The 7th Global Conference on Polymer and Composite Materials (PCM 2020) & (GNN 2020) The 2nd International Conference on Graphene and Novel Nanomaterials

November 1-4, 2020

**Online Conference (Microsoft Teams Meeting)** 



# PCM2020 & GNN2020 CONFERENCE PROGRAM

## November 1-4, 2020 China Standard Time (GMT+8:00)

**ONLINE-Microsoft Teams Meeting** 

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## **Part I Conference Schedule Summary**

November 2	1, 2020
MS Teams: http://www.commonword.com/integrationalized teams.com/integrationalized teams/integrationalized teams/integrationali	ttp://www.academicconf.com/teamslink?confname=pcm2020
10:00-12:00	MS Teams Online Conference Testing and Ice Breaking
15:00-17:30	MS Teams Online Conference Testing and Ice Breaking
November	2, 2020
09.00-09.05	WELCOME SPEECH (PCM 2020)
07.00 07.05	Prof. Esteban Broitman, SKF Research & Technology Development, the Netherlands
09.05-09.10	WELCOME SPEECH (GNN 2020)
07.05-07.10	Prof. Tingkai Zhao, Northwestern Polytechnical University, China
09.10-09.55	Keynote Speech 1: Carbon Dots as Versatile Drug Nanocarriers in Modern Medicine
07.10-07.55	Prof. Roger M. Leblanc, Department of Chemistry, University of Miami, USA
	Keynote Speech 2: Intensity of Singular Stress Fields (ISSFs) in Pull-out Test and
09:55-10:40	Micro-bond Test
	Prof. Nao-Aki Noda, Kyushu Institute of Technology, Japan
10:40-10:50	BREAK
	Keynote Speech 3: Mechanical Properties of Polymers and Composite Materials
10:50-11:35	Measured at the Macro-, Micro-, and Nanoscales
	Prof. Esteban Broitman, SKF Research & Technology Development, the Netherlands
	Keynote Speech 4: Development and Application of a Novel Sample In-Answer Out
11:35-12:20	(SIAO) System Based on a cartridge and Magnetic Nanoparticles
	Prof. Nongyue He, Southeast University, China
12:20-14:00	LUNCH BREAK
14.00.10.00	
14:00-19:00	<b>Ural Session 1:</b> Graphene and NanoMaterials (1)

#### November 3, 2020

08:30-12:40	Oral Session 2: Graphene and NanoMaterials (2)			
12:25-14:00	LUNCH BREAK			
14:00-18:55	<b>Oral Session 3:</b> Polymers and Composite Materials: Synthesis, Characterization			
November 4	4, 2020			
00 00 10 55				

08:30-12:55	<b>Oral Session 4:</b> Fibers, Multi-Functional Composites and Novel Applications
12:40-14:00	LUNCH BREAK
14:00-18:55	<b>Oral Session 5:</b> Applications in Energy, Biomaerials, Medicine, and Food Industry
18:55-19:00	<b>CLOSING SPEECH (PCM2020)</b> <i>Prof. Esteban Broitman, SKF Research &amp; Technology Development, the Netherlands</i>
19:00-19:05	CLOSING SPEECH (GNN 2020) Prof. Tingkai Zhao, Northwestern Polytechnical University, China

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## **Part II Keynote Speeches**

Keynote Speech 1: Carbon Dots as Versatile Drug Nanocarriers in Modern Medicine



Prof. Roger M. Leblanc

Professor and Chair Department of Chemistry, University of Miami, USA

**Biography:** Roger M. Leblanc received his B. S. in chemistry in 1964 and Ph. D. in physical chemistry in 1968 from Université Laval, Canada. In 1994, he moved to University of Miami, where he has been a professor at Department of Chemistry since then. At University of Miami, he was Chair of Department of Chemistry from 1994 to 2002, and he is reappointed as Chair from 2013 to present. Dr. Leblanc has published 534 scientific articles in peer-reviewed journals, and he has given more than 430 presentations at medical and scientific conferences around the world.

Dr. Leblanc has very rich experiences in materials chemistry, especially in the area of preparation of new materials and their bio applications development. He also has a strong background in physical chemistry, with a sound expertise in key research areas for this application, in particular in surface chemistry, microscopy (Brewster Angle microscopy, epi-fluorescence imaging, atomic force microscopy, and transmission electron microscopy) and spectroscopy (UV/vis, fluorescence, and infrared reflectionabsorption spectroscopy).

