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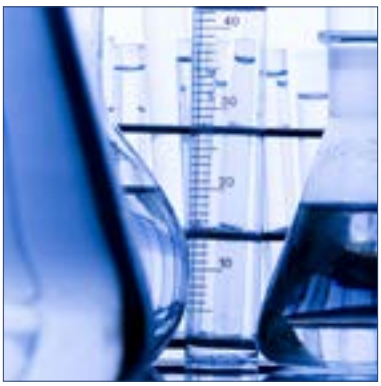
e-Poster

# ChEMEN 2018



Annual Spring Conference and Expo on

# Chemical Engineering: From Materials Engineering to Nanotechnology

April 04-05, 2018 | Miami, USA

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## Electron transport behavior in ZnO-based TCO films embedded with Ag nanoparticles

**Po-Shun Huang** and **Jung-Kun Lee**
University of Pittsburgh, USA

In regime of highly-doped TCOs, their carrier (electron) concentration strongly depends on the shallow donor states created by the amount of extrinsic doping impurities. However, those impurities create equal amount of positively-charged point defects in the TCO lattice that tend to scatter electrons, resulting in the degradation of carrier mobility. Thus, this conundrum between carrier concentration and carrier mobility limits the development of highly-doped transparent conducting oxides (TCOs) films. In this study, we fabricated Ag nanoparticles (NPs) via a surfactant-free solution method, and pre-mix with Al-doped ZnO sol-gel (the Al-doping is approx. 0.1 at. %). We report that electrons can be donated from Ag nanoparticles (NPs) into this ZnO-based TCO matrix without deteriorating the carrier mobility significantly. An increasing Ag content (0.7 vol. %) results in rising electron concentration up to 4×1020 $cm^{-3}$ while the mobility remains 10 to 20 $cm^2$/V.s, which is rarely seen in traditional TCO films prepared by solution methods that contain such high carrier concentration according to several electrical properties of TCO films reported historically. Furthermore, the Hall-effect measurements with function of temperature suggests us that the energetic barrier for this electron donation from Ag NPs at room temperature is synonymous with the Schottky barrier at the metal-oxide interface. Those evidence suggest us that electrons donated from Ag NPs can overcome this energetic barrier at the metal-oxide interface and further transport in the polycrystalline ZnO-based TCO matrix with relatively less positively-charged defects. Therefore, the carrier mobility remains as the same as that of oxide matrix and are eventually collected by our conductivity measurement tool. It is noted that the optical transmittance of such composite films in the visible wavelengths is above 85 % as the electrical resistivity is slightly less than $10^{-3}$ Ω.cm.

### Speaker Biography

Dr. Po-Shun Huang studied metal oxide thin film depositions and low-dimensional nanomaterials via wet chemistry method during his PhD work with Prof. Jung-kun Lee in the Department of Mechanical Engineering and Materials Science at the University of Pittsburgh. Dr. Huang had in-depth knowledge and hangs-on experience in multi-functional oxides, nano-composites for the application of optoelectronics, and has develop several thin-film characterization skills. After PhD study, He worked as a R&D engineer in a startup company affiliated with Lawrence Berkeley National Laboratory at Berkeley, CA, mainly focusing on the polymeric conformal coating via CVD method on the AFM cantilevers for the application of liquid AFM. His interest includes low-dimensional nanomaterials for energy-harvesting devices, photovoltaic materials, and solution-based methods for electrically active thin-films.

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*Notes:*

# Accepted Abstracts

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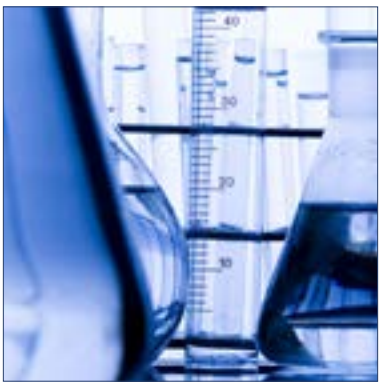

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## Synthesis and characterization of emulsion polymerized polyaniline doped with DBSA

