Abstract book for the proceedings of the 3rd International conference on structural nano composites (NANOSTRUC 2016), 12-15 September 2016, Aberdeen, UK.

STAROST, K., NJUGUNA, J. (eds.)

2016

NANOSTRUC 2016

International Conference on Structural Nano Composites
12-15 Sept 2016 in Aberdeen, United Kingdom

Abstract Book

ROBERT GORDON UNIVERSITY • ABERDEEN

Editors: Kristof Starost & James Njuguna
Contact: k.starost@rgu.ac.uk, j.njuguna@rgu.ac.uk
Robert Gordon University, Aberdeen AB10 7AQ, UK

Preface

Dear Colleagues,

Welcome you to Aberdeen. It is our great pleasure to welcome you to NANOSTRUC 2016 at Robert Gordon University and many thanks for your contributions to this Conference. The theme of NANOSTRUC 2016 conference is on 'Nanoscience and Nanotechnologies – Recent Advances towards Nanoproducts and Applications'. The conference is aimed to promote activities in various areas on materials and structures by providing a forum for exchange of ideas, presentation of technical achievements and discussion of future directions. The key sessions are on Application of Nanomaterials and Nanocomposites, Functional Nanocomposites, Graphene and Carbon-based Nanocomposites, Metallic and Metals Oxide Nanocomposites, Sustainability - Nanosafety & Environment, Toughness of Polymer Nanocomposites, Biocomposites and Nanofibres and on Fibre Reinforced Composites. The conference benefits from key note lectures focused on topical issues in nanosciences and nanotechnology.

We would like to acknowledge the hard work, professional skills and efficiency of the Organising Committee and Steering Committee which ensured the successful organisation. It is more so to the conference contributors authors, sponsors and supporters.

Welcome to the NANOSTRUC 2016 and wish you a stimulating Conference and a fruitful time here at Robert Gordon University, Aberdeen.

Yours sincerely,

James Njuguna, Conference Chair

Scientific Committee

Jinbo Bai – *CNRS Ecole Centrale Paris, France*

Kanda Balasubramanian – *Defense Institute of Advanced Technology, India*

Maria Blazquez – *Inkoa, Spain*

Aravid Dasari – *Nanyang Technological University, Singapore*

Raj Das – *University of Auckland, New Zealand*

Andrzej Gałęski – *Polish Academy of Sciences, Poland*

Youssef Habibi - *Luxembourg Institute of Science and Technology, Luxembourg*

Susheel Kalia – *University of Bologna, Italy*

Dirk Lehmhus – *University of Bremen, Germany*

Conor McCarthy – *University of Limerick, Ireland*

Ajay Mishra – *University of South Africa, South Africa*

Satyendra Mishra – *North Maharashtra University, India*

James Njuguna – *Robert Gordon University, UK*

Maria Peeler – *Washington State Department of Ecology, USA*

Sergio Pezzin – *State University of Santa Catarina, Brazil*

Krzysztof Pielichowski – *Cracow University of Technology, Poland*

Davide Roncato – *Centro Ricerche FIAT (CRF), Italy*

Vijay Srivastava – *Indian Institute of Technology, Varanasi, India*

Sabu Thomas - *Mahatma Gandhi University, India*

Raquel Verdejo – *Consejo Superior de Investigaciones Científicas (CSIC), Spain*

Paul Wambua – *Dedan Kimathi University, Kenya*

Marcel Weil – *Karlsruhe Institute of Technology, Germany*

Jianqiao Ye – *Lancaster University, UK*

Session Chairs

Application of Nanomaterials and Nanocomposites - 1 - *Krzysztof Pielichowski - Cracow University of Technology, Poland*

Functional Nanocomposites 1 – *Sekhar Chandra Ray - University of South Africa, South Africa*

Sustainability – Nanosafety & Environment - 1 – *Ketan Pancholi - Robert Gordon Univ., United Kingdom*

Graphene and Carbon-based Nanocomposites - 1 - *Sabelo Mhlanga - University of South Africa, South Africa*

Toughness Polymer Nanocomposites *-Krzysztof Pielichowski - Cracow University of Technology, Poland*

Functional Nanocomposites - 2- *Christine Edward (Robert Gordon Univ., United Kingdom)*

Application of Nanomaterials and Nanocomposites - 2 - Kalia Susheel *(Indian Military Academy, India)*

Graphene and Carbon-based Nanocomposites -2 – *Evelien Frijns (VITO nv, Belgium)*

Biocomposites and Nanofibres - *Youssef Habibi (Luxembourg Institute of Science and Technology, Luxembourg)*

Metallic and Metals Oxide Nanocomposites -2 - *Radhakrishna Prabhu (Robert Gordon Univ., United Kingdom)*

Fibre Reinforced Composites - *Ketan Pancholi (Robert Gordon Univ., United Kingdom)*

Poster session - Sponsored by

Organising committee

James Njuguna – *Robert Gordon University, UK*

Ajay Mishra – *University of South Africa, South Africa*

Youssef Habibi - *Luxembourg Institute of Science and Technology, Luxembourg*

Nadimul Faisal – *Robert Gordon University, UK*

Urenna Ekeh – *Robert Gordon University, UK*

Kristof Starost – *Robert Gordon University, UK*

Monday 12th September 2016

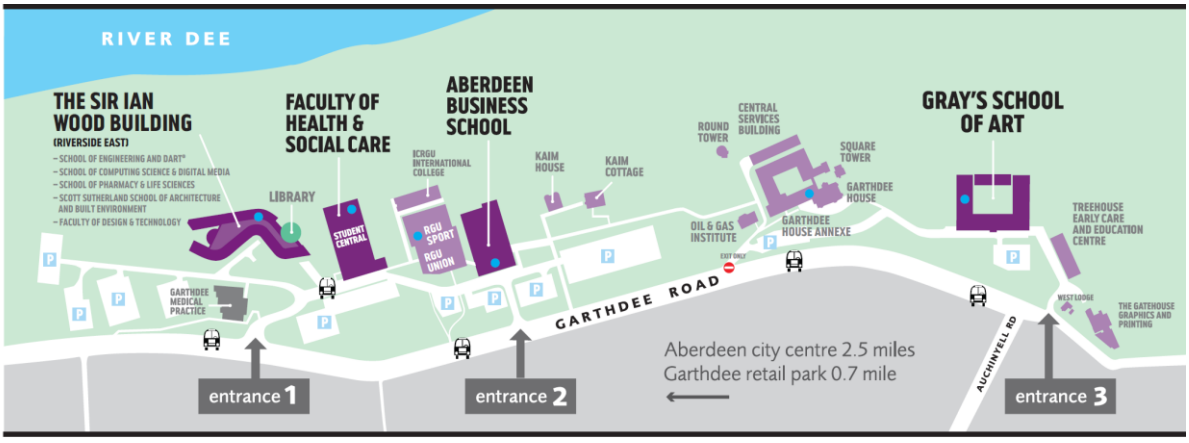
Registration & Reception

Time **Venue: The Sir Ian Wood Building, Atrium, Room N240, Garthdee Campus**

16:00-18:30 **Pre-Registration + Drinks and Canapés Reception**

POSTER SESSION

supported by



Tuesday 13th September 2016

08:00 – 09:00	**Registration (Atrium, Room N240)**
9:00-09:20	**Welcome (Room N242)**
	Session 1.1: Application of Nanomaterials and Nanocomposites -1 (Room N242) Chair-Krzysztof Pielichowski (Cracow University of Technology, Poland)
09:15-09:55	**Nanotechnology in Water Applications** Ajay Mishra (*University of South Africa, South Africa*)
09:55 -10:30	**Temperature Controlled Theranostics for Cancer Therapy** Clare Hoskins *(Keele University, United Kingdom)*

10:30-11:00	**Coffee/Tea Break (Atrium, Room N240)**	
	Session 1.2: Functional Nanocomposites -1 (Room N345) Chair - Sekhar Chandra Ray *(University of South Africa, South Africa)*	**Session 2.1: Sustainability - Nanosafety & Environment (Room N344)** Chair – Ketan Pancholi *(Robert Gordon Univ., United Kingdom)*
11:00-11:30	**Technological Advancements in Nanofiller Reinforced Self-Healing Polymer Composites for Automotive and Aerospace Applications** Pankaj Kumar, (Technical Polymers Material, New Delhi, India)	**Sustainable Bioplastics from Microbes and Waste** Christine Edwards and Linda Lawton (*Robert Gordon University, United Kingdom)*
11:30-11:50	Cyclodextrins as versatile tools for the synthesis of RuO_2/TiO_2 composites with controlled pore structure and enhanced catalytic performance Rudina Bleta, Sébastien Noel, Ahmed Addad, Anne Ponchel and Eric Monflier *(University of Artois, France)*	Thermoplastic Starch/PVA Films Reinforced with Cellulose Nanofibers from Oil Palm Empty Fruit Bunches (OPEFBs) Farah Fahma and Sugiarto Sugiarto *(Bogor Agricultural University, Indonesia)*
11:50-12:10	Flexural strength and elastic modulus recovery in self-healing concrete repaired by inorganic solutions Ana Dolores Carrillo González, *(Politecnico di Torino, Italy Universidad Central de Venezuela, Venezuela)*	Thermoplastic Starch/PVA Films Reinforced with Cellulose Nanofibers from Oil Palm Empty Fruit Bunches (OPEFBs) Farah Fahma and Sugiarto Sugiarto *(Bogor Agricultural University, Indonesia)*
12:10-12:30	Investigations on mechanism of self-healing and cavity filling in case of steel inoculated with sea shell powder Parvaiz Habibullah *(Interdisciplinary Res. in Met. & Mat. for Adv. Appl., Pakistan)*	The effect of talc, organically modified montmorillonite (OMMT) and wollastonite (WO) on nanoparticle release due to mechanical drilling from polypropylene (PP) nanocomposites Kristof Starost, Evelien Frijns, Jo Van Laer, Nadimul Faisal, Ainhoa Egizabal, Cristina Elizextea, Inge Nelissen, Maria Blazquez and James Njuguna *(Robert Gordon Univ., United Kingdom; VITO nv, Belgium; Tecnalia, Spain; INKOA SISTEMAS, Spain)*
12:30-12:50	Thermo-mechanical and structural properties of Ag-Cu and ZnO reinforced polylactide nanocomposite films Yasir Arfat and Jasim Ahmed *(Kuwait Institute for Scientific Research (KISR), Kuwait)*	Waste to Want: Polymer nanocomposites using nanoclays extracted from Oil based drilling mud waste Urenna V. Adegbotolu, Kyari Yates, Kerr Matthews, Krzysztof Pielichowski, Agnieszka Leszczynska, Thomsz Majak, James Njuguna *(Robert Gordon University, United Kingdom; Cracow University of Technology, Poland)*
12:50-14:00	**Lunch (Atrium, Room N240)**	
	Session 1.3: Graphene and Carbon-based Nanocomposites -1 **(Room N345)** Chair - Sabelo Mhlanga *(University of South Africa, South Africa)*	**Session 2.2: Toughness Polymer Nanocomposites (Room N344)** Chair-Krzysztof Pielichowski *(Cracow University of Technology, Poland)*

14:00-14:20	Release of carbon nanotubes from a polyamide nano-composite during milling Evelien Frijns *(VITO nv, Belgium)*	Designing of Hybrid Structured Glass Laminated Transparent Nano Composites through Vacuum infusion Technique Arindam Mukherji *(SP Advanced Engineering Materials Ltd, India)*
14:20-14:40	Nitrogen functionalized bi-layer graphene for spintronic application Sekhar Chandra Ray *(University of South Africa, South Africa)*	On the mechanical influence of Boehmite nanoparticles on reinforced epoxies Media Ghasem Zadeh Khorasani, Dorothee Silbernagl and Heinz Sturm *(Bundesanstalt für Materialforschung und -prüfung, Germany)*
14:40-15:00	Surface modification of carbon nanofibers, graphene platelets and mixtures of both by plasma polymerization of propylene (C.A. Covarrubias-Gordillo, F. Soriano-Corral, C.A. Ávila-Orta, P. A. De León-Martínez, V. Cruz-Delgado (*Centro de Investigación en Química Aplicada, Mexico)*	Feasibility of plasma treated clay in clay/polymer nanocomposites powders for use Laser Sintering (LS) Alaa Almansoori, Cornelia Rodenburg, Candice Majewski and Ryan Seabright *(University of Sheffield, United Kindgom)*
15:00-15:20	Silk fibroin/gold nanoparticles: a new example of biopolymer-based nanocomposites Sylvie Noinville, Adrien Garnier and Alexa Courty *(Université Pierre et Marie Curie, France)*	Development of graphene-filled polymer nanocomposites for enhanced thermal conductivity Syed Sohail Akhtar, Annas Bin Ali, Mohammad Usama Siddique, Abulfazal M. Arif and Amir Al Ahmad (*King Fahd University of Petroleum and Minerals, Dhahran, Saudi Arabia)*
15:20-16:00	**Coffee/Tea Break (Atrium, Room N240)**	
	Sesssion 1.4: Functional Nanocomposites -1 (Room N345) Chair – Christine Edward ***(****Robert Gordon Univ., United Kingdom)*	**Session 2.3: Application of Nanomaterials and Nanocomposites -2 (Room N344)** Chair - Kalia Susheel *(Indian Military Academy, India)*
16:00-16:30	**Structural and nonlinear optical property of $BaSnO_3$ nanopowder prepared by solid state ceramic method** Jibi John, V.P.Mahadevan Pillai, Anitta Rose Thomas, Reji Philip and Radhakrishna Prabhu *(University of Kerala, India; Raman Research Institute, India; Robert Gordon University, United Kingdom****)***	**Nanotechnology Needs in Oil and Gas Industry Applications** Babs Oyeneyin *(Robert Gordon Univ., United Kingdom)*
16:30-16:50	Hybrid sol-gel/polyaniline coatings reinforced with nano-ZnO particles for corrosion protection of Mg alloys Aurelie Dupuis, Emmanuel Aragon and François-Xavier Perrin *(Université de Toulon, France)*	Dynamically mechanical and nano-impact (fatigue) analysis of touch screen thin films deposited on polyethylene terephthalate substrate Nadimul Faisal, Saurav Goel, Caoimhe Kelly and Richard Fu *(Robert Gordon University, United Kingdom; Queen's University, Belfast, United Kingdom; University of Northumbria, United Kingdom)*
16:50-17:10	Ferroelectricity and electromechanical coupling behavior at twist boundaries in PbTiO3	Influence of carbon nanotubes dispersion in the processing and performance properties of Pre-Impregnated materials for Space

	Xiaoyuan Wang (China Academy of Engineering Physics, China)	Applications Susana P. Fernandes- *(INEGI- Institute of Science and Innovation in Mechanical and Industrial Ingineering, Portugal)*
17:10-19:00	**POSTER SESSION – Drinks and Canapés Reception** (Atrium, Room N240)	

Wednesday 14th September 2016

	Session 1.5: Keynote Lectures (Room N242) Chair - Ajay Mishra (*University of South Africa, South Africa)*	
9:00-9:45	**Polymer Nanocomposites with Layered Silicates - Up- Scaling of Production and Recycling** Krzysztof Pielichowski (*Cracow University of Technology, Poland)*	
09:45-10:30	**Nanocelluloses: Emerging Biobased Building Blocks for Nanostructured Materials** Youssef Habibi *(Luxembourg Institute of Science and Technology, Luxembourg)*	
10:30 - 11:00	**Coffee/Tea Break (Atrium, Room N240)**	
	Session 1.6: Graphene and Carbon-based Nanocomposites -2 (**Room N345)** Chair – Evelien Frijns *(VITO nv, Belgium)*	**Session 2.4: Application of Nanomaterials and Nanocomposites - 2 (Room N342)** Chair – Youssef Habibi *(Luxembourg Institute of Science and Technology, Luxembourg)*
11:00-11:30	**Chitosan-Based Nanocomposite Beads for Drinking Water Production** Sabelo Mhlanga *(University of South Africa, South Africa)*	**Biocomposites and Their Applications** Kalia Susheel *(Indian Military Academy, India)*
11:30-11:50	Synthesis of graphene oxide and its effect on properties of Polyaniline in presence of HNO_3 and absence of HNO_3 Preetam Bharadiya, Vijay Chaudhari and Satyendra Mishra *(North Maharashtra University, India)*	The Wheat Grain as a cemented granular material: Nanoscale investigation of its mechanical properties Karsta Heinze, Jean-Yves Delenne, Matthieu George and Valérie Lullien-Pellerin *(Laboratoire Charles Coulomb, UMR5221 CNRS/UM (L2C), France; Université de Montpellier, France)*
11:50-12:10	Nonenzymatic Amperometric determination of glucose by CuO nanobelt graphene composite modified glassy carbon electrode Kempahanumakkagari Sureshkumar, Sreeramareddy Muralikrishna, Zhou Yan, Carlos Fernandez and Thippeswamy Ramakrishnappa *(Jain University, India; China University of Petroleum, China; Robert Gordon University, United Kingdom)*	Routes to Graphene based Sensors Ha-Duong and Asaf Avnon, *(FraunhoferIZm, Germany)*
12:10-12:30	Nature and application of magnetically active nanostructured organic thin films	Influence of pectins and xyloglucan on structure of bacterial cellulose

	Gunther Hennrich *(Universidad Autonoma de Madrid, Spain)*	membranes Monika Szymańska-Chargot, Monika Chylińska, Justyna Cybulska, Piotr M. Pieczywek and Artur Zdunek *(Polish Academy of Sciences, Poland)*
12:30-12:50	Multi-scale numerical simulation and experimental validation of elastic properties of laminate composites based Carbon NanoTubes Ahmed El Moumen, Mostapha Tarfaoui and Khalid Lafdi *(ENSTA Bretagne, IRDL, France; University of Dayton Research Institute, USA)*	Prototype Development of the Vibro-Impact Capsule Robot for Pipeline Inspection Yang Liu *(Robert Gordon Univ., United Kingdom)*
12:50-14:00	**Lunch (Atrium, Room N240)**	
	Session 1.7: Metallic and Metals Oxide Nanocomposites -2 (Room N345) Chair - Radhakrishna Prabhu *(Robert Gordon Univ., United Kingdom)*	**Session 2.5: Fibre Reinforced Composites (Room N342)** Chair – Ketan Pancholi *(Robert Gordon Univ., United Kingdom)*
14:00-14:20	Determination of hall effect parameters of gallium arsenide and gallium manganese arsenide by van der pauw geometry Ndiritu Francis, Kimei Solomon and Kirui Michael *(Egerton University, Kenya)*	Flexural strengthening of reinforced concrete deep beams using carbon fiber polymers Aya Al-Asi, Mu'Tasim Aabdel-Jaber and Maha Alqam *(The University of Jordan, Jordan)*
14:20-14:40	Deposition of CuFeS2 and CuFeS22 thin films and nanocrystals using dialkyldichalcogenophosphinatometal precursors Sajid N. Malik, Abdul Qadeer Malik, Mohammad Azad Malik and Khuram Shahzad Ahmad *(National University of Sciences and Technology (NUST), Pakistan; University of Manchester, United Kingdom; Fatima Jinnah Women University, Pakistan)*	Nanostructure of the polymer-graphene composites J.Janicki1, R.Fryczkowski1, M.Gorczowska1, M.Baczek1, Cz. Slusarczyk *(University of Bielsko-Biala, Poland)*
14:40-15:00	Surface modification of TiO_2–Ag hybrid nanoparticles using microwave assisted polymerization in the presence of bis (2-hydroxyethyl)-terephthalate (BHET) Patricia Adriana de León-Martínez, Florentino Soriano, Carlos Alberto Ávila-Orta, Pablo González-Morones, Antonio Serguei Ledezma-Pérez and Carlos Andrés Covarrubias-Gordillo *(CIQA -Centro de Investigación en Química, Mexico)*	Interpretation of the Effect of Ablative Environment on the Ablation Resiskastatance of C/P Composites Jamal Zamani and M. R. Ashani *(K.N.Toosi university of Technology, Iran; Tehran University, Iran)*
15:00-15:20	Magneto-resistive Behaviour in Fe-catalyst based Multi Wall Carbon Nanotubes Sekhar Chandra Ray *(University of South Africa, South Africa)*	Shear strengthening of reinforced concrete deep beams using carbon fiber-reinforced polymer composites Hana Al-Ghanim, Maha Alqam and Mu'Tasim Aabdel-Jaber *(The University of Jordan, Jordan)*
15:20-15:40	The influence of nanoclay loading on the thermal stability, flame retardant and mechanical properties of polyamide/nanoclay nanocomposites prepared by	Computational Study of Nanostructured Composite Materials for Photonic Crystal Fibre Sensors

	melt processing Shohel Siddique, Kyari Yates and James Njuguna *(Robert Gordon Univ., United Kingdom)*	*Jincy Johny, Radhakrishna Prabhu and Wai Keung Fung* *(Robert Gordon Univ., United Kingdom)*
15:40-16:00	**PRESENTATIONS PROGRAMME CLOSURE & GALA DINNER BRIEFING (Room N345)**	
16:00-16:30	**Coffee/Tea (Atrium, Room N240)**	
19:30 - 23:30	**GALA DINNER DANCE** **(including Poster Awards)** **Venue - Mercure Aberdeen Ardoe House Hotel and Spa** 	**GALA DINNER DANCE** **(including Poster Awards)** **Venue - Mercure Aberdeen Ardoe House Hotel and Spa**
19:30	**Dinner Reception**	
20:00		**Dinner Followed by Live Music by a 4 Piece Band + a Scottish Ceilidh**
23:30	**Coach Pick Up and Drop (Schoolhill – City Centre (at 19:00) and Garthdee Campus (19:15))**	

Table of Content

Nanoscale Sovereignty in Waste Water Chemistry

A. K. Mishra*

Nanotechnology and Water Sustainability Research Unit, College of Science, Engineering and Technology, University of South Africa, Florida Campus, Johannesburg, Jo-burg, South Africa

Nano size materials offer unique and sometimes unexpected material properties. This means that at the nano scale, materials can be 'tuned' to build faster, lighter, stronger, more efficient and stimuli responsive materials. Such properties of nanomaterials provide a platform for eco-toxicological based research investigations. Polymers are natural or synthetic compounds of high molecular weight. Polymers range from natural biopolymers such as DNA and proteins to synthetic plastic such as polystyrene. Polymers have a range of applications in areas such as coatings, adhesives, packaging materials, foams, textiles, composites, and industrials fibers to electronic devices, biomedical and optical devices. In addition, polymers have been employed in wastewater treatment, toxic metal removal and enrichment of precious metals from hydrometallurgical liquids. Nanomaterials in water research have been extensively utilized for the treatment, remediation, and pollution prevention. The focus of the lecture will to provide an overview of the nanoscale materials for waste water chemistry as futuristic materials.