The innovative work of Dr. Leblanc's multidisciplinary team has long focused on the development of novel nanomaterials such as carbon dots. After synthesis, purification and characterization by various spectroscopies and microscopies, we are especially interested in the application of carbon dots in drug delivery to treat Alzheimer's disease, bone mineralization process and many types of cancer. Except for drug delivery, our research group is also investigating the application of 2D or 3D printing, biosensing, photocatalysis and cosmetics using carbon dots. Another focus of our research group is the study of surface chemistry of organic and biological supramolecular complexes using Langmuir monolayer technique.

**Abstract:** Carbon dots (CDs) with size less than 10 nm have recently triggered great attention in the research of material science and biomedical engineering due to their unique properties such as small size, excellent photoluminescence (PL), high water-dispersity, biocompatibility, nontoxicity and abundant surface functionalities. In this presentation, I will firstly introduce diverse preparations of CDs. Extensive structural characterizations have been used to hypothesize comprehensive structural models for 3 distinct CD species that represent both top-down and bottom-up approaches in order to optimize their properties and applications.

Then, I will mainly focus on many excellent biomedical applications of the CDs recently developed in our lab: (1), *in vivo* experiment suggested that glucose-based CDs could cross the blood-brain barrier (BBB) due to the presence of glucose transporter proteins on the BBB; (2), a drug delivery system of carbon nitride dots conjugated with an anti-cancer therapeutic drug and a targeting molecule was capable of effective treatment against diffuse large B-cell lymphoma both *in vitro* and *in vivo* revealing efficient therapeutic capabilities with minimal toxic side effects; (3), metformin-derived CDs showed

a unique nucleus targeting property, which suggests a huge potential for future nucleus-targeting drug delivery; (4), CDs have constantly shown the capability to inhibit the formation of amyloid precursor protein (APP), beta-amyloid (A $\beta$ ) and A $\beta$  fibrils. CDs are promising nanomedicine and drug nanocarriers to treat Alzheimer's disease (AD); (5) a pilot study showed a versatile nanocarrier could be assembled via the direct conjugation between distinct CDs to fulfill multitasks.

**Keywords:** Carbon Dots; Nanocarrier; Blood-Brain Barrier; Drug Delivery; Cancer Treatment; Alzheimer's Disease; Nanoparticle Assembly

Acknowledgements: Professor Roger M. Leblanc thanks the support from National Science Foundation under the grant 1809060 and 2041413. Also, authors gratefully acknowledge the great support from University of Miami, USA.

## Keynote Speech 2: Intensity of Singular Stress Fields (ISSFs) in Pullout Test and Micro-bond Test



Prof. Nao-Aki Noda

## Kyushu Institute of Technology, Japan

**Biography:** Nao-Aki Noda received his Ph.D. degree in Mechanical Engineering from Kyushu University, Japan in 1984. He has been doing research and teaching at Kyushu Inst. Tech., Kitakyushu, Japan, 1984-87, He is an author of Theory of Elasticity useful for engineers and a co-author of Safety Engineering for Workers in Industry and other several books. He is a co-editor of Stress Intensity Factors Handbook, vol. 4 & 5, Advances in Finite Element Analysis for Computational Mechanics. He is a recipient of Outstanding Paper Medal of Japan Soc. Tech. Plasticity, Sokeizai Industry Technology award from the Materials Process Tech. Ctr., a fellow of JSME (Japan Soc. Mech. Engrs.) and a fellow of JSAE (Soc. Automotive Engrs. Japan), JSMS Award for Academic Contribution and JSME Materials and Mechanics Division Award. He Achievements include researches in stress analysis for notched material testing specimens, and development for large ceramics structures used for steel manufacturing machinery and special bolt-nut connection improving anti-loosening and fatigue strength.

**Abstract:** In fiber reinforced composites, the fiber/matrix combination produces certain mechanical properties that cannot be achieved by either of the constituents acting alone. Pull-out and micro-bond tests are commonly used to investigate the interface properties by using the average interface stress without considering the singular stress fields (ISSFs). In this talk, therefore, the ISSF at the fiber entry/end points is discussed since the ISSF may control the interface debonding for pull-out and micro-bond tests. It is found that the ISSFs of pull-out test can be predicted from the ISSF of the micro-bond test conveniently used because the ISSF of micro-bond test is about 1.5 times of the ISSF of pull-out test under the same fiber geometry. Suitable testing geometry is proposed for micro-bond test since the ISSF is very sensitive to the knife gap under the small dimension commonly used.

