**

**N. K. Lokanath and M. K. Hema**

Department of Physics  
University of Mysore  
Mysuru, India  
E-mail: hemamk38@gmail.com

The variation of synthesis conditions makes possible to create metal nanoparticles with different morphologies: spheres, ellipsoids, nanorods, nanotriangles, nanoplates, prisms, cubes, nanoparticles with shells. In the present investigation, thermal decomposition approach is used to prepare CoO nanocrystals (CoONcs) with different morphologies using benzoylacetate cobalt complex as precursor. Crystals of benzoylacetate cobalt complex coordination environment exhibits 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. Experiment was performed at different temperatures to obtain different morphology of CoONcs. SEM results revealed that the morphology of synthesized CoONcs at 1000°C forms nano-flower shape, 900°C as nano-hybrids, 800 °C as nano-chain, and 700°C as nano-cube structures. The shape of a nanocrystal enables to 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**

**Marianne C. Tarun and Matthew D. McCluskey**

Department of Physics and Astronomy  
Washington State University  
Pullman, Washington, United States of America  
E-mail: mtarun@hct.ac.ae

Strontium titanate ( $\text{SrTiO}_3$ ) 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  $\text{SrTiO}_3$  samples were annealed at  $1200^\circ\text{C}$  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.