*Corresponding author: mishrak@unisa.ac.za

Temperature Controlled Theranostics for Cancer Therapy

Clare Hoskins*

Keele University, School of Pharmacy, Hornbeam Building, Newcastle Under Lyme, ST5 6DB, United Kingdom

Pancreatic cancer is the 4th most aggressive cancer in the western world with less than 34% of patients surviving past 5 years. Lack of specific symptoms results in delayed diagnosis. Theranostics are new platforms, which offer simultaneous diagnosis and therapy resulting in a decrease in treatment time. Here treatments are conugated onto diagnostics by stimuli responsive binding allowing for controlled drug release resulting in a rapid and localised clinical effect. Hybrid nanoparticles are composed of an iron oxide core surrounded by a rigid gold shell. These particles undergo manipulation due to inherent magnetism of the core whilst laser irradiation of their gold shell results in localised heating due to surface plasmon resonance. Hence, they can be utlilised as diagnostics using MRI and laser irradiation can be used as a trigger for drug release. In our studies, we designed hybrid nanoparticles (50 nm) capable of drug loading onto their surface (3:1:0.25, Drug:Fe:Au). By exploiting the gold surface-to-drug interaction of a range of novel Bisnaphtalamido based agents a system with heat triggered drug release was produced. In vitro studies of these formulations on human pancreatic adenocarcinoma cell lines (BxPC-3 & Panc-1) showed the novel formulations possess a 10-fold lower IC50 value when compared with the free drug after only 24 h. These cytotoxicity studies combined with cellular uptake studies showed the formulations to be significantly more effective compared with gemcitabine. In vivo trials have commenced to further elucidate their viability for use as theranostics in pancreatic cancer therapy.

*Corresponding author: c.hoskins@keele.ac.uk

Technological Advancements in Nanofiller Reinforced Self-Healing Polymer Composites for Automotive and Aerospace Applications

Pankaj Kumar

Technical Polymers Material, New Delhi, India

The growth in Asia Pacific of customized Engineering Polymer Composites in newer highly differentiated demands of specialty applications has been observed in recent years due to developments in the polymer matrix materials, customized laying & type of fiber and performance additives. Composites differ from traditional material because they comprise of minimum two distinct different materials, one being fibers and other is matrix material which could be a modified engineering polymer .The combination of these discrete materials cannot be predicted by simply summing up of properties of the components as they function interactively to make new combinations that drive composite materials to newer demanding applications requiring high strength ,superior customized performance and light weight. These Smart 3D Composite materials with advanced Engineering Polymers offer good vibrational damping, low coefficient of thermal expansions, corrosion resistance, enhanced electrostatic dissipative properties due to which they are customized for specialized requirements in transport industry, especially automotive, railways and aerospace applications. Composites are resistant to fatigue and provide both design and fabrication flexibility which can significantly decrease the number of parts required for that application, reduce labor cost and enhance performance & aesthetics by replacing traditional materials. The push for economic usage of fuel has made light weight a priority in every mode of transport from bicycles to large aircraft.

**Corresponding author: pkumar@technicalpolymers.in*

Cyclodextrins as Versatile Tools for the Synthesis of RuO2/TiO2 Composites with Controlled Pore Structure and Enhanced Catalytic Performance

Rudina Bleta[1*], Sébastien Noel[1], Ahmed Addad[2], Anne Ponchel[1], Eric Monflier[1]

[1] *University of Artois, France*
[2] *University of Lille, France*

Creating self-assembled nanostructured materials with well-defined architectures and enhanced catalytic performance is an essential requirement for applications in the field of heterogeneous catalysis. The catalytic efficiency strongly depends on the pore structure of the support, the size and composition of individual metal nanoparticles, as well as the metal-support interactions. Titanium dioxide (TiO2) has proved to be an important support owing to its high surface area, chemical and thermal stability, as well as ability to strongly interact with various metal nanoparticles. In this study, we present a new and simple approach for the preparation of RuO2/TiO2 composites that employs the supramolecular assemblies formed between the randomly methylated β-cyclodextrin (RaMeβ-CD) and the block copolymer P123 as soft templates , the TiO2 nanocrystals as building blocks and the native β-CD as dispersing agent. We show that CD-based assemblies provide a versatile and easily accessible toolbox with different functionalities for generating supported catalysts with controlled pore architecture and uniform metal distribution. The efficiency of those catalysts was evaluated in the liquid phase hydrogenation of methyl oleate (MO, C18:1) to methyl stearate (MS, C18:0) under mild conditions (50 °C, 40 bar H2). Control of ruthenium dispersion into the large pores of RaMeβ-CD-P123-templated TiO2 material enhanced catalyst activity, imparted selectivity for the hydrogenation of the internal C=C bond and permitted catalyst separation and reuse without loss of activity and selectivity.

**Corresponding author: rudina.bleta@univ-artois.fr*

Flexural Strength and Elastic Modulus Recovery in Self-Healing Concrete Repaired by Inorganic Solutions

A.D. Carrillo*[1,2], J. Tulliani[3], A. Formia[3], P. Antonaci[4]

[1] *Student of Faculty of Architecture and Urbanism, Universidad Central de Venezuela, Barquisimeto, Venezuela*

[2] *Department of Architecture and Design, Politecnico di Torino, Turin, Italy*

[3] *Department of Applied Science and Technology (DISAT), Politecnico di Torino, Turin, Italy*

[4] *Department of Structural, Geotechnical and Building Engineering (DISEG), Politecnico di Torino, Turin, Italy*

Concrete is the most widely used construction material over the word because of its high compressive strength and low cost. However, it is sensitive to crack formation because of its limited tensile strength. These cracks endanger the durability of concrete buildings as aggressive liquids and gases may penetrate into the matrix along these cracks and cause further damage. Hence, inspection, maintenance and repair of concrete cracks are all indispensable. For these reasons, the self-healing ability would be desirable for concrete.

In this research, cementitious hollow tubes were produced by extrusion and used as healing agent containers that were embedded in the mortar matrix to obtain self-healing properties. Based on the results of preliminary mechanical tests, sodium silicate, potassium silicate and Primal (a commercial acrylic resin) were first selected as healing agents. To determine their efficiency, three-point bending test were performed on samples with the different healing agents and load, as well as, stiffness recovery indexes were determined. It was first observed that modulus of rupture and elastic modulus were not affected because of the presence of the capsules inside the samples with respect to plain mortar samples.

The best results were achieved with the sodium silicate solution. The Load Recovery Index, ranged from +7.4% to +27.6% and the Stiffness Recovery Index, ranged from +5.8% to +37.3%, one month after damaging the samples. After six months of rest, the Load Recovery Index ranged from +17.1% to +70.9% and the Stiffness Recovery Index, ranged from +15.7% to +53.6%. A longer time for repairing seemed to increase the efficiency of sodium silicate as a healing agent.

Corresponding author: anacarrillogv@gmail.com

Investigations on Mechanism of Self-Healing and Cavity Filling in Case of Steel Inoculated with Sea Shell Powder

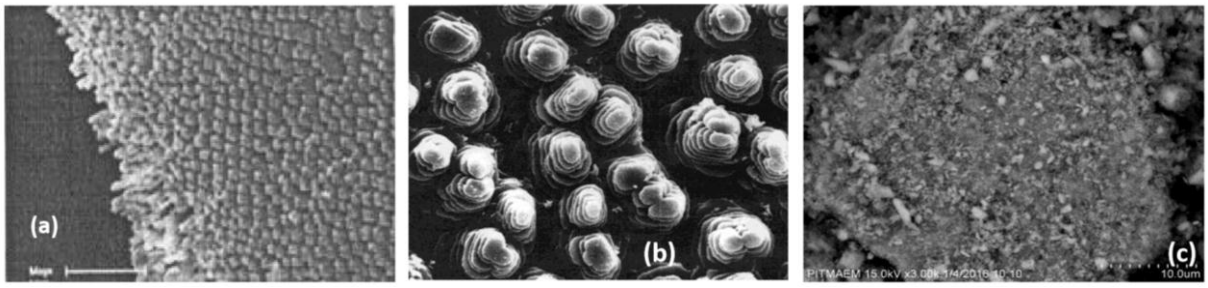
Parvaiz Habibullah[1], Ghazala Siddiqui[2], Saadat Anwar Siddiqi[3]

[1] *Interdisciplinary Res. in Met. & Mat. for Adv. Appl., Lahore, Pakistan*

2. Director, Centre of Excellence, University of Karachi, Karachi, Pakistan

3. Interdisciplinary Research Centre in Biomedical Materials, COMSATS, Lahore, Pakistan

Recently scientists have come up with some stuffs that can repair themselves. One of the models for this research comes from steel inocculated with seashells powder. Seashells are comprised largely of a brittle ceramic material (calcite, the stuff of chalk) in the form of microscopic slates. Shells, such as the abalones, are reinforced with a kind of protein mortar. Scanning electron microscope pictures of calcite prisms of Mytilus edulis shell and of lime crystals of surface turbo snail, at 1500□, are shown respectively in (a) and (b).



We utilized the seashell powder, Composition: Moisture = 0.280%, L.O.I @950 oC (as CO2) = 39.92%, SiO2 = 5.980%, Al2O3 = 2.558%, Fe2O3 = 0.518%, CaO = 47.86%, MgO = 2.232%, Na2O = 0.582%, K2O = 0.0356%, PO4)-3 = 0.030%, Estimated crude protein = 1.12%, for our researches, SEM image at 3000□ (c). We are identifying the protein and mechanism how the protein mortar stretches itself into ligaments that bridge the gap, with the help of scanning electron microscope (SEM).

*Corresponding author: drpervaiz.h@gmail.com

Thermo-mechanical and Structural Properties of Ag-Cu and ZnO Reinforced Polylactide Nanocomposite Films

Yasir Arfat[1*] and Jasim Ahmed[1]

[1]*Kuwait Institute for Scientific Research (KISR), Shuwaikh, Safat, Kuwait, 13109, Kuwait*

Plasticized polylactic acid (PLA) based nanocomposite films were prepared by incorporating polyethylene glycol (PEG) and two selected nanoparticles (NPs) [silver-copper (Ag-Cu) alloy (<100 nm) and zinc oxide (ZnO) (<50 and <100 nm)] through solvent casting method. Thermal properties of the nanocomposites films were investigated using differential scanning calorimeter (DSC) and thermogravimetric (TG) analyzer. The addition of 20% PEG to the neat-PLA decreased the glass transition temperature (Tg) significantly from about 60 to 17 °C, whereas the melting temperature (Tm) did not drop significantly. Metallic nanoparticles increased the Tg, however, Ag-Cu alloy exhibited a greater increase than ZnO nanocomposite films. Particle size of ZnO NP did not show significant difference in the Tg values of the films. The Tm value of the nanocomposite films was not influenced by the NP. The addition of plasticizer initiated the crystallization (cold and melt) of the PLA/PEG blend, which was substantially improved by incorporation of NP in the composite films, in particular, 1wt% loading. Non-isothermal crystallization was significantly affected by the cooling and heating rate. Thermogravimetric analysis data indicated that only Ag-Cu alloy could improve thermal stability of nanocomposite films. The crystallinity of the nanocomposites (NCs) was significantly influenced by NP incorporation as evidenced from DSC and X-ray diffraction (XRD) analysis. The PLA nanocomposite reinforced with NPs exhibited much higher tensile strength than that of PLA/PEG blend. Melt rheology of NCs exhibited a shear-thinning behaviour. The mechanical property drastically reduced with a loading of NPs, which is associated with degradation of PLA. SEM micrographs exhibited that both Ag-Cu alloy and ZnO NPs were dispersed well in the PLA film matrix. Furthermore, nanoparticles significantly influenced the UV barrier and the transmittance of plasticized films.

**Corresponding author: yasir.arfat123@gmail.com*

Release of Carbon Nanotubes from a Polyamide Nano-composite During Milling

Evelien Frijns*

Environmental Risk and Health Unit, VITO nv, Mol, BE-2400, Belgium

Multi Walled Carbon NanoTubes (MWCNTs) are commonly used in polymer formulations to improve tensile strength, electrical and thermal conductivity, fire resistance and other properties. Nowadays nanocomposites are widely used in industry and concerns have been raised about the potential release of CNTs when the nanocomposites are mechanically stressed. After release CNTs can pose a risk to workers and consumers because of the high aspect ratio and bio persistent nature. Potential CNT release from a polyamide (PA) nanocomposite was studied in a CNC milling machine in an industrial setting. The released particles were characterized by measuring real-time particle number and mass concentration using a Condensation Particle Counter (CPC) and a light-scattering laser photometer. Airborne milled particles were collected using an cowl head air sampler and analyzed using electron microscope (STEM and TEM). Electron microscopic analysis was performed to find out if CNTs were completely embedded in the PA matrix, CNTs were protruding from the PA matrix and if CNTs were free-standing. Results showed lower mass and particle number concentrations during the milling of a PA with a CNT filler compared to the milling of a neat PA. This could be explained by improved mechanical properties of the CNT composite reducing the dust release during milling. Electron microscopic analysis did reveal protruding CNTs, but no free-standing CNTs were found. Protruding CNTs could break off from the matrix and become free-standing. After inhalation free-standing and protruding CNTs may directly come in contact with lung cells and induce toxic reactions.

Corresponding Author: evelien.frijns@vito.be

Nitrogen Functionalized bi-layer Graphene for Spintronic Application

Sekhar C. Ray[1,*], N. Soin[2], S. S. Roy[3], W. F. Pong[4] and A. M. Strydom[5]

[1] *Department of Physics, College of Science, Engineering and Technology, University of South Africa, Private Bag X6, Florida, 1710, Science Campus, Christiaan de Wet and Pioneer Avenue, Florida Park, Johannesburg 1710, South Africa*

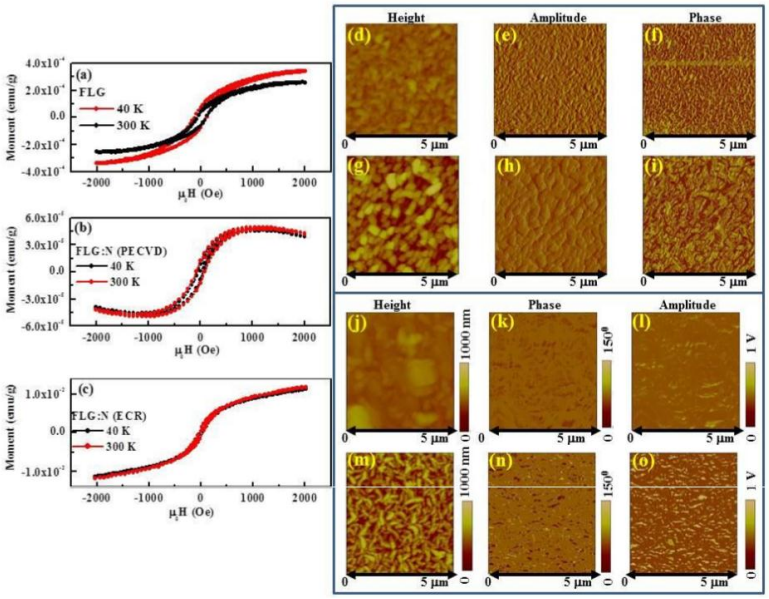
[2] *Energy and Environmental Technologies (IREET), Knowledge Centre for Materials Chemistry (KCMC) University of Bolton, Deane Road, Bolton BL3 5AB, United Kingdom.*

[3] *Department of Physics, School of Natural Sciences, Shiv Nadar University, Gautam Budh Nagar 203207, UP, India.*

[4] *Department of Physics, Tamkang University, Tamsui 251, Taipei, Taiwan,*

[5] *Highly Correlated Matter Research Group, Physics Department, University of Johannesburg, PO Box 524, Auckland Park 2006, South Africa*

We have studied the electronic structure and magnetic properties of plasma enhanced chemical vapour deposition (PECVD) and high density electron cyclotron resonance (ECR) plasma-assisted CVD functionalized bilayer graphene and hence elucidated the possibility of spintronic application. It is observed that the magnetic moment of ECRCVD functionalized bi-layer graphene is higher than PECVD functionalized bi-layer graphene and is due to high density nitrogen is functionalized with bi-layer graphene. The magnetic force microscopy image shows that the magnetic domains are higher in case of ECR-CVD functionalized bi-layer graphene. These results are also correlated with the electron field emission current and Raman spectroscopy results; where we observed that the emission current and defects are higher ECR-CVD functionalized bi-layer graphene.