**Keywords:** Fiber Reinforced Composites; Micro-Bond Test; Fiber Pull-Out; Intensity of Singular Stress Field (ISSF); Fiber/Matrix Interface

## Keynote Speech 3: Mechanical Properties of Polymers and Composite Materials Measured at the Macro-, Micro-, and Nanoscales



Prof. Esteban Broitman

SKF Research & Technology Development, 3430 DT Nieuwegein, The Netherlands

**Biography:** Esteban Broitman holds a Ph.D. in Physics from the University of Buenos Aires (Argentina), and a Docent (Habilitation) degree in Tribology from Linköping University (Sweden). He has been doing research and teaching at the University of Buenos Aires (Argentina), The College of William & Mary (USA), Carnegie Mellon University (USA), Linköping University (Sweden), and Invited Professor at University of Sao Pablo (Brazil), and the Chinese Academy of Sciences (CAS - China). He is presently a Senior Scientist in the area of Coatings at the SKF Research and Technology Development Center in Netherlands. His activities focus on the use of advanced surface engineering to control friction and wear at the macro-, micro-, and nano-scales of coatings like DLC, nanocomposites, and softer materials like soft metals and polymers.

**Abstract:** During the last decade, novel polymers and composite materials have been developed for applications as micro- and nanodevices. In these applications, conventional mechanical characterization techniques like tensile, compression and bending tests are inapplicable due to the size of the samples. Nanoindentation technique, widely used to characterize the mechanical properties of hard metals and ceramics has started to be used also to characterize polymers and composite materials. Recently, a review has been published by the author comparing mechanical measurement techniques at different scales: *"Indentation Hardness Measurements at Macro-, Micro-, and Nanoscale,"* Tribology Letters vol 65 (2017) p.23.

In this talk, the application of indentation techniques to measure the hardness, elastic modulus, and creep of polymers and composite materials is discussed. A comparison between nanoindentation results and macroscopic properties is offered. Finally, typical mistakes in the measurements of these materials are also critically examined. Challenges and future perspectives in the application of nanoindentation to characterize mechanical properties of polymers and composite materials are suggested.

## Keynote Speech 4: Development and Application of a Novel Sample In-Answer Out (SIAO) System Based on a cartridge and Magnetic Nanoparticles



## Prof. Nongyue He

State Key Laboratory of Bioelectronics, School of Biological Science and Medical Engineering, Southeast University, P.R. China

**Biography:** Nongyue He completed his PhD degree from Nanjing University, China. Initially, he joined Southeast University, Nanjing and Nanjing Medical University, Nanjing as a postdoctoral researcher. But since 2000, he emerged as a professor in State Key Laboratory of Bioelectronics, School of Biomedical Science and Medical Engineering, Southeast University, Nanjing. His research interests are focused on biochips and biosensors, functional nanomaterials, controlled drug release and tissue engineering. He gained several awards like the Award for Excellent Teachers in Chinese Universities (2002), the Second Grade Award for Natural Science (2015), the Second Grade Award for Advance in Science and Technology (2014) of Chinese Ministry of Education; the Second Grade Award for Technology Invention (2013) of Hunan Province; Chien-Shiung Wu Award (2002) of Southeast University; the First Grade Award for Advance in Science and Technology (2017) of Nanjing City, Jiang; and the First Grade Award of Endoscopic Medical Tech-Science in China (2008). He has published more than 300 scientific journal articles, 6 books, and more than 55 patents.

Abstract: Because it has many advantages such as rapidity and accuracy, nucleic acid detection is applied for infectious disease diagnosis more and more. On the other hand, the prevention, control, diagnosis and treatment of infectious diseases have become a global focus for public health. While the traditional methods for pathogen testing have some major disadvantages including the need for highly skilled staff and expensive instrumentation, while procedural aspects are complex and sensitive to the environment. These shortcomings have greatly limited the application of traditional testing in on site pathogen detection. In recent years, an automatic integrated nucleic acid detection system based on real-time PCR is developed by our research group to conduct point-of-care testing of infectious pathogens. The home-made detection system collects fluorescence data in each PCR cycle through an integrated dual-channel fluorescence detection module and then real-time fluorescence curves are drawn by the software, which can tell the results of the diagnostics after some processing and analysis. In this paper, we present a new point-of-care-testing (POCT) system based on magnetic nanoparticles that enable sample in-answer out (SIAO) automated real-time testing for pathogens. Various performance tests were conducted on the instrument. Nucleic acid extraction efficiencies of SIAO versus manual systems were 95.49% and 84.33%, respectively. Real-time PCR by two methods (TaqMan-based probe and SYBR green dye) in the SIAO system was achievable, with comparable results to the manual method. Nucleic acid testing with the SIAO system was repeatable and better than with manual testing. The SIAO system had good anti-pollution performance with easy avoidance of inter-assay cross contamination. Finally, use of the SIAO system for adenovirus detection produced similar results to LightCycler2.0 system assay findings. The amplification plots and Ct values suggested similar amplification plots shapes for adenovirus testing with the SIAO system and with real-time fluorescence PCR testing and commercial instrument post-manual nucleic acid extraction. Collectively, these findings indicate that testing with the SIAO system is virtually equivalent to that of manual extraction with commercial system testing.