**Alok Gupta**
Malaviya National Institute of Technology, India

In this paper polyaniline (PANI) has been made through polymerization of aniline using emulsion polymerization technique. The polymerization is carried out in an emulsion comprising water and a non-polar or weakly polar organic solvent (Xylene) in the presence of the functionalized protonic acid dodecyl benzene sulphonic acid (DBSA). It is found that using the emulsion polymerization technique, conducting PANI-DBSA complexes can be produced that exhibit high molecular weight, good conductivity and high solubility in organic solvents in the electrically conducting state. Electrically conducting polyaniline PANI-DBSA prepared by an inverted emulsion polymerization in which DBSA played both roles of surfactant and dopant. Fourier transform infrared FTIR. spectroscopy for the PANI-DBSA showed the existence of hydrogen bonding between PANI and DBSA which indicates the existence of PANI. UVV is spectra was performed to check the doping level of DBSA. The electrical conductivity measurement, TGA test and measurement of viscosity was also studied in the paper.

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## Low power dual ion beam sputtered high endurance resistive switch with memristive behavior

**Amitesh Kumar, Mangal Das, Brajendra S Sengar, Md Arif Khan, Abhinav Kranti** and **Shaibal Mukherjee**
Indian Institute of Technology Indore, India

The memory effects in a memristor can be realized through the switching behavior between two distinct resistance states, low resistance state (LRS) and high resistance state (HRS) driven by low pulse voltages. ZnO-based thin films such as undoped ZnO, Mg-doped ZnO, Na-doped ZnO and Mn-doped ZnO have attracted considerable interest as promising resistive switching materials. Gallium doping electrically modulates the behavior of ZnO to suit low power switching behavior. Non-lattice oxygen ions and oxygen vacancies as detected by XPS are found to play important role in imparting forming-free resistive switching behavior.

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## The application of the new LBET method to the comprehensive analysis of the microporous structure of carbonaceous and mineral adsorbents

**Mirosław Kwiatkowski, Katarzyna Zarebska** and **Paweł Baran**
AGH University of Science and Technology, Poland

The LBET method entails a wider spectrum of information on the analyzed structure of the micropores and the processes occurring on the surface of the adsorbent what provides a unique tool enabling a precise characterization of the structure of the porous materials. The LBET method might be used not only as a competitive tool in comparison with the DR and BET methods, porosimetric measurements and others, but also as a valuable complement to these, making it possible to obtain an almost full spectrum of useful information on the structure of the analyzed materials. Such precise information enables an optimal selection of methods and conditions of the production process of carbonaceous and mineral adsorbents.

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## Synthesis and characterization of $SnO_2$ nanofiller from recycled expanded polystyrene

**Olusola Olaitan Ayeleru[1], Freeman Ntuli[1], Williams Kehinde Kupolati[2]** and **Peter Apata Olubambi[1]**
[1] University of Johannesburg, South Africa
[2] Tshwane University of Technology, South Africa

An efficient way to derive values from waste polymers is through the development of blends and nanocomposites from the wastes. This will help to enhance the mechanical properties of the recycled polymers that are often lost when other methods of recycling are employed. The aim of this study is to prepare and characterize $SnO_2$ nanofiller from recycled expanded polystyrene wastes (rEPS). The rEPS was obtained from the University of Johannesburg recycling facility. The rEPS was dispersed in benzene and was sonicated for about 20 minutes. Afterwards, $SnCl_4.2H_2O$ was added to the mixture and sonicated for another 20 minutes. It was then subjected to heat at a temperature of 250 °C for 3 hours. The resulting product was characterized using SEM, EDX, FTIR, TEM, XRD and BET. Based on the results obtained, spherical-shaped particles between 5 µm and 50 µm were obtained from the SEM analysis, the EDX showed that tin, chlorine and oxygen were all present in the synthesised nanofiller while only carbon and oxygen were present in the control experiment. The FTIR analysis showed the wider band at around 3400 $cm^{-1}$ and the peak at 1630 $cm^{-1}$. The TEM showed a particle size between 7 and 12 nm and the XRD indicated that the material is crystalline with tetragonal shape and the BET showed isotherm with a microporous adsorbent. This work demonstrated an efficient method to upcycle waste polymer in an economical way while the properties of the polymers would still be retained.