*Corresponding author: Raysc@unisa.ac.za

Surface Modification of Carbon Nanofibers, Graphene Platelets and Mixtures of Both by Plasma Polymerization of Propylene

C.A. Covarrubias-Gordillo, F. Soriano-Corral, C.A. Ávila-Orta, P. A. De León-Martínez, V. Cruz-Delgado

Centro de Investigación en Química Aplicada Blvd. Enrique Reyna 140, Saltillo, Coahuila, 25253, Mexico

Surface modification of carbon nanoparticles (CNPs) by plasma polymerization of propylene was studied aiming to enhance affinity to produce polymer nanocomposites with high thermal conductivity. For this purpose, carbon nanofibers (CNF), graphene platelets (GP) and mixtures CNF:GP (using ratios of 9:1, 8:2 and 7:3) were modified. The power of the plasma reactor (60 w), reaction time (60 min) and reactor pressure of 2 x 10-1 mbar, were constant through all experiments, while the surface area and sp2 hybridization spots were the studied variables. The CNPs were previously treated by sonication in gas phase, the process of deagglomerated particles was evaluated by dynamic light scattering (DLS). Meanwhile, the surface modification was characterized by transmission electron microscopy (TEM), infrared spectroscopy (IR), Raman spectroscopy, solvent dispersion tests and thermogravimetric analysis (TGA). Such characterizations indicate a significant deagglomeration by increasing the surface area exposed of CNPs, also, the presence of crosslinked polypropylene clusters generated on the surface of the CNPs after treatment was observed. All NPs exhibit similar modification percentages (4-5 wt-%), however, while an increment ocurrs in the surface area and sp2 hybridization spots (with increasing GP concentration), the ratio ID / IG shows an increase in the covalent modification.

**Corresponding author: posgrado2014.103@ciqa.edu.mx*

Silk Fibroin/Gold Nanocrystals: A New Example of Biopolymer-Based Nanocomposites

Sylvie Noinville*, Adrien Garnier, Alexa Courty

Sorbonne Universités, UPMC Univ Paris 06, CNRS, UMR8233, MONARIS, Université Pierre et Marie Curie, 4 place Jussieu, F-75005 Paris, France.

The dispersion of nanoparticles in ordered polymer nanostructures can provide control over particle location and orientation, and pave the way for engineered nanomaterials that have enhanced mechanical, electrical, or optical properties. Here we used silk fibroin, a natural biopolymer, to embed gold nanocrystals (NCs), so as to obtain well-ordered structures such as nanowires and self-assembled triangular nanocomposites. Monodisperse gold NCs synthesized in organic media 1,2 are mixed to silk fibroin and the obtained nanocomposites are characterized by UV-visible spectroscopy, transmission electron microscopy (TEM), scanning electron microscopy (FEG-SEM), atomic force microscopy (AFM) and Infrared spectroscopy. Surface plasmon absorption study of gold NPs shows that the optical properties of gold NCs-silk nanocomposites is blue shifted compared to gold NPs. The size and distribution of gold NCs can be well controlled by the presence of silk fibroin giving nanowires and also self-assembling into triangular nanocomposites as characterized by TEM, FEGSEM and AFM. The strong interaction between gold NCs and silk fibroin is also revealed by the conformation change of silk protein in presence of gold NCs, as shown by FTIR analysis 3,4. The self-assembly of such nanocrystals into organized arrays with enhanced collective properties will provide new nanoplasmonic devices.

(1) Courty, A.; Mermet, A.; Albouy, P. A.; Duval, E.; Pileni, M. P. Nature Materials 2005, 4, 395.
(2) Andrieux-Ledier, A.; Tremblay, B.; Courty, A. Journal of Physical Chemistry C 2013, 117, 14850.
(3) Wojcieszak, M.; Percot, A.; Noinville, S.; Gouadec, G.; Mauchamp, B.; Colomban, P. Journal of Raman Spectroscopy 2014, 45, 895.
(4) Noinville, S.; Revault, M. Conformations of proteins adsorbed at liquid-solid interfaces. In Principles and practice : Proteins at solid-liquid interfaces; Springer-Verlag: Berlin Heidelberg, 2006; pp 119.

Corresponding author: sylvie.noinville@upmc.fr

Structural and Non Linear Optical Property of BaSnO3 Nanopowder Prepared by solid state ceramic method

Jibi John[1,] V.P.Mahadevan Pillai[1*], Anitta Rose Thomas[2], Reji Philip[2] and Radhakrishna Prabhu[3]

[1]*Department of Optoelectronics, University of Kerala, India*
[2] *Raman Research Institute, India*
[3] *Robert Gordon University, School of Engineering, Aberdeen, AB10 7GJ, United Kingdom*

Alkaline earth stannates with the general formula RSnO3 (R = Ba, Sr and Ca) are important material systems inview of their interesting physical properties and perovskite structures. Perovskite-type oxides have a simple and flexible structure that is easy for ionic substitution, carrier doping and oxygen non-stoichiometry, which can form a vast set of technologically important materials for a wide variety of industrial applications. BaSnO3 is a cubic perovskite-type oxide that behaves as an n-type semiconductor with a wide band gap of 3.4 eV and remains stable at temperatures up to 10000C. It has wide applications such as thermally stable capacitors, humidity sensors, gas sensors, etc. BaSnO3 doped with a few percent of La exhibits unusually high electrical mobility of 320 cm2(Vs)-1 at room temperature and superior thermal stability at high temperatures.

BaSnO3 powder was prepared by solid state ceramic method. X-ray diffraction pattern of the prepared sample presents the characteristic peaks of cubic phase of BaSnO3. The average size of the crystallites, estimated by Debye Scherrer's formula, was found to be 49 nm indicating the nanostructured nature. The SEM image shows a porous surface morphology with grains of cuboidal structure with well defined grain boundaries. UV-Visible spectra shows BaSnO3 powder exhibit high reflectance in the 400-700 nm range. The open aperture Z-scan measurements are carried out in the present sample using 5 ns laser pulses at 532 nm from a frequency doubled Nd: YAG laser. The normalized transmission decreases at higher laser intensities indicating an optical limiting behavior. From numerical fitting the effective third order absorption coefficient βeff and saturation intensity Isat are found to be 6.9 x 10 -11 m/W and 9.0 x 1012 W/m2, respectively. These values indicate a high optical limiting efficiency, comparable to that of graphene and its metal hybrids.

**Corresponding author: vpmpillai9@gmail.com*

Hybrid Sol-gel/Polyaniline Coatings Reinforced with Nano-ZnO Particles for Corrosion Protection of Mg alloys

Aurelie Dupuis[1*], Emmanuel Aragon[1] and François-Xavier Perrin[1]

[1] *Laboratoire MAPIEM EA 4323, Seatech-Ecole d'Ingénieurs, Université de Toulon, CS 60584, Toulon, 83041, France*

A way to reduce the jet fuel consumption is an application of lighter materials in the aircraft construction. Magnesium is seen as the primary candidate for substantial weight reduction due to its low density and good mechanical properties. However, engineering applications of magnesium have been limited mainly due to the poor corrosion resistance of magnesium alloys. Several coating applications have been developed in order to improve corrosion resistance of Mg alloys and a very promising approach is hybrid organic-inorganic sol-gel coatings. Active corrosion inhibiting components are often added to the protective corrosion system in order to assure prolonged protection even in the case of partial damage of the coating.

Polyaniline (PANI) has been extensively studied as protective coating for metals and alloys and has remarkable capability to protect steel in acid, alkaline and neutral environments. In the last decade, nanoparticles like nano-SiO2, nano-TiO2, nano-Al2O3 and nano-ZnO have been used to improve the mechanical properties as well as the anticorrosion performance of the organic paints. Among inorganic nanoparticles, nano ZnO particles have received great attention because of their unique electrical, catalytic, electronic and optical properties, high stability and environmental friendly feature, as well as low cost and extensive applications in different fields.

The aim of this work is so to test corrosion protection of sol-gel coatings reinforced with a combination of PANI and nano-ZnO pigments on Magnesium alloys. Optimization of nano-ZnO and PANI proportions as well as their dispersion in the sol-gel coating have been studied. Corrosion resistance properties of the coatings was investigated by electrochemical measurements and by the study of evolution of coating under salt spray exposure. A special attention will be paid to the self-healing properties of the hybrid coatings.

**Corresponding Author: aurelie.dupuis@univ-tln.fr*

Ferroelectricity and Electromechanical Coupling Behavior at Twist Boundaries in $PbTiO_3$

Xiaoyuan Wang

Institute of Systems Engineering, China Academy of Engineering Physics, Mianyang, Sichuan Province, China

Since perovskite oxide ceramics are usually polycrystalline materials, grain boundaries are one of the most important planar defects within the material. Grain boundaries considerably affect electronics and ferroelectric properties of perovskites. In this study, atomic and electronic structures as well as ferroelectricity at Σ5(001) twist grain boundaries in ferroelectric PbTiO3 have been investigated using first-principles (ab initio) density-functional theory calculations within the local density approximation. The twist-boundary structure with the coincidence site lattice of O-Pb and O-O is found to be energetically favorable. At the twist boundary, rectilinear spontaneous polarization along the normal direction to the boundary is highly enhanced because of the locally strengthened covalent Pb-O bond, which predominates ferroelectricity in PbTiO3. Interestingly, we found vortex or toroidal polarization in the twist-boundary plane coexisting with the rectilinear polarization. The vortex polarization arises from rotational in-plane displacement induced by the twisted misorientation of lattices. An applied tensile strain tends to increase the rectilinear polarization, especially at the twist boundary. On the other hand, the vortex polarization is suppressed upon application of a tensile strain and finally disappears at a critical strain in the TiO2 layer of the boundary, whereas the PbO layer exhibits the opposite tendency.

**Corresponding Author:* xjtuwxy@gmail.com

Polymer Nanocomposites with Layered Silicates - Up- Scaling of Production and Recycling

Krzysztof Pielichowski* and Tomasz Majka

Cracow University of Technology, ul. Warszawska 24, Krakow, 31155, Poland

Lab-scale preparation of polymer nanocomposites with layered silicates has been developed in the last two decades and the most important factors that contribute to the structure of polymer-based clay nanocomposites identified. They include molecular weight of polymer, the type and concentration of organic modifier and the processing conditions of the polymer melt to secure intercalation or exfoliation of layered silicates. Processing conditions depend on the temperature, pressure, extruder's screw diameter and length which governs the throughput of the processing equipment. However, most of the experiments are laboratory-scale and the question how to up-scale the process toward industrial production scale still remains not fully answered.

Another issue that requires more research attention is recycling of polymer nanocomposites. Among different methods, pyrolysis seems to be an interesting alternative. Hence, we have developed a novel method of polypropylene/montmorillonite nanocomposites recycling by pyrolysis to produce pyrolysed montmorillonite (MMT) that can be re-used in the preparation of polymer composites. Interestingly, the polypropylene composites with recycled MMT display still improved mechanical properties compared to the neat polymer.

References:

1. K. Pielichowski, T. M. Majka, A. Leszczynska and M. Giacomelli, Optimization and Scaling up of the Fabrication Process of Polymer Nanocomposites: Polyamide 6/ Montmorillonite Case Study, in 'Structural Nanocomposites – Perspectives for Future Applications' (Ed. James Njuguna), pp. 75-104, ISBN 9783642403217, Springer-Verlag Berlin Heidelberg 2013.
2. T.M. Majka, O. Bartyzel, K.N. Raftopoulos, J. Pagacz, A. Leszczyńska, K. Pielichowski, Recycling of polypropylene/montmorillonite nanocomposites by pyrolysis, Journal of Analytical and Applied Pyrolysis, in press (http://dx.doi.org/10.1016/j.jaap.2016.04.005).

Corresponding Author: kpielich@pk.edu.pl

Nanocelluloses: Emerging Biobased Building Blocks for Nanostructured Materials

Youssef Habibi

Luxembourg Institute of Science and Technology, Materials Research and Technology, Department, 5, avenue des Hauts-Fourneaux, Esch-sur-Alzette, L-4362, Luxembourg

Since their first isolation in 1940s by Randy, nanocrystalline cellulose start attracting the attention of the material community. Later during 1980s, Turbark group's succeeded in extracting a new kind of nanocellulose, called at that time microfibrillated cellulose, stimulating further the interest toward these renewable building blocks. Nowadays with the emergence of the green portfolio, numerous efforts are being focused on the use of materials from renewable resources, and we are attesting a huge and unprecedented interest for nanocellulose. This interest is due to their renewability and biodegradability, in addition to their appealing intrinsic properties such as low density, outstanding mechanical properties. Moreover, nanocelluloses possess spectacular optical properties originating from their ability to self-organize into liquid crystalline arrangements. All these impressive properties allow their use in wide range of applications.

This keynote presentation will provide an overview on nanocellulose followed by few examples related to their processing using various techniques to access useful nanostructured materials for different applications.

**Corresponding Author: Youssef.Habibi@list.lu*

Chitosan-Based Nanocomposite Beads for Drinking Water Production

ML Masheane[1,2], LN Nthunya[1,2], SS Sambaza[2], SP Malinga[2], EN Nxumalo[1], BB Mamba[1] and SD Mhlanga[1*]

[1]Nanotechnology and Water Sustainability Research Unit, College of Science, Engineering and Technology, University of South Africa, Florida, 1709, Johannesburg, South Africa.
[2]Department of Applied Chemistry and the DST/Mintek Nanotechnology Innovation Centre-Water Research Node, University of Johannesburg, P.O. Box 17011, Doornfontein, 2028, South Africa.

Potable drinking water is essential for the good health of humans and it is a critical feedstock in a variety of industries such as food and pharmaceutical industries. For the first time, chitosan-alumina/functionalised multiwalled carbon nanotube (f-MWCNT) nanocomposite beads were developed and investigated for the reduction of various physicochemical parameters from water samples collected from open wells used for drinking purposes by a rural community in South Africa. The water samples were analysed before and after the reduction of the identified contaminants by the nanocomposite beads. The nanocomposite beads were effective in the removal of nitrate, chromium and other physico-chemical parameters. Although, the water samples contained these contaminants within the WHO and SANS241 limits for no risk, the long-term exposure and accumulation is an environmental and health concern. The reduction of these contaminants was dependent on pH levels. At lower pH, the reduction was significantly higher, up to 99.2% (SPC), 91.0% (DOC), 92.2% (DO), 92.2% (turbidity), 96.5% (nitrate) and 97.7% (chromium). Generally, the chitosan-alumina/f-MWCNT nanocomposite beads offer a promising alternative material for reduction and removal of various physico-chemical parameters for production portable water.

**Corresponding Author: mhlansd@unisa.ac.za*

Synthesis of Graphene Oxide and its Effect on Properties of Polyaniline in Presence of HNO_3 and Absence of HNO_3

Preetam Bharadiya, Vijay Chaudhari* and Satyendra Mishra

University Institute of Chemical Technology, North Maharashtra University, India

Graphene is two dimensional-atomically thick material having sp2 domains which impart it interesting electrical and electronic properties. Functionalization of graphene by oxygenated groups ie. Graphene oxide (GO) enhance its mechanical strength and chemical reactivity that has ability to tune the physic-chemical properties of other material. In this report, nanocomposite of GO with polyaniline (PANI) is prepared by solution blending technique. Multifunctional role of GO viz. as modifier, dopant, as well as template is exploited. Briefly, in addition to enhancement in electrical conductivity as well as its role as dopant, GO also affect the aspect ratio and overall morphology of PANI/GO composite that project it as template. PANI/GO nanocomposites were prepared by in-situ oxidative polymerisation in presence of HNO3 and absence of HNO_3 using Ammonium persulfate as an oxidizing agent, water as a solvent and GO as a filler with varying concentration. The nanocomposites were characterised by Fourier Transform Infrared spectroscopy (FTIR),X-ray Diffraction (XRD), Field Emission Scanning Electron microscopy (FESEM), Raman Spectroscopy, Thermal Gravimetric Analysis (TGA), Current-Voltage characteristics (I-V), Conductivity. FESEM reveal nanotube and nanorod morphology of nanocomposites. I-V characteristics show non-ohmic behaviour and ohmic behaviour of nanocomposites.

*Corresponding Author: vijay.rchaudhari@gmail.com

Nonenzymatic Amperometric Determination of Glucose by CuO Nanobelt Graphene Composite Modified Glassy Carbon Electrode

Kempahanumakkagari Sureshkumar[1], Sreeramareddy Muralikrishna[1], Zhou Yan[2], Carlos Fernandez[3*] and Thippeswamy Ramakrishnappa[1]

[1]Center for Nano and Material Science, Global Campus, Jain University, Jakkasandra (P), Kankapura (T), Bangalore-560001, Karnataka, INDIA
[2]Department of Chemistry, School of Science, China University of Petroleum (East China) Qingdao, China
[3]School of Pharmacy and Life Sciences, Robert Gordon University, Garthdee Road, Aberdeen AB10 7GJ, United Kingdom

We have successfully developed for the first time an electrochemical sensor for glucose by using a simple and effective design of growing CuO nanobelts graphene composites (CuO@G). The as-prepared composites were characterized by Powder X-ray powder diffraction (PXRD) Field emission scanning electron microscopy (FESEM) and Transmission electron microscopy (TEM). The prepared composite material exhibits higher electro catalytic activity for the oxidation of glucose compared to chemically reduced graphene (C rGO) and bare CuO nanobelts. This may be due to high catalytic active sites and high electron transfer rate provided by the CuO nanobelts graphene composite network. The optimized protocol has linearity with current response and glucose concentration in the range 0.5 – 6.5 µM and detection limits were found to be 0.05 µM (3σ). The method exhibits fast response time (less than 5s) along with good reproducibility and selectivity towards glucose in the presence of other electro active compounds that are normally present in blood serum like dopamine, ascorbic acid, uric acid and sodium chloride. The protocol has been successfully applied for glucose determination in clinic human blood serum samples.

**Corresponding Author: c.fernandez@rgu.ac.uk*

Nature and Application of Magnetically Active Nanostructured Organic Thin Films

Gunther Hennrich

Universidad Autonoma de Madrid, Spain

The emerging field of organic spintronics consists of the implementation, detection, and manipulation of spin transitions in novel materials. The advantages of organic thin film (TF) materials in terms of structural variability, mechanical flexibility, processability, lightness, etc. are evident.1 The presence of accessible triplet states in organic semi-conductors has been identified as the origin of the magnetic activity,2 and the macroscopic order of the molecular building units is of vital importance.3 We have recently reported on the magnetic response of TF devices formed by liquid crystalline benzene-based discotics as studied by Faraday rotation spectroscopy.4 Our latest advances in magneto-optical materials resulted in TFs based on similar octopolar mesogens or even simpler linear structures.5 The molecules consist of an electron rich benzene nucleus, substituted with flexible alkyl/alkoxy chains, and peripheral electron withdrawing groups (EWG).6 In all cases they form good quality TFs by self-assembly. In order to rationally design magnetically active materials it is crucial to relate the supramolecular order that the individual building units adopt to the observed magnetism. Our current study of phenylacetylenes of varying symmetry (octopolar, wedge shaped and linear) suggests that the simplification of the structural motif yields an increased magnetic response. Here we present a number of tolane derivatives that form smectic liquid crystals and study the magneto-optical activity of the respective TFs, molecular structures of crstalline and LC phenylacetylenes.

References

1 B. Hu, L. Yan and M. Shao, Adv. Mater., 2009, 21, 1500.
2 A. Köhler and S. Bässler, Mater. Sci. Eng. R, 2009, 66, 71.
3 J. K. Grey et al., ACS Nano, 2014, 8, 10559.
4 S. Vandendriessche et al. Chem. Mater., 2013, 25, 1139.
5 G. Hennrich, T. Verbiest et al. manuscript submitted.
6 G. Hennrich, T. Verbiest, J. L. Serrano, J. L. et al., Angew. Chem. Int. Ed., 2006, 45, 4203.

**Corresponding Author: gunther.hennrich@uam.es*

Multi-scale numerical simulation and experimental validation of elastic properties of laminate composites based Carbon NanoTubes

Ahmed El Moumen[1*], Mostapha Tarfaoui[1] and Khalid Lafdi[2]

[1]*ENSTA Bretagne, IRDL, Ensta Bretagne, Brest, 29200, France*
[2]*University of Dayton Research Institute, USA*

The principal objective of this investigation is the prediction of the elastic moduli of laminate composites containing a random distribution of carbon nanotubes (CNTs) using numerical and experimental approaches. Homogenization technique based on the representative volume element is used. To construct a representative model of composites, a set of microscope observation was considered to identify the periodicity of composites. These have been used to construct the representative volume element, on which the numerical homogenization was carried out. The effect of the distribution and the CNTs volume fractions were studied. The results of numerical homogenization were compared and validated with experimental data. Experimental characterization is based on the use of tension and shear tests to obtain the nine elastic moduli of laminate composites with and without CNTs reinforcement. We have also used the Flatwise tension and open hole tension tests. The analytical approach consists in using the homogenization models to estimate the elastic properties of the composite from the knowledge of their constituents. Finally, a comparison between different approaches, experimental, numerical and analytical, is planned.

Session 1.7 –Metallic and Metals Oxide Nanocomposites – 2 – Radhakrishna Prabhu

Determination of Hall Effect Parameters of Gallium Arsenide and Gallium Manganese Arsenide by Van Der Pauw Geometry

Ndiritu Francis, Kimei Solomon and Kirui Michael*

Egerton University, Njoro, Kenya, Nakuru, 20115, Kenya

Gallium Arsenide (GaAs) has been used widely in electronic industry to make diodes and transistors. As a semiconductor, it can be doped up with impurities with magnetic properties such as manganese to increase its electron conductivity. The storage capacity of the electronic devices made of gallium manganese arsenide (Ga1-xMnxAs) and the proportion of manganese atoms is worth studying. Here, GaAs was doped at different manganese levels, x, and the charge carrier concentrations at varied applied magnetic fields was investigated using Van der Pauw configuration. The tests were conducted at room temperature of 230C with magnetic field, 0.9 ≤ B ≤ 3.6mT and direct current of 1.19A. All the samples were studied for their hall voltage VH, carrier mobility μ, hall resistivity ρH and charge carrier concentration for different values of x. It was determined for Ga1-xMnxAs, 10% ≤ x ≤ 20% range, has maximum hall resistivity at B≈ 1.9 mT. For x=10%, ; x=20%, and for x=1%, the applied magnetic field has no effect on hall resistivity at initial states until B≈1.7mT. Beyond this point, magnetic field increases linearly with the hall resistivity to a maximum of . Maximum hall resistivity for x=50% was at . For , carrier mobility , was of order of while for , was of order . It was found out that the most probable doping percentage of GaAs with Mn dopants is approximately 20% and 10% as they show a hysteric response to an applied magnetic field. It suggests a good doping level of GaAs for making of volatile memory chips.

*Corresponding Author: mskirui@egerton.ac.ke

Deposition of CuFeS2 and CuFeS22 Thin Films and Nanocrystals Using Dialkyldichalcogenophosphinatometal Precursors

Sajid N. Malik[1, 2], Mohammad Azad Malik[1], Abdul Qadeer Malik[2] and Khuram Shahzad Ahmad[3*]

[1]*School of Materials, The University of Manchester, Oxford Road, Manchester M13 9PL, United Kingdom*
[2]*School of Chemical and Materials Engineering (SCME), National University of Sciences and Technology (NUST), Islamabad 44000 Pakistan*
[3]*Environmental Sciences Department, Fatima Jinnah Women University, The Mall, Rawalpindi 46200 Pakistan*

CuFeS2 and CuFeSe2 are low band gap, earth abundant and environment friendly representatives of I-III-VI2 semiconductors which are being explored for thermoelectric, solar photovoltaics and spintronics applications. The research work presented herein reports the deposition of CuFeS2 and CuFeSe2 thin films and nanoparticles using dialkyldichalcogenophosphinatometal complexes as molecular precursors. Copper and iron complexes belonging to diphenyldiselenophosphinatometal [Mx(Ph2PSe2)y] and diisobutyldithiophosphnatometal [Mx(iBu2PS2)y] family (where M = Cu, Fe), have been synthesized in high yield by an efficient and reproducible method. Characterization of the as synthesized complexes has been done using mass spectrometry, NMR (1H and 13C) spectroscopy, FTIR spectroscopy and elemental analysis. Degradation behavior of these complexes as a function of temperature was studied using thermogravimetric analyses. These complexes have been used as molecular precursors for deposition of CuFeS2 and CuFeSe2 thin films by aerosol assisted chemical vapor deposition (AACVD). Depositions experiments were performed at four different temperatures (350, 400, 450 and 500 °C) to evaluate the influence of deposition temperature on morphology, diameter, stoichiometry and crystallographic phase of deposited material. Similarly, parametric studies were also undertaken to investigate the effect of solvent and carrier gas flow rate on quality of deposited thin films. Characterization of thin films was carried out by p-XRD, SEM, AFM and EDX analysis. Significant variation in grain size, shape, stoichiometry and phase structure was observed by varying the deposition parameters, particularly the deposition temperature. Similarly, these molecular precursors have also been used for colloidal preparation of CuFeS2 and CuFeSe2 nanoparticles. Effect of various nanoparticles growth

parameters i.e growth temperature, reaction duration and precursors concentrations has been investigated. Nanocrystals were characterized by p-XRD studies, UV-Vis-NIR spectroscopy, Raman spectroscopy, TEM, EDX analysis, and XPS techniques. It was demonstrated that mean diameter, morphology and band gap of the nanocrystals could be controlled by judicious choice of the growth parameters.

Corresponding Author: chemist.phd33@yahoo.com

Surface Modification of TiO_2–Ag Hybrid Nanoparticles Using Microwave Assisted Polymerization in the Presence of bis (2-hydroxyethyl)-terephthalate (BHET)

P. A. De León-Martínez*, F. Soriano-Corral, C.A. Ávila-Orta, C.A. Covarrubias-Gordillo,

Antonio S. Ledezma-Pérez

Centro de Investigación en Química Aplicada Blvd. Enrique Reyna 140, Saltillo, Coahuila, 25253, Mexico

Titanium dioxide doped silver nanoparticles (nTiO2-Ag) were surface-modified by microwave-assisted polymerization in order to determine the influence of the modification on the morphological, physicochemical and bactericide properties of the nTiO2-Ag/PET hybrid. During the microwave assisted polymerization process, antimony oxide as initiator and bis-(2-hydroxyethyl)-terephthalate (BHT) as monomer were used. The modified and unmodified nanoparticles were analysed by Fourier transform infrared spectroscopy (FTIR), X-ray diffraction (XRD), thermogravimetric analysis (TGA), transmission electron microscopy (TEM) and electron diffraction. A thin layer of PET coating in the surface of the nanoparticles were observed, which, was quantified by TGA giving a value of 40 wt-%, with respect to neat nanoparticles. On the other hand, the XRD analysis and electron diffraction showed a change of the crystalline microstructure of Ag after the modification process; i.e. traces of silver oxide were found. This oxidation was attributed to the presence of oxygen ions and radicals generated during microwave polymerization, oxidizing slightly from Ag0 to Ag+1. Additionally, the bactericide properties of surface-modified nanoparticles with PET were evaluated and compared to unmodified nanoparticles using Escherichia coli and Staphylococcus aureus. In conclusion the presence of the thin layer of PET on the nTiO2-Ag did not change significantly the bactericide activity, showing an excellent performance similar to nanoparticles without modification with higher affinity to PET.

*Corresponding Author: palm2128@gmail.com

Magneto-resistive Behaviour in Fe-catalyst based Multi Wall Carbon Nanotubes

Sekhar Chandra Ray

Department of Physics, UNISA, Florida Campus, Johannesburg, 1710, South Africa

INTRODUCTION

The Fe-catalyst based multiwall carbon nanotubes (MWCNTs) were synthesized using catalytical chemical vapor deposition (CVD) process. Magneto-resistance behaviour is observed from measurement of DC resistance with temperature at different applied magnetic field.

EXPERIMENTAL STUDY

The magnetization (M) was measured versus applied magnetic field strength (H), using a commercial physics properties measurement system (PPMS) at a temperature of 305 K; whereas the DC resistance are measured at different applied magnetic field using Superconducting quantum interference device (SQUID).

RESULTS AND DISCUSSION

The temperature dependent resistance of Fe-catalyst based multiwall-CNT shows metallic behaviour. The minimum resistance is occurred at 12.6 K and 50 K. The maximum resistance is observed at 4.2 K. This behaviour is generally equivalent to the resistivity behaviour observed in metal added with magnetic impurities. As MWCNTs is metallic in nature and Fe is used as catalyst, hence the interaction between the magnetic impurities and conduction electron at low temperature gives rise to the increase in resistance after 12.6 K. The DC resistance value increases with increase of applied magnetic field. The magnetic field dependent magnetization shows an anisotropic behaviour which is convinced from the difference saturation magnetization value obtained due to application of magnetic field in parallel direction and perpendicular direction to the MWCNTs surface.

CONCLUSION

In conclusion Fe-catalyst based MWCNTs shows the anisotropic behaviour and temperature versus resistance shows the Kondo like resistive behaviour.

REFERENCES

1. Journal of Nano science and Nanotechnology, Vol.9, 1–7, 2009

ACKNOWLEDGMENTS

The author S.C.R. acknowledges to National Research Foundation (NRF), South Africa for financial support.

**Corresponding Author: Raysc@unisa.ac.za*

The Influence of Nanoclay Loading on the Thermal Stability, Flame Retardant and Mechanical Properties of Polyamide/Nanoclay Nanocomposites Prepared By Melt Processing

Shohel Siddique[1*], Kyari Yates[2] and James Njuguna[1*]

[1]*School of Engineering, Robert Gordon University, Riverside East, Garthdee Road, Aberdeen, AB10 7GJ United Kingdom*

[2]*School of Pharmacy and Life Sciences, Robert Gordon University, Aberdeen, AB10 7GJ, UK*

This review paper aims to provide better understanding of the catalysing effect of nanoclay during the combustion of polyamide 6 (PA6)/montmorillonite (MMT) clay nanocomposites. The catalytic behaviour of different flame retardant additives present in MMT such as, some mineral compounds, halogenated compounds, phosphorus-based flame retardants, nitrogen-based flame retardants, silicon-based flame retardants, and nanometric particles are discussed here which shows better thermal and mechanical properties. Each flame retardant additive uniquely influences phase reactions depending on its loading in MMT and its ability to form complex compounds associated with the PA6 matrix. However, the mechanisms of all these flame retardant additives can be classified into two groups: gas-phase-active and condensed-phase-active; which are discussed.

The flame/fire behaviour of polymeric nanocomposites is characterised by their ignitability, flame spread time, and heat release. This review article also highlights the three commonly used test methods for analysis of polymer nanocomposites flammability, that is: UL94 horizontal and vertical burning test, limiting oxygen index (LOI), and cone calorimeter.

References:

1. Leszczyńska A Njuguna J Pielichowski K Banerjee J R 2007 Polymer/montmorillonite nanocomposites with improved thermal properties: Part II. Thermal stability of montmorillonite nanocomposites based on different polymeric matrixes. Thermochimica Acta, Volume 454, Issue 1, Pages 1-22

2. Leszczyńska A Njuguna J Pielichowski K Banerjee J R 2007 Polymer/montmorillonite nanocomposites with improved thermal properties: Part I. Factors influencing thermal stability and mechanisms of thermal stability improvement. Thermochimica Acta, Volume 453, Issue 2, Pages 75-96

3. Dasari, A., J Njuguna, 2016. Functional and Physical Properties of Polymer Nanocomposites. John Wiley & Sons.

4. Zope IS, Dasari A, Guan F, Yu Z, 2016. Influence of metal ions on thermo-oxidative stability and combustion response of polyamide 6/clay nanocomposites. Polymer 2016;92:102-113

Corresponding Author: s.a.siddique@rgu.ac.uk, j.njuguna@rgu.ac.uk

Sustainable Bioplastics from Microbes and Waste

Christine Edwards * and Linda Lawton

Pharmacy and Life Sciences, Robert Gordon University, Garthdee Rd, Aberdeen, AB10 7GJ, United Kingdom

Plastics are ubiquitous in everyday life and offer increasing technological and medical advances to improve/extend quality of life. However, with current global production of 311 m tonnes per annum, and forecast increase to 1,124 m tonnes by 2050, reflecting an 8% to 20% of oil demand exceeding that used by the aviation industry. Use of fossil fuel as raw materials combined with the high energy demand for their production (accounting for 15% total carbon budget by 2050) is not sustainable.

Petrochemical based plastics are non-biodegradable resulting in severe global pollution (an estimated 10-20 million tonnes per annum entering the world's oceans) causing damage to marine ecosystems, associated industries and public health. Consequently, plastic pollutants will continue to accumulate from over 150 million tonnes in the oceans today, rising to potentially 250 million tonnes by 2025 with the suggestion that there will be a greater mass of plastic than fish in the sea by 2050, unless action is taken. In addition to the polymers themselves, most plastics contain additives such as the lead in PVC,posing further hazards to the environment and human health.

The combination of decreasing fossil fuel reserves, environmental pollution coupled to increase in demand for plastics has led to the need for a shift to exploiting bio-based, biodegradable plastics for long term sustainability, and protection of the environment.

A range of microbes produce monomers and polymers suitable for plastic production, but as a consequence of the high price of production, and the controversial use of food crops for this purpose, the current market share of bioplastics is limited to 0.2%. This paper presents strategies for exploiting microbes grown on waste substrates for production of polyhydroxalkanoates (PHAs), a group of polyesters produced mainly as storage compounds in bacteria where biosynthesis is triggered by nutrient limitation and stress.

*Corresponding Author: c.edwards@rgu.ac.uk

Synthesis and Application of Amine-Functionalized Silica-Carbon Hybrid Nanocomposites for the Removal of Cu(II) in Acidic Environments

A Etale[1*], N Tavengwa[2], H Tutu[2] and S Mhlanga[1]

[1]*Nanotechnology and Water Sustainability Research Unit, College of Engineering, Science and Technology, University of South Africa, Johannesburg, South Africa*
[2] *Molecular Sciences Institute, School of Chemistry, University of the Witwatersrand, Private Bag X3, WITS 2050, Johannesburg, South Africa*

A novel amine-functionalized inorganic-organic hybrid adsorbent was synthesised for the removal of Cu ions in acidic conditions such as those characterising acid mine drainage (AMD). Synthesis was via a three-step process involving coating of silica nanoparticles (NPs) with carbon, oxidation of the carbon layer and grafting of hexamine to the silica-carbon composites. Transmission electron micrographs revealed that the adsorbent comprised spherical particles in the nanometre range while spectroscopic analyses confirmed the presence of amine, carboxyl and hydroxyl groups. Nitrogen sorption isotherms revealed a considerable decrease in particle area as a result of carbonisation and hexamine grafting. 52% of Cu ions in solution were retained by the adsorbent at pH 3 in a reaction that achieved equilibrium in 45 minutes, and followed the pseudo-second-order kinetics. Metal removal increased with initial concentrations and isotherms were fitted by the Freundlich model which gave an adsorption capacity of 0.016 mmol g-1. Cu removal increased with pH although adsorption at pH 5 was higher than at pH 7 and 9 (62, 57 and 57% respectively). The adsorbent also selectively bound Cu from a multi-elemental solution indicating that it could be applied for the selective removal of Cu from AMD-contaminated waters.

**Corresponding Author: aetale@gmail.com*

Thermoplastic Starch/PVA Films Reinforced with Cellulose Nanofibers from Oil Palm Empty Fruit Bunches (OPEFBs)

Farah Fahma* and Sugiarto Sugiarto

Department of Agroindustrial Technology, Bogor Agricultural University, Bogor, 16680

Indonesia

Thermoplastic starch/PVA films were successfully prepared by reinforcing with cellulose nanofibers (CNF) from OPEFBs. The X-ray diffraction profiles of the films showed that the crystallinity of thermoplastic starch/PVA films influenced with increasing CNF content. The physical and mechanical properties changes indicate that the CNF was successfully dispersed into thermoplastic starch/PVA matrix and achieved strong filler-matrix interaction.

Corresponding Author: farah_fahma@yahoo.com

The Effect of Talc, Montmorillonite (MMT) and Wollastonite (WO) on Nanoparticle Release due to Mechanical Drilling from Polypropylene (PP) Composites

Kristof Starost[1*], Evelien Frijns[2], Jo Van Laer[2], Nadimul Faisal[1], Ainhoa Egizabal[3], Cristina Elizextea[3], Inge Nelissen[2] Maria Blazquez[4], James Njuguna[1*]

[1] *Centre for Advanced Engineering Materials, School of Engineering, Robert Gordon University, Aberdeen, AB10 7GJ, United Kingdom*
[2] *VITO NV, Boeratang 200, 2400 Mol, Belgium*
[3] *TECNALIA, Mikeletegi pasealekua, 2 E-20009, Donostia Spain*
[4] *INKOA SISTEMAS, SL. Ribera de Axpe 11, Edificio D1, Dpto 208. 48950, Bizkaia Spain*

The use of sillicate nanofillers as mechanical reinforcements in polymers is increasingly being well established throughout literature. This has generated an influx into various commercial industries such as the automotive industry. However, there is still an insufficient understanding on how these fillers effect the release of nanoparticles to evaluate and quantify the full risks associated to nanorelease and nanoparticle exposure. In this study, the effect on nanorelease due to drilling on Polypropylene (PP) reinforced with 20% Talc, 5% montmorillonite (MMT) and 5% wollastonite (WO) is investigated. With 5% WO, equivalent tensile properties with a 10 % weight reduction were obtained relative to the reference 20% Talc sample. The materials were fabricated through a twin screw extruder. The nanorelease studies were undertaken using the controlled drilling methodolgy for nanoparticle exposure assessment developed within the SIRENA life project. Measurements were taken using CPC, SMPS and DMS50 equipment for real-time characterization and measurements. The particle number concentration (of particles <100nm) and particle size distribution (4.87nm – 562.34nm) of the particles emitted during drilling were evaluated to investigate the effect of the silicate fillers on the particles released. The nano-filled samples exhibited a 33% decrease (MMT sample) or a 30% increase (WO sample) on the average particle number concentration released in comparison to the neat polypropylene sample. The size distribution data displayed a substantial percentage of the particles released from the PP, WO and MMT samples to be around 10nm, whereas the Talc sample appeared to emit larger particle diameters. No independent nanoparticles of the fillers were found in the microscopy (SEM) analysis on samples collected within the test chamber.

The work is part of EC project named Simulation of the release of nanomaterials from consumer products for environmental exposure assessment (SIRENA, Pr. No. LIFE 11 ENV/ES/596) and QualityNano (Grant Agreement No:INFRA-2010-262163).

**Corresponding Author: k.starost@rgu.ac.uk; J.njuguna@rgu.ac.uk*

Waste to Want: Polyamide nanocomposite using nanoclays nanofillers reclaimed from oil and drilling fluids and cuttings waste – Thermal properties

Urenna V. Adegbotolu[1*], Kyari Yates[1], Kerr Matthews[1], Krzysztof Pielichowski[2], Agnieszka Leszczynska[2], Thomsz Majak[2], James Njuguna[1]

ISchool of Engineering, Robert Gordon University, Aberdeen, AB10 7GJ, UK
2School of Pharmacy and Life Sciences, Robert Gordon University, Aberdeen, AB10 7GJ, UK
3Department of Chemistry and Technology of Polymers, Cracow University of Technology, ul. Warszawska 24, 31-155 Krakow, Poland

In the oil and gas industry oil based mud is often used due to high temperature and high pressure well drilling. However, after its use, the drilling mud becomes part of the waste generated and a large portion of it ends up in land fill. Some of these waste include, produced water, and used drilling fluid, drill cutting and slop. This paper focuses on a new innovative method of utilizing solid extracts including bentonite from oil and gas drilling wastes by separating the recoverable minerals, water and oil. The recovered minerals, are chemically processed, modified and next used as nanofiller reinforcement to develop advanced lightweight materials. In particular, two- and three-phased composites were prepared using nanofillers nano-silica (nano-SiO_2) and nano-clay and micro glass-spheres to reinforce polyamide (PA6) and its glass-fibre reinforced thermoplastic composites. The polyamide composites are manufactured using injection moulding process. In this paper we will present initial findings from the pilot study geared towards the drilling fluid waste recycling and re-use of extracted minerals as nanofillers.