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## Fabrication of $ZrO_2$ nanofiller from polystyrene polymer waste as reinforcement

**Olusola Olaitan Ayeleru[1], Freeman Ntuli[1], Williams Kehinde Kupolati[2]** and **Peter Apata Olubambi[1]**
[1] University of Johannesburg, South Africa
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Rapid generation of non-biodegradable polymer wastes (NBPW) has posed serious environmental and economic challenges which are now issues of global concern. This study explored the application of nanofiller material from polystyrene polymer waste (PPW) through upcycling recycling process method of the waste material and its incorporation as reinforcement materials in road construction. The PPW sample from a recycling facility in Johannesburg was thermally treated to upcycle the wastes. The PPW sample was dispersed in an organic solvent, $Zr(NO_3)_4$ and was heated. A corresponding control experiment was carried out in the absence of $Zr(NO_3)_4$. Afterwards, $ZrO_2$ nanofiller was obtained from the resulting product of the first experiment and another product was obtained from the control experiment and both were characterized by SEM, EDX, TEM, FTIR, BET, XRD and TGA. This work demonstrated an alternative route of upcycling NBPW in a cost-effective and environmentally friendly ways.

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## Properties of P (HB-HV) / nanodiamonds as material for orthopedic use

**Rubén Jesus Sánchez Rodríguez, Gabriel Rodrigues de Almeida Neto, Fabrício Moreira Almeida, José Gregório Cabrera Gomez** and **Mariana Valinhos Barcelos**
North State Fluminense University, Brazil

This current study aims to develop a biocomposite to be used as an orthopedic device, using poly(3-hydroxybutyrate-co-3-hydroxyvalerate) P(HB-HV), a biodegradable copolymer, with 94%HB and 6%HV, as matrix; and nanodiamonds (ND) with primary grains of 4-6nm, as reinforcement. The nanodiamonds were previously encapsulated by P(HB-HV) and specimens were prepared using an injection molding machine. The biocomposite P(HB-HV) probes were analyzed by XRD, TGA, flexural testing and compresion DMA tests. The distribution of nanodiamonds on the specimen fracture surface were investigated by SEM. The SEM micrographs allowed us to concluded that the encapsulation of nanodiamonds by P(HB-HV) was successfully performed, promoting a better interface and distribution in the polymeric matrix. The presence of ND in the polymeric matrix decreased the P(HB-HV) crystallinity, inhibiting the crystallite growth. The mechanical properties obtained from flexural test and DMA of the injection-molded specimens were promise to material for bone filling Evaluated by in vitro testing, all formulations were non-cytotoxic.

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## Modeling and simulation in Materials Science

**Chinta Sanjay**
GITAM University, India

Important advances in multi-scale computer simulation techniques for computational materials science have been made in the last decade as scientists and engineers strive to imbue continuum-based models with more-realistic details at quantum and atomistic scales Materials modelling and simulation aims to develop fundamental relationships between the atomic structure and properties of molecules and materials. Simulation modelling has been used in a wide range of physical and social sciences and engineering fields, ranging from nuclear fusion to economic forecast to space shuttle design. For different types of situations and systems, different types of models are used. In classifying simulations, there are important distinctions among the types of models that are being simulated, and among the types of program structures that are used to carry out the simulation. Computer modelling and simulation are known to aid design of new materials, processes and products. A model is a conceptual description of an entity or a phenomenon, quantified using the relevant laws of science with allowable approximations and simplifications. The four important sequential steps involved in any modelling are conceptualization, simplification, representation and finally quantification. Essentially, a model provides the basis for simulation to create an image of a real system or a phenomenon. Modern computers have made simulation attractive to the extent that 'virtual reality' has become possible. Sound numerical simulations are almost equivalent to performing real experiments and therefore referred to as 'numerical experiments'. A real experiment is a direct dialogue with the system of interest and therefore expected to be naturally reliable.