References

1. Silva, F., Njuguna, J., et al (2013). The influence of multiscale fillers reinforcement into impact resistance and energy absorption properties of polyamide 6 and polypropylene nanocomposite structures. Materials & Design, 50, 244-252
2. Adegbotolu, U. V., Njuguna, J., et al. (2014). Waste to Want: Polymer nanocomposites using nanoclays extracted from Oil based drilling mud waste. In IOP Conference Series: Materials Science and Engineering (Vol. 64, No. 1, p. 012023). IOP Publishing.
3. Mouti, Z., Westwood, K., Kayvantash, K., & Njuguna, J. (2010). Low velocity impact behavior of glass filled fiber-reinforced thermoplastic engine components. Materials, 3(4), 2463-2473.

**Corresponding Author. u.v.ekeh@rgu.ac.uk; J.njuguna@rgu.ac.uk*

Designing of Hybrid Structured Glass Laminated Transparent Nano Composites through Vacuum Infusion Technique

Arindam Mukherji

SP Advanced Engineering Materials Ltd, Jalgon, 425001, India

Glass is the most commonly used transparent material. However, glass is not suitable in applications where low weight, high strength is required. The present invention comprises a method of making a Transparent Glass Laminated Nano composite product. The product contains a Bi-directionally oriented E-Glass Fabric an essentially bidirectional yarn woven fabrics is stretched Bi-directionally by specially fabricated steel frame associated with both co and counter rotating device. These fibers include glass fibrics/cloths or mixtures of any of these. The synthetic fiber may be any synthetic silica based oven waived bi-directional or Uni-directional fabrics. Engaged gear provided in the device develops uniform tension on fabric, in both direction. Nano particle dispersed resin to be used is formulated with their respective curing agents and extenders. The formulated resin contains 0.1-0.5% of Nano additives and the product composed from 5-10 % of Glass fabric, be¬tween 10 to 20 % of ordinary glass, and between 60 -80 % of the product is the Nano particles dispersed formulated resin, all measured by volume.

**Corresponding Author: drmukherji@gmail.com*

On the Mechanical Influence of Boehmite Nanoparticles on Reinforced Epoxies

Media Ghasem Zadeh Khorasani*, Dorothee Silbernagl and Heinz Sturm

Bundesanstalt für Materialforschung und -prüfung, Unter den Eichen 87, Berlin, 12205, Germany

Boehmite nanoparticles are in the focus of interest when there is a need to improve matrix dominated properties of fiber reinforced composites. Recently found is an increase of crack resistance, compressive strength and reduction of shrinkage due to boehmite nanoparticles. In order to understand the mechanism behind these enhancements more details concerning the micro- and nanoscopic contact mechanics are required. To get insight into the structure-property relationship at first place more investigations on mechanical properties of boehmite itself are necessary. However, information about mechanical properties of boehmite is rare and the experiment found is not well defined. In this study, the young's modulus of boehmite was measured for the first time by means of force-distance curve (FDC) mapping in the atomic force microscope (AFM). For this purpose three different preparations of Boehmite are used. A macroscopic crystal obtained from a mineral, a hydrothermal synthetized film on aluminum and commercial spray dried nanoparticles in different polymer matrices are chosen. The force distance curves obtained from all three mentioned samples were in a good agreement with each other. A calculation of the modulus of boehmite´s single crystal based on molecular dynamics finite element methods (MDFEM) leads, as expected, to a higher modulus. For the hydrothermal film repeated indentation on the same position shows plastic deformation, this vanishes after several probed FDC. This effect can be attributed to a deformation along the slip plane spanned by the (100) and (001) direction. Using boehmite nanoparticles in an epoxy matrix, where the orientation of the particles is random, such anisotropic modulus leads to a high variation in local stress distribution. Further investigations on fractured surfaces will try to achieve a deeper understanding of the effectiveness of such particles to distribute the crack propagation energy. This requires also a more realistic model of particles and polymer.

Corresponding Author: media.ghasem-zadeh-khorasani@bam.de

Feasibility of plasma treated clay in clay/polymer nanocomposites powders for use Laser Sintering (LS)

Alaa Almansoori[1], Ryan Seabright[1], C Majewski[2], and C Rodenburg[1]

[1]*Material Science and Engineering Department, University of Sheffield*
[2] *Mechanical Engineering Department, University of Sheffield*

The addition of small quantities of nano-clay to is known to improve mechanical properties of the resulting nano-composite. However, achieving a uniform dispersion and distribution of the clay within the base polymer can prove difficult.

A demonstration of the fabrication and characterization of plasma-treated organoclay/Nylon12 nanocomposite was carried out with the aim of achieving better dispersion of clay platelets on the Nylon12 particle surface. Oxygen-plasma etching was used to enhance the compatibility between clays and polymers to ensure a uniform clay dispersion in composite powders. A hot press was then used to process the composite powders into tensile test specimens.

Hot stage microscopy (HSM) was employed to optimize processing conditions. Morphological studies using Low Voltage Scanning Electron Microscopy (LV-SEM) were undertaken to characterize the fracture surfaces and clay dispersion in powders and final composite specimens.

Thermogravimetric analysis (TGA) testing performed on different clay loading samples indicated an enhancement of the thermal stability for both EC/N12 and NEC/N12 nanocomposites.

The influence of the clay ratio and the clay plasma treatment process on the mechanical properties of the nano-composite was studied by tensile testing. The composite fabricated from (3% EC/N12) powder showed a modest (10%) improvement in elastic modulus compared to the composite made from (3% NEC/N12) powder. Most notably however is that the variation between tests is strongly reduced when etch clay is used in the composite. We attribute this to a more uniform distribution and better dispersion of the plasma treated clay within polymer powders and ultimately the composite.

**Corresponding Author: ammalmansoori1@sheffield.ac.uk*

Development of Graphene-Filled Polymer Nanocomposites for Enhanced Thermal Conductivity

S. S. Akhtar[1*], A. Bin Ali[1], M. U. Siddique[1], A. F. M. Arif[1], Amir Al-Ahmad[2]

[1]*Department of Mechanical Engineering, King Fahd University of Petroleum and Minerals, Dhahran 31261, Saudi Arabia*
[2]*Center of Excellence in Renewable Energy, Research Institute, King Fahd University of Petroleum and Minerals, Dhahran 31261, Saudi Arabia*

The room-temperature thermal conductivity of carbon-based materials span an extraordinary large range. Recently graphene has attracted both academic and industrial interest because it can produce a significant improvement in properties even at low filler content. However, the potential use of graphene to enhance thermal conductivity is restricted by the large interfacial thermal resistance between the polymer and graphene boundaries. In the present paper, we report the effect of size, weight fraction and thermal interfacial resistance of graphene nanoplatelets (GnPs) on the thermal conductivity of polysulphone (PSU) composites. It is predicted that two factors which can greatly affect the thermal conductivity of graphene composites are interfacial thermal resistance and graphene platelet size. With 10 wt% GnPs having platelet thickness of 12 nm and the average lateral size of 3000 nm , the experimentally measured thermal conductivity of PSU composite reaches to a value of 1Wm-1 K-1, which is more than double the thermal conductivity of pure PSU. Morphological characterization of the composites is also studied using scanning electron microscope and X-Ray diffraction. An effective medium approximation is used to predict the thermal conductivity of GnPs filled PSU composites with interfacial thermal resistance. The goal of our in-house code is to predict the thermal conductivity of such polymer-based composites by taking into consideration the effect of thermal interfacial resistance and aspect ratio of the GnPs in PSU matrix. The comparisons between the experimental and predicted results show very good agreement. Numerical calculations of different sets of composites show very interesting predictions concerning the effects of the GnPs aspect ratio, weight fraction and the interfacial thermal resistance on the thermal conductivity of GnPs filled PSU composites.

**Corresponding Author: ssakhtar@kfupm.edu.s*

Nanotechnology Needs in Oil and Gas Industry Applications

Babs Oyeneyin

The Robert Gordon University, Riverside East, Garthdee Road, Aberdeen, AB10 7GJ, United Kingdom

The oil industry is stepping up its exploration and extending its activities into new terrains including the hostile extremely deepwater environments in order to reduce the expected gap between demand and supply of hydrocarbons in the next decade. The asset teams are being challenged to reduce cost and be more operationally efficient to guarantee the oil/gas flow assurance. Nanotechnology has been identified as one of the key technologies required to achieve these objectives.

In this presentation the potential for nanotechnology application across the ‘’supply chain’’ of the oil industry operations from exploration through to well construction and reservoir management/monitoring to production flow assurance will be showcased with example of key potentials and application areas.

The presentation will end with new nanotechnology R& D initiatives at RGU with opportunities for collaboration with other institutions.

**Corresponding Author: b.oyeneyin@rgu.ac.uk*

Dynamically Mechanical and Nano-impact (Fatigue) Analysis of Touch Screen Thin Films Deposited on Polyethylene Terephthalate Substrate

Nadimul Faisal[1*], Saurav Goel[2], Caoimhe Kelly[2] and Richard Fu[3]

[1]*School of Engineering, Robert Gordon University, Aberdeen, United Kingdom*
[2]*Queen's University, Belfast, United Kingdom*
[3] *University of Northumbria, United Kingdom*

Nano-scale touch screen thin film have not been thoroughly investigated in terms of dynamic impact analysis under various strain rates. This research is focused on two different thin films, Zinc Oxide (ZnO) film and Indium Tin Oxide (ITO) film, deposited on Polyethylene Terephthalate (PET) substrate for the standard touch screen panels. Dynamic Mechanical Analysis (DMA) was performed on the ZnO film coated PET substrates. Nano-impact (fatigue) testing was performed on ITO film coated PET substrates. Other analysis includes hardness and the elastic modulus measurements, atomic force microscopy (AFM), Fourier Transform Infrared Spectroscopy (FTIR) and the Scanning Electron Microscopy (SEM) of the film surface.

Ten delta of DMA is described as the ratio of loss modulus (viscous properties) and storage modulus (elastic properties) of the material and its peak against time identifies the glass transition temperature (Tg). Thus, in essence the Tg recognizes changes from glassy to rubber state of the material and for our sample ZnO film, Tg was found as 388.3 K. The DMA results also showed that the Ten delta curve for Tg increases monotonically in the viscoelastic state (before Tg) and decreases sharply in the rubber state (after Tg) until recrystallization of ZnO takes place. This led to an interpretation that enhanced ductility can be achieved by negating the strength of the material.

For the nano-impact testing using the ITO coated PET, the damage started with the crack initiation and propagation. The interpretation of the nano-impact results depended on the characteristics of the loading history. Under the nano-impact loading, the surface structure of ITO film suffered from several forms of failure damages that range from deformation to catastrophic failures. It is concluded that in such type of application, the films should have low residual stress to prevent deformation, good adhesive strength, durable and good resistance to wear.

**Corresponding Author:* n.h.faisal@rgu.ac.uk

Influence of Carbon Nanotubes Dispersion in the Processing and Performance Properties of Pre-Impregnated Materials for Space Applications

Susana P. Fernandes-Silva and Nuno Rocha

INEGI- Institute of Science and Innovation in Mechanical and Industrial Ingineering, Rua Dr. Roberto Frias 400, Porto, 4200-465, Portugal

Research on unidirectional prepregs doped with carbon nanotubes have gained a significant impact on carbon fibre reinforced polymer (CFRP) manufacturing, due to possible of providing them as important building block for multifunctional composites manufacturing. One of the most relevant potential applications of such materials is for Spacecraft structures. In Space applications, CFRP materials brought important advantages in the replacement of metallic structures, such as lightweight, excellent mechanical performance and corrosion resistance. Nevertheless, the use of CFRP as substitutes of aluminium are still limited, mainly due to their low electrical and thermal dissipative properties in the through-thickness direction. When subjected to Space environments, the surface of these materials is constantly bombarded by electrical (electron flux, vacuum, magnetic fields etc) and thermal (solar radiation and heat generated by electronics) hazards, which results in charges accumulations on both the surface and inside the material and/or temperature gradients. These hazards are likely to promote the failure or even damage the CFRP structure. Taking the previous statement into account, research in multifunctional composites with superior electrical and thermal becomes attractive for Space applications.

This research work was focused in the development of a production method of Space relevant pre-impregnated materials through dip solution approach, where the carbon fibre tow (from intermediate to ultra-high modulus) is immersed in a solventless epoxy resin bath. Processing parameters were optimised and related with relevant characteristics of Space qualified materials (high stiffness carbon fibres and high viscosity resin system).

To improve electrical and thermal behaviours, multiwalled carbon nanotubes (MWCNT) with different functionalisations were incorporated in the epoxy resin. The pre-impregnation processing characteristics and parameters of the different modified resin samples with different types of carbon fibres were discussed. The results showed that the resin viscosity is highly dependent on the MWCNT functionalization, consequently affecting the carbon fibre wettability and processing.

**Corresponding Author: ssilva@inegi.up.pt*

Biocomposites and their Applications

Kalia Susheel*

Department of Chemistry, Army Cadet College Wing, Indian Military Academy, Dehradun, 248007, India

Natural fiber-reinforced biocomposites have received much attention because of many properties such as low cost, low density, nonabrasive, combustible, nontoxic, and biodegradation. The lack of good interfacial adhesion between fibers and matrix, low melting point, and water sensitivity make the use of natural fiber-reinforced composites less attractive. Surface modification of natural fibers can improve the surface roughness and moisture resistance and the compatibility between hydrophilic natural fibers and hydrophobic polymer matrices. There are many chemical treatments which can alter the wettability of natural fibers but the appropriate handling and disposal of the large amounts of hazardous chemicals that is often involved is unattractive and results in an additional cost to the production. Surface modification of natural fibers by alternative green methods to increase the compatibility between natural fibers and polymer matrices may outshine the chemical treatments for effective industrial applications. Biografting of natural organic molecules on natural fibers is one of the best environmentally friendly methods. Applications of such green composite materials include biomedical applications, structural applications, consumer products, food packaging, transportation, and textile, sports & leisure industry.

*Corresponding Author: susheel.kalia@gmail.com

The Wheat Grain as a Cemented Granular Material: Nanoscale Investigation of its Mechanical Properties

Karsta Heinze[1*], Jean-Yves Delenne[2], Matthieu George[1] and Valérie Lullien-Pellerin[2]

[1]*Laboratoire Charles Coulomb, UMR5221 CNRS/UM (L2C), Place Pierre Viala, Montpellier, France*

[2]*IATE, CIRAD, INRA, Montpellier SupAgro, Université de Montpellier, 34060, Montpellier, France*

The wheat grain is a natural composite material of worldwide importance for human nutrition. The major part of the grain is the endosperm, which contains starch in form of granules, surrounded by a protein matrix. In order to obtain food products such as flour, the wheat grains must be milled under high forces to disintegrate this compact structure. The quantity and quality of the milling products depend highly on the fragmentation behavior of the endosperm. Specifically, the nanoscale properties of the starch and protein components, and their interaction determine the fracture pathways inside the endosperm.

We apply a multiscale experimental and modeling approach to investigate the nanomechanical properties of the composing polymers and the way they influence grain fragmentation. The nanomechanical properties are analyzed directly inside sliced grains with two atomic force microscopy (AFM) methods. An AFM abrasion assay is used to target the distinct biopolymers starch and gluten inside the grain and study their abrasive hardness. Complementary to this, an AFM contact resonance setup is applied to acquire maps of the local mechanical properties of a representative view of the composite structure.

Understanding the nanomechanical properties of these different components and their interaction is crucial to explain the grain milling behavior. We aim to link the observed nanomechanics of specific grain samples to their milling behavior, which was determined with a laboratory mill. Finally, numerical simulation of the fragmentation of a representative element volume will be employed to connect the nanoscale and macroscale mechanical properties.

**Corresponding Author: kmheinze@univ-montp2.fr*

Routes to Graphene Based Gas Sensors

Ha-Duong Ngo and Asaf Avnon

Fraunhofer IZm, Berlin, 12459, Germany

Graphene owns a selection of properties making it an obvious candidate for nanoelectromechanical systems (NEMS). The outstanding mechanical properties of graphene comprising high stiffness, low mass and high strength bring about to high resonant frequencies. This provides the possibility of frequency strain tuning through high-sensitivity mass detection. Here, we explore a possible pathway to utilize those outstanding properties into building an ultra-sensitive sensor.

**Corresponding Author: Asaf.Avnon@izm.fraunhofer.de, Ha-Duong.Ngo@izm.fraunhofer.de*

Influence of Pectins and Xyloglucan On Structure of Bacterial Cellulose Membranes

Monika Szymańska-Chargot*, Monika Chylińska, Justyna Cybulska, Piotr M. Pieczywek and Artur Zdunek
Institute of Agrophysics Polish Academy of Sciences, Lublin, Poland

Cellulose itself is the most abundant natural polymer. Cell wall of every plant on Earth is made from polysaccharide composite with cellulose as a scaffold. This polymer has unique properties: high mechanical strength and relatively low density. Tensile strength of cellulose fibril is 7.7 GPa which is two times higher than that of steel wire or Kevlar fibre. For nanocomposite technologies to processed forms of native cellulose are used: microfibrilated cellulose, cellulose nanocrystals or nanocellulose. Furthermore, currently, cellulose I, the native crystalline morphotype of cellulose, is receiving an increased attention due to its potential use in bioenergy.

Cellulose microfibrils are heterogeneous. A schematic model of cellulose microfibrils involves a high crystalline core surrounded by less crystalline region and interrupted by amorphous form of cellulose. Physicochemical behaviour, i.e.: accessibility for chemical derivatization, swelling and water binding and also mechanical properties of cell wall, which directly influence textural properties of plant tissue depends on degree of cellulose crystallinity. Whereas, bacterial cellulose (BC) which are produced by some bacteria as biofilm and therefore its properties are different then the plant one. BC microfibrils achieve microns in length, have a large aspect ratio with a morphology depending on the specific bacteria and culturing conditions.

Nanocomposites of bacterial cellulose produced by Acetobacter xylinus are consider to mimic cellulose composites to be found in natural plant cell walls. A model materials composed of bacterial cellulose cultured in medium with addition apple pectin and tamarind xyloglucan were used. The aim of investigations was to determine the influence of various concentration of non-cellulosic polysaccharides (pectins and xyloglucan) on cellulose microfibrils structure and arrangement. The cellulose structure, microfibrils diameters and mechanical properties of bacterial cellulose membranes was obtained.

Acknowledgements

This work was partially funded by The National Centre for Research and Development - Poland (grant no. LIDER/300/L-6/NCBR/2015)

**Corresponding Author: m.szymanska@ipan.lublin.pl*

Prototype Development of the Vibro-Impact Capsule Robot for Pipeline Inspection

Yang Liu

The Robert Gordon University, Riverside East, Garthdee Road, Aberdeen, AB10 7GJ, United Kingdom

This paper introduces a current research project being carried out in the Robert Gordon University for developing the prototype of a vibro-impact capsule robot for pipeline inspection. The project aims to address the technical bottlenecks encountered by current pipeline technologies with a particular focus on oil and gas industry. In order to verify this concept, a dummy capsule prototype driven by internal vibro-impact forces with a diameter of 80 mm was designed for testing in a 2.5 meter long section of 140 mm nominal diameter clear PVCu pipe with a flow velocity 0.4 m/s. CFD analysis was conducted for optimizing geometric parameters of the capsule shape in order to minimize the resistance forces from fluid. By using the experimental rig, the capsule prototype was tested for various flow rates, and the experimental results were compared with CFD simulations.

**Corresponding Author: y.liu8@rgu.ac.uk*

Flexural Strengthening of Reinforced Concrete Deep Beams Using Carbon Fiber Polymers

Aya Al-Asi, Mu'Tasim Aabdel-Jaber* and Maha Alqam

The University of Jordan, Amman, Jordan

This work studies the flexural strengthening of reinforced concrete deep beams using two types of externally bonded Carbon Fiber-Reinforced Polymer (CFRP) composites. To achieve the best strengthening scheme, ten reinforced concrete deep beams were casted of 400×190 mm cross section with 1,900 mm length. Beams were separated into four strengthened groups in addition to a control beams group. Two groups were strengthened using laminates CFRP with two different schemes and the other two groups were strengthened using wrap CFRP, also, with two different schemes. Each beam was subjected to two loading points until failure. Tests results showed that using carbon fiber reinforced polymers enhanced the ductility, delayed the appearance of flexure and shear cracks and increased the ultimate load for all schemes at different percentages. It was found that the best strengthening scheme was the double layer sheet; it achieved 51% increase in the ultimate load compared with the control beams group.

*Corresponding Author: mutasim100@hotmail.com

Nanostructure of the Polymer-Graphene Composites

J.Janicki[1]*, R.Fryczkowski[1], M.Gorczowska[1], M.Baczek[1], Cz. Slusarczyk[1]

[1]*University of Bielsko-Biala, Institute of Textile Engineering and Polymer Materials, Willowa 2, 43-309 Bielsko-Biala, Poland*

PVDF and PET is a polymer of high chemical resistance, good mechanical strength, and additionally is easy in processing. Its properties prefer it to be used in technical solutions where you need a long-term chemical and thermal resistance for outdoor conditions. Graphene is a planar sheet of sp 2-bonded carbon atoms in a hexagonal network. It can be considered as the final member of the series of fused polycyclic aromatic hydrocarbons, such as naphthalene and anthracene. There are many publications that describe the testing of composites in which graphene is used as an additive to polymers to improve their properties. These results indicate that using the graphene may increase the mechanical strength of the composite, the thermal and electrical conductivity. The combination of the properties of PVDF and PET and graphene suggests that the resulting composite will be a new material for technical applications. In the literature there are no reports on the receiving polymer-graphene fiber nanocomposite. Mixtures prepared by their own patent. In the process of thermoforming there were obtained fibers with very interesting properties containing graphene. This paper will present the results of nanocomposites determining by SEM, structural studies WAXS and SAXS, and DSC thermal analysis.

**Corresponding Author: jjanicki@ath.bielsko.pl*

Interpretation of the Effect of Ablative Environment on the Ablation Resistance of C/P Composites

Jamal Zamani[1*] and M. R. Ashani[2]

[1]*K.N. Toosi university of Technology, Tehran, Iran*
[2]*Tehran University, Tehran, Iran*

This paper presents an extensive study of the ablation properties and thermal stability of four groups of carbon fiber/phenolic resin composites (C/P) composed of different material, such as p-toluene Sulfonic acid (PTSA) and polyvinyl Butyral resin (PVB). In order to investigate the effect of various ablative environment on the ablation properties of the C/P composites, the ablation tests were performed with both plasma and oxyacetorchtylene torch.

The ablation test results reveal that the use of polyvinyl Butyral resin in the C/P composites (C/P/PVB) has improved the ablation resistance and the erosion rate (mm/s) of these specimens is 15% and 22% lower than the other specimens in both plasma and oxyacetylene. Also it was finded that, because of the presence of oxidation agent in oxyacetylene ablative invironment, oxygne, we had 15% increase in the erosion rate of C/P composites. From comparison of these two different ablation test method, this could be find that the mass reduction of composites has increased with changing the torch from plasma to oxyacetylene respectively, except in C/P/PVB samples.

**Corresponding Author: zamani@kntu.ac.ir*

Shear Strengthening of Reinforced Concrete Deep Beams Using Carbon Fiber-Reinforced Polymer Composite

Hana Al-Ghanim, Maha Alqam and Mu'Tasim Aabdel-Jaber*

The University of Jordan, Amman, Jordan

This experimental investigation deals with shear strengthening of reinforced concrete deep beams using the externally bonded Carbon Fiber-Reinforced Polymer (CFRP) composites. The current study; therefore, evaluates the effectiveness of four various configurations of shear strengthening with two different types of CFRP materials including sheets and laminates. For this purpose, a total of 10 specimens of deep beams were cast and tested. The shear performance of the strengthened beams is assessed regarding the cracks' formation, modes of failure, ultimate strength and the overall stiffness. The obtained results demonstrate the effectiveness of using the CFRP technique on enhancing the shear capacity of deep beams; however, the efficiency varies depending on the material used and the strengthening scheme adopted. Among the four investigated schemes, the highest increase in the ultimate strength is recorded by using the continuous wrap of two layers of CFRP sheets, exceeding a value of 86%, whereas an enhancement of 36% is achieved by the inclined CFRP laminates.

Corresponding Author: mutasim100@hotmail.com

Computational Study of Nanostructured Composite Materials for Photonic Crystal Fibre Sensors

Jincy Johny, Wai Keung Fung and Radhakrishna Prabhu*

[1]*Robert Gordon University, School of Engineering, The Sir Ian Wood Building, Garthdee Road, Aberdeen, AB10 7GJ, United Kingdom*

Photonic Crystal Fibres (PCFs) are gaining popularity in recent years, owing to their specialized geometrical structure (core-air hole cladding) and unique properties, which include their guiding mechanisms and modal characteristics. The inherent capabilities of PCFs can be exploited for different applications such as sensing, optical communication, etc. Propagation and guiding characteristics of PCFs can be tuned by altering various structural parameters like air hole size, shape, position, etc.

Nanostructured materials will provide special optical properties which can revolutionise current optical sensing technologies. Nanostructuring of PCF air holes is expected to reduce the fibre confinement losses and also improve its effective mode area. Furthermore, addition of composite materials (liquid crystal and glass) on to the cladding holes manipulates PCF transmission and polarization properties, enabling them to operate within the photonic bands having highest sensitivities. The higher wavelengths of the optical spectrum are of particular interest for fibre-optic sensing applications due to their improved sensitivity and accuracy compared to other spectral regimes. Hence, there arises a need to closely investigate the effect of nanostructuring of composite materials on various parameters of the PCF sensor.

Simulations were conducted on a hexagonal PCF designed using COMSOL MULTIPHYSICS 5.1. The simulations helped in analysing the effect of different liquid crystal materials on PCF parameters such as effective area, spectral width, etc. Altering refractive index of liquid crystal material filled into the cladding holes of PCF resulted in shifting and broadening of the photonic bandgap. Further study carried out by changing the size (nano size), shape (circular, elliptical) and distribution of the PCF holes also resulted in a shift in photonic bandgap, accompanied with a reduction in confinement losses. Hence, through the simulations it was identified that the spectral positions and photonic bandgaps can be tuned by nanostructuring the PCF holes and changing its material infiltrations.

**Corresponding Author: r.prabhu@rgu.ac.uk*

The Estimation of Quantitative Parameters of Oligonucleotides Immobilization on Mica Surface

T. I. Sharipov* and R. Z. Bakhtizin

Department of Physical Electronics and Nanophysics, Bashkir State University, Ufa, Russia

Immobilization of nucleic acids on the surface of various materials is increasingly being used in research and some practical applications. Currently, the DNA chips technology is rapidly developing. To create DNA chips a major component is attachment the DNA or DNA fragments - oligonucleotides - on the surface. The basis of the immobilization process can be both physical adsorption and chemisorption. A useful way to control the immobilization of nucleic acids on a surface is to use atomic force microscopy (AFM). It allows you to investigate the topography of the surface by its direct imaging with high resolution. Typically, to fix the DNA on the surface of mica are used polyvalent cations which mediate the interaction between the negatively charged mica surface and the DNA molecules. In our work we have developed a method for estimation of quantitative parameter of immobilization of oligonucleotides is their degree of aggregation depending on the fixation conditions on the surface of mica. The results on study of aggregation of oligonucleotides immobilized on mica surface will be presented. The single oligonucleotides molecules have been imaged clearly, whereas their surface areas have been calculated and calibration curve have been plotted.

*Corresponding Author: sha-T@yandex.ru

Synthesis of Polyurethane Nanocomposite Materials from Green Chemistry for the Removal of Contaminants in Water

Hilary Ezuruike* and Rui Krause

Department of chemistry, Rhodes University, Grahamstown, South Africa

Two different polymers, synthetic and natural that are hydrophobic and hydrophilic, respectively were chemically combined and enhanced by chain extender to form polyurethane composites. The purpose was to modify their respective properties and make them compatible for synergistic effect. The use of chain extender and acetone (as a precipitating solvent) was observed to have eliminated possible visible phase separation and enhanced miscibility. Though, the combination of hydrophilic and hydrophobic polymers to make them compatible and miscible has been reported to be difficult in many literatures.

The FT-IR spectra of the composites show that carbonyl stretching bands of the hydrophobic polylactide (PLA) component tend to be wider with declined intensities following an increase in hydrophilic chitosan (CH) content. It suffixes to point out that, there exist intermolecular hydrogen bondings or interactions between the functional groups of these two components of the composite which indicate miscibility. To further confirm the FT-IR results, DSC technique was used. SEM result agrees with the results established by the other techniques suggesting that there exists no macroscopic phase separation of the composite materials. However, nanoparticles with controlled particle sizes were prepared and added as fillers to form polyurethane nanocomposite materials. The nanoparticles inclusion provided the composites with stability and also serves as antimicrobials.

TEM images displayed the nanocomposite structure with dispersed nanomaterials embedded in the matrix.

The efficiency and effectiveness of the polyurethane nanocomposite was tested on the removal of model organic pollutants in drinking water.

Corresponding Author: g13e0002@campus.ru.ac.za

Preparation and characterization of epoxy-clay nanocomposite and its application as anticorrosive coating

Jenaro Leocadio Varela-Caselis[1*], José Alberto Galicia-Aguilar[2], Efraín Rubio-Rosas[1] and Marco Morales-Sanchez[2]

[1]*Centro Universitario de Vinculación/Benemérita Universidad Autónoma de Puebla, Mexico*

[2]*Facultad de Ingeniería Química/Benemérita Universidad Autónoma de Puebla, Mexico*

Epoxy-clay nanocomposites have become a very interesting topic among researchers because nanoclays have a positive effect on the mechanical, thermal and especially barrier anticorrosive performance of the polymers. In this study, an epoxy-clay nanocomposite was synthesized using a quaternary ammonium-modified montmorillonite clay and diglycidyl ether of bisphenol A (DGEBA) type epoxy resin, in order to produce anti-corrosive epoxy coating. The montmorillonite clay was added to epoxy resin at loadings 0.5, 1, 3 and 5 wt%, and were dispersed using forced agitation-sonication, after that, the mixture was deposited on cold rolled carbon steel coupons and cured. The nanocomposite coatings obtained have been characterized by scanning electron microscopy (SEM), spectroscopy Fourier transform infrared (FTIR), X-ray diffraction (XRD), thermogravimetric/scanning calorimetry analysis (TGA/DSC). Anticorrosive-properties of the nanocomposite were evaluated using electrochemical impedance spectroscopic (EIS) methods.The X-ray analysis showed that exfoliation occurred for the MMT in the polymer matrix, the SEM analysis showed that MMT was homogenous dispersed in the polymer matrix and the coatings were uniform. The FTIR analysis showed the characteristic bands of epoxy resin and MMT in the composite. The time course of impedance parameters studies show that coating corrosion resistance is improved as the amounts of montmorillonite are increased to 5 wt%. The best performance of this coating was achieved at 3 and 5 wt% clay concentration.

**Corresponding Author: genaro.varela@correo.buap.mx*

Thermal, Mechanical and Crystallization Behaviour of Nanostructured Banana Fiber-filled Poly (ε-caprolactone)/Chitosan Biocomposites

Ephraim Vunain* and Ajay Mishra

Nanotechnology and Water sustainability Research Unit, University of South Africa, Johannesburg, South Africa

The development of new materials for different applications especially biodegradable composites have received a lot of attention in recent years. In this study, composites based on ε-caprolactone (PCL)/chitosan (CT) and banana fiber (Musa species) were prepared using the melt mixing technique and characterized. The mechanical, thermal and crystallization behaviour of the banana fiber-filled ε-caprolactone/chitosan-based nanocomposites were studied. Scanning electron microscopy (SEM) and X-ray diffraction analysis were used to characterize the biofiller particles and synthesized composites. Proper dispersion of the biofiller leads to an improvement in properties of the nanocomposites such as better thermal properties, higher tensile modulus and increased crystallization rate. Synthesized biocomposites could be used in a range of applications.

*Corresponding Author: evunain@gmail.com

Conductive Diamond Powder – SiO_2 Nanotubes Composite, A Promising Platinum Support for Methanol Fuel Cell Applications

Nicolae Spataru*, Crina Anastasescu, Tanta Spataru, Petre Osiceanu and Cornel Munteanu

Institute of Physical Chemistry of the Romanian Academy, Bucharest, Romania

Despite the tremendous amount of research work channeled so far towards finding active, noble metal-free, electrocatalytic materials, it appears that platinum still remains the main choice for high efficiency direct methanol fuel cell applications. Finding ways to minimize noble metal loading, while upholding high catalytic activity, would make conspicuous contribution to the foretold major upswing in the utilization of such energy-conversion systems. The most straightforward approach seems to be the deposition of electrocatalyst particles on a plethora of support materials, among which various forms of carbon (including glassy carbon, graphite, nanotubes, microspheres, and conductive diamond) are a natural choice.

A strategy that could allow obtaining stable, high surface area electrode materials was initiated by the observation that sol-gel chemistry provides a simple way to embed various electrochemically active species in a robust silica matrix. The lack of intrinsic electron conductivity of the SiO2 network could be compensated by the dispersion into the bulk of the material of different types of carbonaceous structures. By appropriately adjusting the obtaining conditions it is possible, at least in principle, to control oxygen stoichiometry in order to create on the SiO2 particles surface semiconducting nanodomains. From this perspective, the use of silica nanotubes appears to be particularly auspicious because structural deformations necessary to achieve their characteristic shape induce significant lattice stress, leading to the formation of a non-negligible number of defects with beneficial effects on the surface conductivity.

With an eye to fuel cell applications, the present work was aimed at scrutinizing the potential assets as support for platinum particles of a composite obtained by embedding conductive boron-doped diamond powder (BDDP) into a SiO2 nanotubes (SiO2NT) matrix. To assess the attractiveness of such materials from a more practical point of view, methanol and carbon monoxide anodic anodic oxidation in acidic media were used as test-reactions.

Corresponding Author: nspataru@icf.ro

Influence of Pectins and Xyloglucan on Structure of Bacterial Cellulose Membranes

Monika Szymańska-Chargot*, Monika Chylińska, Justyna Cybulska, Piotr M. Pieczywek and Artur Zdunek

Institute of Agrophysics Polish Academy of Science, Lublin, Poland

Cellulose itself is the most abundant natural polymer. Cell wall of every plant on Earth is made from polysaccharide composite with cellulose as a scaffold. This polymer has unique properties: high mechanical strength and relatively low density. Tensile strength of cellulose fibril is 7.7 GPa which is two times higher than that of steel wire or Kevlar fibre. For nanocomposite technologies to processed forms of native cellulose are used: microfibrilated cellulose, cellulose nanocrystals or nanocellulose. Furthermore, currently, cellulose I, the native crystalline morphotype of cellulose, is receiving an increased attention due to its potential use in bioenergy.

Cellulose microfibrils are heterogeneous. A schematic model of cellulose microfibrils involves a high crystalline core surrounded by less crystalline region and interrupted by amorphous form of cellulose. Physicochemical behaviour, i.e.: accessibility for chemical derivatization, swelling and water binding and also mechanical properties of cell wall, which directly influence textural properties of plant tissue depends on degree of cellulose crystallinity. Whereas, bacterial cellulose (BC) which are produced by some bacteria as biofilm and therefore its properties are different then the plant one. BC microfibrils achieve microns in length, have a large aspect ratio with a morphology depending on the specific bacteria and culturing conditions.

Nanocomposites of bacterial cellulose produced by Acetobacter xylinus are consider to mimic cellulose composites to be found in natural plant cell walls. A model materials composed of bacterial cellulose cultured in medium with addition apple pectin and tamarind xyloglucan were used. The aim of investigations was to determine the influence of various concentration of non-cellulosic polysaccharides (pectins and xyloglucan) on cellulose microfibrils structure and arrangement. The cellulose structure, microfibrils diameters and mechanical properties of bacterial cellulose membranes was obtained.

Acknowledgements

This work was partially funded by The National Centre for Research and Development - Poland (grant no. LIDER/300/L-6/NCBR/2015).

**Corresponding Author: m.szymanska@ipan.lublin.pl*

Interpretation of the Effect of Ablative Environment on the Ablation Resistance of C/P Composites

Jamal Zamani[1*] and M. R. Ashani[2]

[1]*K.N.Toosi University of Technology, Iran*

[2]*Tehran University, Iran*

This paper presents an extensive study of the ablation properties and thermal stability of four groups of carbon fiber/phenolic resin composites (C/P) composed of different material, such as p-toluene Sulfonic acid (PTSA) and polyvinyl Butyral resin (PVB). In order to investigate the effect of various ablative environment on the ablation properties of the C/P composites, the ablation tests were performed with both plasma and oxyacetorchtylene torch.

The ablation test results reveal that the use of polyvinyl Butyral resin in the C/P composites (C/P/PVB) has improved the ablation resistance and the erosion rate (mm/s) of these specimens is 15% and 22% lower than the other specimens in both plasma and oxyacetylene. Also it was finded that, because of the presence of oxidation agent in oxyacetylene ablative invironment, oxygne, we had 15% increase in the erosion rate of C/P composites. From comparison of these two different ablation test method, this could be find that the mass reduction of composites has increased with changing the torch from plasma to oxyacetylene respectively, except in C/P/PVB samples.

**Corresponding Author: zamani@kntu.ac.ir*

Synthesis and Characterization of Polyurethane/Bentonite Nanoclay Based Nanocomposites Using Different Diisocyanates: Relation between Mechanical and Thermal Properties

Javier Quagliano*, Javier Bocchio and Víctor Wittemberg

CITEDEF, Buenos Aires, Argentina

Polyurethanes (PUs) and polyurethane nanocomposites (PUNC) with bentonite nanoclay were prepared by the reaction of toluene-2,4-diisocyanate (TDI), dimeryl diisocyanate (DDI) and isophorone diisocyanate (IPDI) with two different polymers: hydroxyl terminated polybutadiene (HTPB) and polytetramethylene ether glycol (PTMEG), and the chains were further extended with 1,4-butanediol (1,4-BDO) to get final PUs and PUNCs. PUNCs were prepared by dispersing within the polymers a commercial and a synthesized bentonite nanoclay by mechanical dispersion. Mechanical properties showed that the addition of a small amount of nanoclay (1%) resulted in a significant increase in tensile strength and consequent reduction in elongation at break (maximum increase of 2.3 and 5-times reduction, respectively, for a HTPB-TDI-BDO based PUNCs). Thermal analysis revealed that the addition of nanoclays improved the thermal stability and increased decomposition temperature of PUNCs around 10°C. We concluded that there is a positive correlation between mechanical and thermal properties as a result of nanoclay addition.