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# Special type of nano gel electrolytes for deep drawing AGM, AGM-VRLA batteries for getting more cycle life compatible with all type of electrical motive power applications

**D Gibson** and **D Shivson**
Neuron Material Science, India

Neuron developed special type of Nano gelling agent based on poly alkyl/aryl silicone oxides and phosphates compounds. By the addition of 4.5 to 25% of Sulphuric acid concentrations, electrolyte will become immobilised, good ionic movements, high conductivity/ very low inter cell impedance(IR characteristics very low ) values, no shedding of active material from the grid plates, no fuming, safe to use end users, easy recombination of $H_2$ and $O_2$ at nascent stage, fast charging up to C5 rate can charge for E-motive power applications. After filling of electrolyte with Neuron-1879 R-SiOX/POR Nano Gel Additives, battery may undergone by regular process manufacturing techniques, after 24 hrs battery start use for regular charge and discharge applications, (R=Alkyl/Aryl substituted).

The above method will enhance the performance of the battery life 60% more cycle power compare with all other battery technology. The above Neuron Nano electrolyte ideally suits all type of AGM or AGM-VRLA, FLA, SMF, Short and tall tubular batteries.

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# Preparation of nanosized particles for Group IB and Group VIII transition metals by chemical reduction in solution

**Walid Daoush**
Al Imam Muhammad Ibn Saud Islamic University, Saudi Arabia

In the presence work, chemical reduction by electroless deposition technique as a method belonged to the bottom up approach of synthesis for a nanosized particles is used for producing a uniform shape and size metallic nanoparticles. A number of metals can be reduced to the metallic state from solutions of their salts by chemical means. These are of group IB such as, silver and copper and of group VIII such as iron, nickel, cobalt, Platinum and palladium. in the elemental form bimetallic form or in the alloyed form. Metals and alloys as submicron size and nanoized particles structures including Pt, Pd, Ag, Cu and Ni as well as Pt-Ni, Fe-Ni, Ni-Co and Fe-Co bimetals or alloys were prepared. by chemical reduction in aqueous solutions. Although the techniques have been used to produce precious metal powders, the ease of chemical reduction from solution and the variety of powders that can be prepared make this aqueous processing technique the preferred approach to build up homogeneous nanoparticles. Chemical precipitation of metal from a solution of soluble salt is used, such as silver and copper particles of which is produced by adding a reducing agent such as formaldehyde to a solution of silver or copper ions. Although many reducing agents are available, those most commonly used to reduce the ions for the metals of group IB and VIII are hypophosphite, borohydride, hydrazine, polyols and aldehydes. Different types of complexing agents were used as a chelating agent for the metals in the bath to prevent hydroxide precipitations as citrates, oxalates, acetates and tartrates. The results reveled that, it is possible to produce nanoparticles consisting of one or more metal with different morphology by appropriate adjustment of the chemistry of the reduction solution. Synthesis of nanosized bimetallics or alloy are also taking place. Studies of the deposition of nickel with other metals such as Pt, Co or Fe were showed that the produced particles are highly homogeneous. The particle size and morphology investigations were performed by SEM, TEM and EDAX analysis. XRD was performed for the investigated particles to identify the chemical composition of the produced particles. The magnetic properties of the obtained particles were investigated by the vibrating sample magnetometer method.

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## Ultrasensitive cell detection based on new supramolecular probes and multifunctional nanocomposites

**Xuemei Wang**
Southeast University, China

The early efficient diagnosis and therapy of some important disease like cancers is still a hot topic in the relative areas involving in patient care and treatments. In this study, we have explored the possibility of the application of new supramolecular probes combining with nano-scaled materials in relevant biomolecular recognition and high-sensitive detection of disease like cancers. Especially, we have developed a new strategy for the fast and high sensitive recognition of the target biomolecules and cancer cells by combining the supramolecular probe and functionalized nano-interface with the spectro-electrochemical study. Our observations demonstrate that the self-assembly of the specific nanocomposites with the new molecular probes could provide a multifunctional interface for the rapid and high selective identification of cancer cells, with a broad detection range and low detection limit. It is evident that different types of cancer cells or bacteria could be readily distinguished on the relevant nanocomposites modified nano-interface, which have the promising application to be adopted as a significant way to detect and identify various kinds of mutant cells and advance the clinic diagnosis and monitoring the treatment of target disease like cancers. Moreover, some ultrasensitive and intelligently multi-functional nanoprobes based on the *in vivo* bio-synthesized nanoclusters for multimodality imaging of cancer cells / exosomes or target tissues have been also explored for the real-time monitoring and dynamic analysis of some disease related biomolecules/cells/tissues.

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