Corresponding Author: jquagliano@citedef.gob.ar

The Use of SERS Markers for Fuel Identification

Dmitry Kopitsyn*, Mikhail Kotelev, Maksim Gorbachevskyy, Ivan Tiunov, Vladimir Vinokurov and Andrei Novikov

Federal State Budgetary Educational Institution of Higher Education «Gubkin Russian State University of Oil and Gas (National Research University) », Russia

Identification of gasoline and diesel fuels is an actual task to prevent illegal acts involving smuggling, forgery, fuel theft, establish liability for environmental disasters, etc. Existing chemical methods of fuel analysis require complex sample preparation, usage of expensive equipment and skilled staff to perform analysis. A promising approach is the use of markers which are added to the fuel at low concentrations for its identification. The concentration of the markers in the fuel must be minimized to eliminate the influence on the consumer properties of fuels. At the same time, it requires a sensitive method of marker detection, which would be able to distinguish different markers. Analytical technique used for this purpose should be able to detect and identify trace levels of markers. All these requirements are met by the SERS method utilizing the solid or colloidal plasmonic substrates. We have investigated the possibility of identifying compounds in fuels such as pyridine, 2-methylimidazole and monomethylaniline in the range of concentration from 1% to 10 ppm. Until recently monomethylaniline was widely applied in Russia as an octane booster. Currently its use is prohibited by Euro 5 standard, therefore, its presence in fuels indicates forgery. For signal detection we used different suspensions of gold nanoparticles and portable Raman spectrometer. We found that markers at levels as small as 10 ppm can be detected and differentiated. Although the proposed markers contain nitrogen atoms, their presence in fuel is not critical because of their low concentration. The advantages of the method also include high-throughput sample preparation and analysis, and the ability to use the cheap portable automated equipment.

*Corresponding Author: kopicin.d@inbox.ru

Measuring Mechanical Double Layers: Comparison of Static (FDC) and Dynamic (ADFS) AFM Methods

Dorothee Silbernagl* and Heinz Sturm

BAM, Berlin, Germany

The ability to map mechanical properties on the submicron scale is crucial for understanding and optimizing composite materials. AFM Force Distance Curves (FDC), a quasi-static method (1 Hz), is a well-established much relied on method for mapping the stiffness of material phases and interphases with a probed volume of the order of 10-12 m3. The common trend has been that the size of phases in composite materials decrease continuously (Nanocomposites). In order to map the mechanical properties of such composites phases and interphases a volume in the range of 10-20 m3 needs to be resolved. For this purpose, dynamic AFM methods have been further developed, such as Amplitude Dependent Force Spectroscopy (ADFS), which has an increased resolution, but applies a theory in order to produce Force-Deformation curves. In order to prove ADFS as a method we have shown the equality of the two methods, FDC and ADFS, by measuring a mechanical double layer with a film thickness distribution (thin polymer film ranging from 0 to 15 nm thickness on a stiff glass substrate) with both methods. This experimental setup was carefully designed to meet the following requirements: first an adequate number of datapoints could be gathered with both methods yielding a similar distribution of film thickness; second a distribution of stiffness could be measured and compared, since a film thickness range correlates with an average stiffness; and most importantly the Force-Deformation Curves show the typical behaviour measuring a composite, which is a different deformation-rate at a specific applied Force, since the substrate contributes more at higher forces. With this feature the curves cannot be transformed into each other by mere scaling, how it would be the case for Force-Deformation curves taken on homogeneous materials and therefore yield a reliable comparison of both methods.

Corresponding Author: dorothee.silbernagl@bam.de

Colorimetric glucose assay based on magnetic particles having pseudo peroxidase-like activity and covered with glucose oxidase

Pavla Martinkova* and Miroslav Pohanka

University of Defense, Hradec Kralove, Czech Republic

Glucose is an essential substrate for many biochemical pathways and necessary for organs functioning. Beside basic physiological function, increased or decreased glucose blood level out of physiological range is important marker for diagnosis of many pathological states and disorders like diabetes mellitus, metabolic syndrome, immune disorders, long-lasting stress or poisoning. Recently, materials with pseudo-enzymatic catalytic activity replacing instable recognition molecules of biological origin have been gaining more attention in construction of novel biosensors, analytical and diagnostic methods. Magnetic particles (MPs) belong to one of these materials with advanced parameters including chemical and thermal stability unlike enzymes themselves. Standard glucose colorimetric assay is based on two reactions catalyzed by enzymes glucose oxidase and peroxidase. Just peroxidase is known as very instable enzyme, hence, in this point of view, our research was focused on invention and optimization of simply and fast method where peroxidase is replaced by MPs with pseudo-peroxidase activity. MPs also serve as carrier of glucose oxidase which is immobilized onto their surface. Spectrophotometric determination of glucose was performed in 96-multiwell plates at wavelength 450 nm and concentration curve replying Michaelis-Menten equation with correlation coefficient 0.996 was achieved. The Michaelis-Menten constant, maximum reaction rate and limit of detection was set to be 0.13 mmol/l, 1.79 pkat and 3.74 µmol/l respectively. Interferences of other sugars such as sucrose, sorbitol, deoxyribose, maltose and fructose as well as effect of substances typical for plasma (ascorbic acid, reduced glutathione, trolox and urea) was assessed and no interference in the assay was revealed when the results compared with positive and negative controls. The presented assay showed corresponding results with reference method with linear dependence and correlation coefficient 0.997. Possibility of repeated used of modified MPs, decreasing of used chemicals and no need to apply peroxidase can be mentioned as advantages over the standard method.

Corresponding Author: pavlamartinkova@seznam.cz

The Influence of Nanoclay Loading on the Thermal Stability, Flame Retardant and Mechanical Properties of Polyamide/Nanoclay Nanocomposites Prepared By Melt Processing

Shohel Siddique[1*], Kyari Yates[2] and James Njuguna[1*]

[1]*School of Engineering, Robert Gordon University, Riverside East, Garthdee Road, Aberdeen, AB10 7GJ United Kingdom*

[2]*School of Pharmacy and Life Sciences, Robert Gordon University, Aberdeen, AB10 7GJ, UK*

This review paper aims to provide better understanding of the catalysing effect of nanoclay during the combustion of polyamide 6 (PA6)/montmorillonite (MMT) clay nanocomposites. The catalytic behaviour of different flame retardant additives present in MMT such as, some mineral compounds, halogenated compounds, phosphorus-based flame retardants, nitrogen-based flame retardants, silicon-based flame retardants, and nanometric particles are discussed here which shows better thermal and mechanical properties. Each flame retardant additive uniquely influences phase reactions depending on its loading in MMT and its ability to form complex compounds associated with the PA6 matrix. However, the mechanisms of all these flame retardant additives can be classified into two groups: gas-phase-active and condensed-phase-active; which are discussed.

The flame/fire behaviour of polymeric nanocomposites is characterised by their ignitability, flame spread time, and heat release. This review article also highlights the three commonly used test methods for analysis of polymer nanocomposites flammability, that is: UL94 horizontal and vertical burning test, limiting oxygen index (LOI), and cone calorimeter.

References:

1. Leszczyńska A Njuguna J Pielichowski K Banerjee J R 2007 Polymer/montmorillonite nanocomposites with improved thermal properties: Part II. Thermal stability of montmorillonite nanocomposites based on different polymeric matrixes. Thermochimica Acta, Volume 454, Issue 1, Pages 1-22

2. Leszczyńska A Njuguna J Pielichowski K Banerjee J R 2007 Polymer/montmorillonite nanocomposites with improved thermal properties: Part I. Factors influencing thermal stability and mechanisms of thermal stability improvement. Thermochimica Acta, Volume 453, Issue 2, Pages 75-96

3. Dasari, A., J Njuguna, 2016. Functional and Physical Properties of Polymer Nanocomposites. John Wiley & Sons.

4. Zope IS, Dasari A, Guan F, Yu Z, 2016. Influence of metal ions on thermo-oxidative stability and combustion response of polyamide 6/clay nanocomposites. Polymer 2016;92:102-113

Corresponding Author: s.a.siddique@rgu.ac.uk, j.njuguna@rgu.ac.uk

Screen-printed Sensor Used for Assay of Acetylcholinesterase Activity Immobilized on Magnetic Particles

Adam Kostelnik[1*], Miroslav Pohanka[1] and Alexander Cegan[2]

[1]*University of Defence, Faculty of Military Health Sciences, Hradec Králov, Czech Republic*

[2]*University of Pardubice, Faculty of Chemical Technology, Hradec Králové, Czech Republic*

Enzyme acetylcholinesterase (AChE) terminates action of neurotransmitter acetylcholine in cholinergic system. Activity of enzyme is commonly assayed by Ellman´s method having some drawbacks like daylight instability of Ellman´s reagent and inability to use enzyme from the mixture repeatedly. Hence, we developed process using N-(3-dimethylaminopropyl)-N'-ethylcarbodiimide hydrochloride to immobilize AChE on the surface of magnetic particles and we are capable use it repeatedly. The repeatability of measurement with magnetic particles with immobilized enzyme showed five cycles without activity change. To assay enzyme activity, we optimized square wave voltammetry method using N-acetyl-L-cysteine and a screen-printed sensor with carbon working electrode doped with Prussian blue was performed. Prussian blue was described to cathodic reduction of H2O2 but applications for thio group containing molecules were described as well. We examined reversible AChE inhibitor tacrine, as a model molecule, and we applied it in a concentration range from 10.00 to 18.75 µM. Limit of detection equal 8.1 µM was found. No further inhibition was observed above the maximal concentration of inhibitor. Interferences by organic solvents were determined using Tween-20, DMSO, isopropyl alcohol and ethanol were tested. We reported DMSO for interference in voltammogram due it is oxidation on electrode, Tween-20 for inhibition of AChE, isopropyl alcohol and ethanol did not show inhibition ability to AChE.

Aknowledgments: A long-term organization development plan 1011 (Faculty of Military Health Sciences, University of Defence, Czech Republic) is gratefully acknowledged..

**Corresponding Author: Kostelnik.Adam@seznam.cz*

Elaboration of Titania Nanotubes on Ti6Al4V Substrate by Electrochemical Anodization for Dental Application

Abdelghani Boucheham[1*], Ahcene Karaali[2] and Amar Manseri[1]

[1]*CRTSE, Algiers, Algeria*

[2]*Constantine 1 University, Algeria*

Nanostructured Titania layers formed on the surface of titanium and titanium alloys by anodic oxidation play an important role in the enhancement of their biocompatibility and osseointegration in the human body. In the current work, highly ordered titania nanotube array films were elaborated on Ti6Al4V medical grade alloys in organic electrolyte containing ethylene glycol, 0.2 wt. % NH4F and 4 vol. % H2O at an applied potential of 60V for different durations. The diameters, lengths and wall thicknesses of the obtained nanotubes were characterized by scanning electronic microscopy (SEM).

**Corresponding Author: aghani.boucheham@gmail.com*

Multi-scale Numerical Simulation and Experimental Validation of Elastic Properties of Laminate Composites Based Carbon NanoTubes

Ahmed El Moumen[1*], Mostapha Tarfaoui[1] and Khalid Lafdi[2]

[1]*ENSTA Bretagne, IRDL, Brest, France*

[2]*University of Dayton Research Institute, USA*

The principal objective of this investigation is the prediction of the elastic moduli of laminate composites containing a random distribution of carbon nanotubes (CNTs) using numerical and experimental approaches. Homogenization technique based on the representative volume element is used. To construct a representative model of composites, a set of microscope observation was considered to identify the periodicity of composites. These have been used to construct the representative volume element, on which the numerical homogenization was carried out. The effect of the distribution and the CNTs volume fractions were studied. The results of numerical homogenization were compared and validated with experimental data. Experimental characterization is based on the use of tension and shear tests to obtain the nine elastic moduli of laminate composites with and without CNTs reinforcement. We have also used the Flatwise tension and open hole tension tests. The analytical approach consists in using the homogenization models to estimate the elastic properties of the composite from the knowledge of their constituents. Finally, a comparison between different approaches, experimental, numerical and analytical, is planned.

**Corresponding Author: aelmoumen@gmail.com*

Dynamically Mechanical and Nano-Impact (Fatigue) Analysis of Touch Screen Thin Films Deposited on Polyethylene Terephthalate Substrate

Nadimul Faisal[1*], Saurav Goel[2], Caoimhe Kelly[2] and Richard Fu[3]

[1]*Robert Gordon University, Aberdeen, UK*

[2]*Queen's University, Belfast, UK*

[3]*University of Northumbria, Newcastle, UK*

Nano-scale touch screen thin film have not been thoroughly investigated in terms of dynamic impact analysis under various strain rates. This research is focused on two different thin films, Zinc Oxide (ZnO) film and Indium Tin Oxide (ITO) film, deposited on Polyethylene Terephthalate (PET) substrate for the standard touch screen panels. Dynamic Mechanical Analysis (DMA) was performed on the ZnO film coated PET substrates. Nano-impact (fatigue) testing was performed on ITO film coated PET substrates. Other analysis includes hardness and the elastic modulus measurements, atomic force microscopy (AFM), Fourier Transform Infrared Spectroscopy (FTIR) and the Scanning Electron Microscopy (SEM) of the film surface.

Ten delta of DMA is described as the ratio of loss modulus (viscous properties) and storage modulus (elastic properties) of the material and its peak against time identifies the glass transition temperature (Tg). Thus, in essence the Tg recognizes changes from glassy to rubber state of the material and for our sample ZnO film, Tg was found as 388.3 K. The DMA results also showed that the Ten delta curve for Tg increases monotonically in the viscoelastic state (before Tg) and decreases sharply in the rubber state (after Tg) until recrystallization of ZnO takes place. This led to an interpretation that enhanced ductility can be achieved by negating the strength of the material.

For the nano-impact testing using the ITO coated PET, the damage started with the crack initiation and propagation. The interpretation of the nano-impact results depended on the characteristics of the loading history. Under the nano-impact loading, the surface structure of ITO film suffered from several forms of failure damages that range from deformation to catastrophic failures. It is concluded that in such type of application, the films should have low residual stress to prevent deformation, good adhesive strength, durable and good resistance to wear.

**Corresponding Author: n.h.faisal@rgu.ac.uk*

Comprehensive Kinetic Analysis for the Reduction of 4-Nitrophenol Using Metal Nanoparticles

Reinout Meijboom* and Rapelang Patala

University of Johannesburg, Johannesburg, South Africa

The compound 4-Nitrophenol found in waste-water streams is mainly the result of industrial and agricultural production. Having adverse health effects associated with it, 4-nitrophenol should be removed from the environment or converted to less hazardous forms as efficiently as possible. Feasible techniques to get rid of this chemical compound are of great research interest. The synthesized nanoparticles encapsulated inside dendrimers (DENs) will be evaluated for catalytic activity against the reaction of 4-nitrophenol reduction. Transition-metal nanoparticles are of fundamental interest and technological importance because of their applications to catalysis. Synthetic routes to metal nanoparticles include evaporation and condensation, and chemical or electrochemical reduction of metal salts in the presence of stabilizers.

Dendrimers are outstanding candidates for template synthesis of nanoparticles (NPs) because of their regular structure and chemical versatility. As a consequence of their three-dimensional structure and multiple internal and external functional groups, higher-generation dendrimers are able to act as hosts for a range of ions and molecules. Monometallic, bimetallic and semiconductor nanoparticles have been synthesized using template approach method.

In this work, the focus has been on comprehensive kinetic analysis of 4-nitrophenol reduction using dendrimer encapsulated metal nanoparticles (DENs).

Corresponding Author: rmeijboom@uj.ac.za

Tunable Softening and Toughening of Individualized Cellulose Nanofibers-Polyurethane Urea Elastomer Nanocomposites

Minwoo Lee, Min Haeng Heo, Young-Wun Kim and Jihoon Shin*

Korea Research Institute of Chemical Technology, Daejeon, Korea

In the present study, a series of elastomeric nanocomposites with superior tensile strength and elongation at break, also exhibiting softening, were successfully prepared via in situ polymerization by homogeneously dispersing individualized cellulose nanofibers (CNF) in a polyurethane urea (PUU) matrix. The nanostructure of this PUU composite, having a specific association with the hard segments covalently linked with the individual nanofibers, was characterized by Fourier transform infrared spectroscopy, small-angle X-ray scattering, differential scanning calorimetry, thermal gravimetric analysis, and scanning electron microscopy. It was very interesting to find that the amount and size of the hard domains in the PUU composite gradually decreased with the introduction of CNF owing to the formation of a covalently networked structure via CNF-PUU molecular interaction, which caused softening and toughening simultaneously. The mechanical properties and the thermo-dimensional stability of the prepared nanocomposites were significantly improved as measured by static tensile testing, dynamic mechanical analysis, and thermomechanical analysis. With only 2 wt % of CNF incorporated in the elastomer, a 10.4-fold increase in tensile strength, 5.5-fold increase in strain-to-failure, and a decrease of 35% in the coefficient of thermal expansion were achieved. It was also very interesting to find that the elastic modulus of the nanocomposite gradually decreased from 8.7 to 4.9 MPa for 1 wt % of CNF, which is mainly responsible for softening. A synergistic combination of such conflicting properties as softening and strengthening in the new nanocomposite materials could have great potential applications.

Corresponding Author: jshin@krict.re.kr

Dimensional Dependent Electronic Properties in Tetragonal Iron Chalcogenides

Ekaterina Mitrofanova* and Artem Mitrofanov

Lomonosov Moscow State University, Moscow, Russia

The discovery of high-temperature (Tc) superconductivity up to 100 K in a monolayer FeSe on SrTiO3 caused a variety of disputes on how superconductivity evolves in such materials from bulk to film, because bulk FeSe exhibits a Tc not higher than 10 K. Moreover, for multilayer FeSe charge carrier doping convert non-superconducting films with various thicknesses into superconductors with Tc up to 48 K. In order to predict changes of electronic structure leading to Tc increase we need to carefully describe electronic structure of low-dimensional iron chalcogenides and understand mechanisms of charge-transfer in such systems. In this work we investigate a change of electronic structure during the transition from bulk material to two-dimensional one for iron chalcogenides (FeSe, FeTe, for 1, 2, 3, 4, 5, 10, 15 layers and bulk material) with ab initio calculations. All calculations were performed using projector augmented plane-wave (PAW) method with PBE exchange correlation potential. Our results present systematization of electronic structure data for bulk and low-dimensional iron chalcogenides. The reported study was funded by RFBR according to the research project No.16-32-00435 мол_а.

*Corresponding Author: Evenuel1@gmail.com

The Adsorption Model of Xyloglucan on Microcrystalline Cellulose

Monika Chylinska[1*], Dawid Myśliwiec[2], Monika Szymanska-Chargot[1] and Artur Zdunek[1]

[1]*Institute of Agrophysics, Polish Academy of Sciences, Lublin, Poland*

[2]*Department of Radiochemistry and Colloid Chemistry, Faculty of Chemistry, Maria Curie-Sklodowska University, Poland*

Interactions among cellulose, hemicellulose and pectins are important for plant cell wall assembly and properties, and as well for industrial applications of these polysaccharides.

Cellulose consists of unbranched polymers of β-linked glucose residues arranged in linear chains. The extended glucan chain polymer forms a flat ribbon- like structure that is further stiffened by Van der Waals forces, as well as intra- and intermolecular hydrogen bonds, leading to a regular crystalline arrangement of glucan chains. The hemicellulose xyloglucan is found in the cell walls of all vascular plants and is the major hemicellulose in the primary cell wall of dicotyledons, where it is believed to play an important role in cell wall structure and function. Pectins, together with hemicelluloses, are matrix components of primary cell wall, it can be extremely heterogeneous between plants, tissues, and even within a single cell wall.

Binding of pectin and xyloglucan on microcrystalline cellulose was investigated in this experiment by adsorption isotherms, zeta potential and scanning electron microscopy (SEM). Analysis of three isotherm models (Langmuir, Freundlich and Fowler-Guggenheim isotherms) showed that the experimental adsorption isotherm was well described via Fowler-Guggenheim model which includes lateral interaction between adsorbate. Adsorption isotherm and zeta potential measurement showed that xyloglucan adsorbed on the microcrystalline cellulose. The equilibrium was reached in about 3-4 hour and the kinetics of adsorption were well described by multiexponential equation. Analysis of the model suggests that two steps can be distinguished: diffusion and reconformation in an adsorbed layer. SEM study showed that xyloglucan may prevent cellulose from aggregation.

The study was partially supported under project no. LIDER/300/L-6/14/NCBR/2015.

**Corresponding Author: m.chylinska@ipan.lublin.pl*

Effect of Thermal Oxidation Temperature on the Corrosion Behavior of Ti6Al4V Alloys for Dental Application

Abdelghani Boucheham[1*], Ahcene Karaali[2] and Yasmina Keriti[3]

[1] *CRTSE, Algiers, Algeria*

[2] *Constantine 1 University, Algeria*

[3] *Faculté de Physique, Bab Ezzouar, Algiers, Algeria*

Thermal oxide layers formed on the surface of titanium and titanium alloys by heat treatment play an important role in the enhancement of their biocompatibility and osseointegration in the human body. For this purpose, we aimed to study in the current work the structural and electrochemical properties of different heat treated Ti6Al4V substrates under oxygen flow in the temperature range of 600°C to 800°C. The roughness, chemical composition and phase composition of synthesized layers were investigated using atomic force microscope (AFM) and X-ray diffraction (XRD). The corrosion behavior of the different oxide layers was evaluated in 0.9 wt. % NaCl solution with neutral pH at room temperature by means of open circuit potential (Eoc), potentiodynamic polarization (PDYN) and electrochemical impedance spectroscopy (EIS).

*Corresponding Author: aghani.boucheham@gmail.com

Introduction to the NANOTEK+ tool for the integrated life cycle assessment of Engineered Nanomaterials

Beatriz Corral[1*] and María Blázquez[2]

[1]*EKOTEK, Erandio, Spain*

[2] *INKOA SISTEMAS, Spain*

Since the boom of new engineered nanomaterials (ENMs) one of the major limitations for assessing their impact throughout a product's life cycle is the absence of a systematic procedure for calculating the characterization factor through the fate, exposure and effects of the nanomaterial. There are multiple methods to do this for traditional chemical substances; however, yet, there is not scientific consensus for most nanomaterials. To reduce this uncertainty, the researches of NANOTEK Project, funded by the Basque Government, have completed a state-of-the-art review on the models for derivatization of characterization factors specifically for nanomaterials and developed a software calculator for the human and freshwater Effect Factors (EF). Furthermore, this software integrates human toxicity and freshwater ecotoxicity data to build up a complete database with nanomaterials and their potential associated risks. This tool has been developed based on the UseTOX® methodology, which is endorsed by the Life Cycle Initiative of the United Nations Environment Program (UNEP) and the Society for Environmental Toxicology and Chemistry (SETAC), and taking into account the latest breakthrough in science as well as the need for stability, parsimony, transparency, reliability and user-friendly interface. The outcomes of NANOTEK Project aim to provide guidelines for ENMs categorization based on their effects on the environment and human health and to support safe-by-design strategies. Version beta of the software is already available and NANOTEK Consortium is currently working on the validation phase of the case studies.

**Corresponding Author: b.corral@ekotek.es*

The Effect of Talc, Montmorillonite (MMT) and Wollastonite (WO) on Nanoparticle Release due to Mechanical Drilling from Polypropylene (PP) Composites

Kristof Starost[1*], Evelien Frijns[2], Jo Van Laer[2], Nadimul Faisal[1], Ainhoa Egizabal[3], Cristina Elizextea[3], Inge Nelissen[2] Maria Blazquez[4], James Njuguna[1]

[1] *Centre for Advanced Engineering Materials, School of Engineering, Robert Gordon University, Aberdeen, AB10 7GJ, United Kingdom*
[2] *VITO NV, Boeratang 200, 2400 Mol, Belgium*
[3] *TECNALIA, Mikeletegi pasealekua, 2 E-20009, Donostia Spain*
[4] *INKOA SISTEMAS, SL. Ribera de Axpe 11, Edificio D1, Dpto 208. 48950, Erandio, Bizkaia Spain*

The use of sillicate nanofillers as mechanical reinforcements in polymers is increasingly being well established throughout literterature. This has generated an influx into various commerical industries such as the automotive industry. However, there is still an insufficient understanding on how these fillers effect the release of nanoparticles to evaluate and quantify the full risks associated to nanorelease and nanoparticle exposure.

In this study, the effect on nanorelease due to drilling on Polypropylene (PP) reinforced with 20% Talc, 5% montmorillonite (MMT) and 5% wollastonite (WO) is investigated. With 5% WO, equivalent tensile properties with a 10 % weight reduction were obtained relative to the reference 20% Talc sample. The materials were fabricated through a twin screw extruder. The nanorelease studies were undertaken using the controlled drilling methodolgy for nanoparticle exposure assessment developed within the SIRENA life project. Measurements were taken using CPC, SMPS and DMS50 equipment for real-time characterization and measurements. The particle number concentration (of particles <100nm) and particle size distribution (4.87nm – 562.34nm) of the particles emitted during drilling were evaluated to investigate the effect of the silicate fillers on the particles released. The nano-filled samples exhibited a 33% decrease (MMT sample) or a 30% increase (WO sample) on the average particle number concentration released in comparison to the neat polypropylene sample. The size distribution data displayed a substantial percentage of the particles released from the PP, WO and MMT samples to be around 10nm, whereas the Talc sample appeared to emit larger particle diameters. No independent nanoparticles of the fillers were found in the microscopy (SEM) analysis on samples collected within the test chamber.

The work is part of EC project named Simulation of the release of nanomaterials from consumer products for environmental exposure assessment (SIRENA, Pr. No. LIFE 11 ENV/ES/596) and QualityNano (Grant Agreement No:INFRA-2010-262163).
**Corresponding Author:* k.starost@rgu.ac.uk

The Influence of Allotrope and Particle Size on the Sensitivity of Carbon Paste Electrodes

Stuart Waddell*, Carlos Fernandez and Radhakrishna Prabhu

Robert Gordon University, Aberdeen, United Kingdom

Carbon paste electrodes find wide application in the field of voltammetric sensing. Certain details about how these electrodes function are clearly understood, for example decreasing particle size tends to increase the current response due to an increase in surface area. However, in an actual electrochemical cell, there are many parameters which can influence the rate of electron transfer and hence the reversibility of the redox process. This study looked at the influence of three main parameters namely: the particle size, the allotrope (graphite or glassy carbon) and the carbon to binder ratio. It was found that glassy carbon has far superior charge transfer kinetics as demonstrated by cyclic voltammetry of ferricyanide. However a higher percentage of carbon was required in order to achieve conductivity. The smallest particle size used (2-12 µm) did indeed have the highest sensitivity and reproducibility, although interestingly there was little difference between the 45 µm and 150 µm graphite particles. In conclusion, an optimised electrode material has been found which could be subsequently modified with transfer mediators specific to a given application.

*Corresponding Author: s.waddell1@rgu.ac.uk

Dynamic Mechanical Analyses for Molecular Level Engineering of Advanced Subsea Polymers

Chinyere Okolo* , Chris Wood and Fawad Inam

Northumbria University, Newcastle Upon Tyne, United Kingdom

Challenging subsea field developments in ultra-deepwaters has significantly pushed the need for reliable engineering materials and products for high pressure and high temperature applications. In subsea well bore where such extreme conditions are prevalent, multifunctional polymers have been successfully deployed in various applications. To achieve thermomechanical performance at such conditions, these polymers are usually altered at molecular levels or nano reinforced to hinder the movement of the polymer backbone chain. This poster presents a study on DMA characterization of engineering polymer with focus on its mechanical behaviour and thermal stability at elevated temperatures.

*Corresponding Author: chichi.okolo@northumbria.ac.uk

Asphaltenes as New Objects for Nanoelectronics

Dolomatov M.Yu.[1,2], Bakhtizin R.Z.[1], Petrov A.M.[1], Shutkova S.V.[1], Dolomatova M.M.[1], Hayrudinov I.R.[2]

[1]*Bashkir State University, Department of Physical Electronics and Nanophysics, 32 Zaki Validi street, 450076 Ufa, Russia*
[2]*Ufa State Petroleum University, ul. Kosmonavtvo ,. 450062*

Modern carbon nanomaterials (carbon nanotubes, graphenes, fullerenes, polycyclic molecules) are products of rather complicated technologies. Therefore development of new not expensive materials on the basis of natural substances, in particular high-molecular compounds of oil – asphaltenes, is actual for nanoelectronics. Asphaltenes are complex materials that are found in grude oil, bitumen and high-boiling hydrocarbons distillates. Usually asphaltenes are composed mainly of polyaromatic carbon with a small amount of vanadium and nickel, which are in porphyrin structures. Molecules of asphaltenes may contain 5-10-member benzene and naphthenic rings in their structure and also have paramagnetic centers. A variety of techniques: electronic phenomenological spectroscopy (EPS), atomic force microscopy (AFM) and quantum chemistry calculations were used to define the structure of oil asphaltenes. It was supposed that asphaltene fraction is a strong donor (ionization potential 4.10-6.70 eV) and an acceptor (electron affinity 1.80-2.50 eV). The structures of asphaltenes fragments were calculated by RHF-6-31G** methods. AFM images of asphaltenes obtained from crude oil showed the presence of structure fragments ranged from 3 to 10 nm, disposed to strong intermolecular interactions. We used doped compounds for formation of wide band gap amorphous semiconductors from a concentrates of asphaltens. Changes of conductivity in dispersed petroleum systems (DPS) were studied during a pyrolysis at 500 K. The numerous experiments defined of conductivity testify about phase transitions dielectric – semiconductor in DPS for range of 360 – 400 K. The main conclusion is paramagnetic phase of asphaltenes is organic amorphous wide band gap semiconductor. Besides this substance can be consider as an organic spin glasses.

**Corresponding Author: dolomatov@gmail.com*

Effects of increasing reusability iterations on morphological, optical and crystallinity properties of trivalent doped TiO2/CNT photocatalysts

SS Mukonza*, EN Nxumalo, BB Mamba, AK Mishra

Nanotechnology and Water Sustainability Research Unit College of Science, Engineering and technology University of South Africa

Trivalent doped semiconductor carbon nanotube (CNT) nanohybrid photocatalysts could provide remediation to environmental pollution caused by organic pollutants [1]. Their application as an alternative water treatment method has led to wide interests in photocatalyst life cycle (LC) and their reusability [2]. An investigation into the optical, morphological and crystallinity properties of sol-gel derived Ln3+-TiO2/CNT nanohybrid was done through different characterisation techniques. The catalyst structure was further analysed after several cycles of use by small-angle x-ray scattering (SAXS), scanning electron microscope (SEM) and Brunauer Emmett Teller (BET) with particular emphasis being placed on porosity, specific surface area (SSA), shape of particle, particle size, orientation of particles, UV-visible absorption, morphology and crystallinity. These properties were further correlated to the kinetics of the various photocatalytic reaction kinetics at every LC stage of the experiment iteration [3]. The impact of increasing the number of iterations on the enhancement factor and the degree of photomineralisation was also investigated by total organic content (TOC) measurements. Comparison between different cycle catalysts and effects associated with changing properties on the photocatalytic activity of the nanohybrid is also made.

REFERENCES

1. Chequer. D.M.F, Dorta. J.D, Palma de Oliveria. D. (2011), Advances in Treating Textile Effluent, Prof. Peter Hauser (Ed.), ISBN: 978-953-307-704-8.
2. Tariq. M.A, Faisal. M, Saquib. M, Muneer. M. (2008), Dyes Pigm. 76, 358-365.
3. Barrocas B, Monteiro O.C, Melo Jorge E.M, Sério S. (2013).Photocatalytic activity and reusability study of nanocrystalline TiO2 films prepared by sputtering technique. J Appl Surf Scie. 264. 111116.

**Corresponding Author: mishrak@unisa.ac.za*

Status and Recent Developments on Nanosafety in Asia: Some Legal Concerns

Md. Ershadul Karim [1, *], Abu Bakar Munir[1], Siti Hajar Mohd Yasin[2], Firdaus Muhammad-Sukki[3]

[1]*Faculty of Law, University of Malaya, 50603 Kuala Lumpur, Malaysia.*
[2] *Faculty of Law, Universiti Teknologi MARA, 40450 Shah Alam, Selangor, Malaysia.*
[3] *School of Engineering, Robert Gordon University, Garthdee Road, AB10 7GJ Aberdeen, United Kingdom*

Tremendous progress and success in terms of exploiting nanotechnologies and its numerous applications can be observed in the context of some of the Asian countries, like Japan, South Korea, China, India, Iran, Taiwan etc. Some countries from the ASEAN have also done noticeable progresses in terms of nanotechnology R & D. However, it is a matter of great concern that the way these Asian countries are interested in exploiting the benefits of nanotechnology R & D, when the issues of safety of engineered nanomaterials is concerned, these countries are found less enthusiastic. Even though this trend is in line with the global trend, regulators in this part of the world cannot remain very reluctant as already burgeoning number of laboratory findings warn the conscious consumers regarding possible adverse effects. In this context, the aim of this paper is to share an overview of the status of safety aspects of nanotechnology in selective Asian countries. Sharing the progress of this issue in a historical setting, this paper will highlight some recent developments in this regard. After discussion on some of the legal challenges involved in these initiatives, this paper will finally put forth some suggestions referring to the progress on nanosafety in other parts of the world, mainly in Europe and North America for the Asian policymakers and regulators.

**Corresponding Author: ershadulkarim@gmail.com*

Novel magnetically separable Nd,I,F-TiO_2/$ZnFe_2O_4$ nanocomposite photocatalysts for degradation of phenolic compounds in water

G. Mamba* and A.K. Mishra

Nanotechnology and Water Sustainability Research Unit, College of Science, Engineering and Technology, University of South Africa, Florida, 1709, Johannesburg, South Africa

Development of magnetically separable, visible light responsive nanocomposite photocatalysts holds the future towards practical exploitation of photocatalysis. Herein, we report on the synthesis of multidoped titania (Nd,I,F-TiO2) hybridised with zinc ferrite (ZnFe2O4) via a two-step preparation route. The prepared materials (Nd,I,F-TiO2/ZnFe2O4) were characterised by various spectroscopic and microscopic techniques such as FT-IR, TEM, SEM, UV-Vis, XRD and XPS and their photocatalytic properties were investigated for the degradation of 4-clorophenol in aqueous solutions. Improved optical and photocatalytic properties were observed upon coupling Nd,I,F-TiO2 and ZnFe2O4 owing to the combined contribution of the individual components of the nanocomposite. Moreover, the nanocomposite was separable using an external magnetic field which made recovery and recycling of the photocatalyst relatively easy.

Corresponding Author: gcmamba@gmail.com

Tunable Softening and Toughening of Individualized Cellulose Nanofibers-Polyurethane Urea Elastomer Nanocomposites

Minwoo Lee, Min Haeng Heo, Young-Wun Kim and Jihoon Shin*

Korea Research Institute of Chemical Technology, Daejeon, Korea

In the present study, a series of elastomeric nanocomposites with superior tensile strength and elongation at break, also exhibiting softening, were successfully prepared via in situ polymerization by homogeneously dispersing individualized cellulose nanofibers (CNF) in a polyurethane urea (PUU) matrix. The nanostructure of this PUU composite, having a specific association with the hard segments covalently linked with the individual nanofibers, was characterized by Fourier transform infrared spectroscopy, small-angle X-ray scattering, differential scanning calorimetry, thermal gravimetric analysis, and scanning electron microscopy. It was very interesting to find that the amount and size of the hard domains in the PUU composite gradually decreased with the introduction of CNF owing to the formation of a covalently networked structure via CNF-PUU molecular interaction, which caused softening and toughening simultaneously. The mechanical properties and the thermo-dimensional stability of the prepared nanocomposites were significantly improved as measured by static tensile testing, dynamic mechanical analysis, and thermomechanical analysis. With only 2 wt % of CNF incorporated in the elastomer, a 10.4-fold increase in tensile strength, 5.5-fold increase in strain-to-failure, and a decrease of 35% in the coefficient of thermal expansion were achieved. It was also very interesting to find that the elastic modulus of the nanocomposite gradually decreased from 8.7 to 4.9 MPa for 1 wt % of CNF, which is mainly responsible for softening. A synergistic combination of such conflicting properties as softening and strengthening in the new nanocomposite materials could have great potential applications.

**Corresponding Author: jshin@krict.re.k*

Synthesis and characterization of polyurethane/bentonite nanoclay based nanocomposites using different diisocyanates: relation between mechanical and thermal properties

Javier Bocchio[1], Víctor Wittemberg[2] and Javier Quagliano[1*]

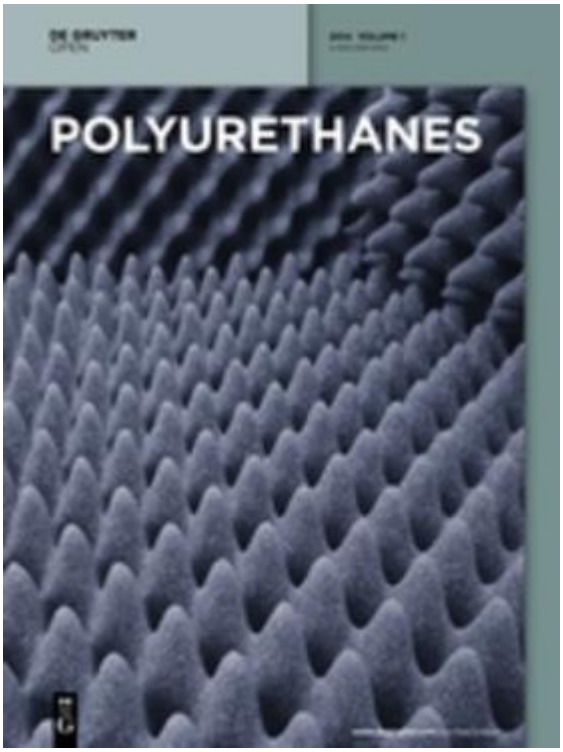
1 División Síntesis Orgánica - Laboratorio de Elastómeros, Departamento Química Aplicada, Instituto de Investigaciones Científicas y Técnicas para la Defensa (CITEDEF), Av. Juan Bautista de Lasalle 4397, Buenos Aires, Argentina.

2 División Química Analítica, Departamento Química Aplicada, Instituto de Investigaciones Científicas y Técnicas para la Defensa (CITEDEF), Av. Juan Bautista de Lasalle 4397, Buenos Aires, Argentina.

Polyurethanes (PUs) and polyurethane nanocomposites (PUNC) with bentonite nanoclay were prepared by the reaction of toluene-2,4-diisocyanate (TDI), dimeryl diisocyanate (DDI) and isophorone diisocyanate (IPDI) with two different polymers: hydroxyl terminated polybutadiene (HTPB) and polytetramethylene ether glycol (PTMEG), and the chains were further extended with 1,4-butanediol (1,4-BDO) to get final PUs and PUNCs. PUNCs were prepared by dispersing within the polymers a commercial and a synthesized bentonite nanoclay by mechanical dispersion. Mechanical properties showed that the addition of a small amount of nanoclay (1%) resulted in a significant increase in tensile strength and consequent reduction in elongation at break (maximum increase of 2.3 and 5-times reduction, respectively, for a HTPB-TDI-BDO based PUNCs). Thermal analysis revealed that the addition of nanoclays improved the thermal stability and increased decomposition temperature of PUNCs around 10°C. We concluded that there is a positive correlation between mechanical and thermal properties as a result of nanoclay addition.

**Corresponding Author: jquagliano@citedef.gob.ar*


JOM
Advanced Materials
and Manufacturing


POLYURETHANES

Authors Index

NANOSTRUC 2016

International Conference on Structural Nano Composites
12-15 Sept 2016 in Aberdeen, United Kingdom

In conjunction with:

AB DN VisitAberdeen

ROBERT GORDON UNIVERSITY ABERDEEN

BREC

UNISA university of south africa

TMS

CSIC
Consejo Superior de Investigaciones Científicas

Nanoscale Horizons

INNOVATION
INNOVATION & TECHNOLOGY TRANSFER
www.greekinnovation.eu

NAFIGATE
nanofibers gateway

SIRENA
LIFE11 ENV/ES/596

Life

ROYAL SOCIETY OF CHEMISTRY

WILEY