## **Part III Oral Presentations**

### Oral Presentation Guidelines

- Online Oral Presentation will be conducted via Microsoft Teams Meeting (Click to see how to join PCM/GNN 2020 via Teams).
- All presenters are requested to reach the Online Session Room prior to the schedule time and complete their presentation on time.
- ↓ All presentation times are shown in China Standard Time (GMT+8:00).
- If a presenter is not able to show up via Teams, the session chair / conference secretary will download and play the pre-recorded video presentation during his/her scheduled presentation time, if listeners have questions about the presentation, please contact the conference secretary to forward the questions.
- If a presenter cannot show up on time or have problem with Internet connect, the session chair has the right to rearrange his/her presentation, and let the next presentation starts.
- ↓ Signed and stamped electronic presentation certificate would be issued via e-mail after presentation

#### **Best Oral Presentations Selection**

The session chair will select one best oral presentation from his/her session based on the following criteria:

- ✓ Research Quality
- ✓ Presentation Performance
- ✓ Presentation Language
- ✓ PowerPoint Design

The Best Presenter will receive an official certificate and a free registration to the PCM/GNN 2021.

## **Session 1\_ Graphene and NanoMaterials (1)**

Time: 14:00-19:00, November 2, 2020

**Session Chairs:** 

14:00-16:25 Dr. Xuge Fan, KTH Royal Institute of Technology, Sweden
16:35-19:00 Assoc. Prof. Mohammad Hatami, Esfarayen University of Technology, Iran

Session Room Link: http://www.academicconf.com/teamslink?confname=gnn2020

14:00-14:25	GNN1165	Carbon based energy storage and conversion materials Prof. Muhammad Arshad, Quaid-i-Azam University Campus Islamabad, Pakistan
14:25-14:40	GNN1148	Enhanced hydrophobic properties of zinc oxide rod coated cotton membrane for self-cleaning and oil/water separation Dr. Diptonil Banerjee, Teerthanker Mahaveer University, India
14:40-15:05	GNN1161	Nano carbon particle preparation and interface property control in supercritical water from waste plastic <i>Prof. Hui Jin, Xi'an Jiaotong University, China</i>
15:05-15:20	GNN1151 (Video)	Quantum phase transition in three dimensional heisenberg antiferromagnet Dr. Hamed Rezania, Razi University, Kermanshah, Iran
15:20-15:45	GNN1153	Graphene based nanofluid applications in combustion engines as nano-fuel, nano-coolant and nano-lubricant Assoc. Prof. Mohammad Hatami, Esfarayen University of Technology, Iran
15:45-16:00	GNN1152 (Video)	The study of Thermodynamics of magnetic insulator Cs <sub>2</sub> CuCl <sub>4</sub> Dr. Hamed Rezania, Razi University, Iran
16:00-16:25	GNN1157 (Video)	Characterization of InSb nanopillars for field emission applications Dr. Filippo Giubileo, CNR-SPIN Salerno, Italy
16:25-16:35		BREAK
16:35-17:00	GNN1146	Fabrication, characterization of suspended graphene with attached masses and their application in ultra-small and sensitive NEMS accelerometers Dr. Xuge Fan, KTH Royal Institute of Technology, Sweden
17:00-17:15	GNN1147	Fractal explanation of Meyer- Neldel rule Dr. Samy Abdelhakim Abdelhamid El-sayed, Benisuef University, Egypt
17:15-17:30	GNN1135	Numerical modelling to asses synergistic wear-corrosion behaviour of nanocomposite coatings Prof. Zulfiqar Khan, Bournemouth University, United Kingdom
17:30-17:55	GNN1156 (Video)	The effect of metal doping/co-alloying on the synthesis of all- inorganic halide perovskite nanocrystals Assoc. Prof. Paola Vivo, Tampere University, Finland
17:55-18:20	GNN1154	Ferroelectric domain walls – novel & reconfigurable 2DEGs Dr. Lukas M. Eng, Institute of Applied Physics, Germany
18:20-18:35	GNN1169	Exfoliation mechanism of Graphene-like MoS <sub>2</sub> prepared by intercalation-detonation method and promising exfoliation for 2D materials <i>Mr. Fan Yang, Xi'an University of Architecture and Technology, China</i>
18:35-19:00	PCM3057	Multiscale material's self-assembly Dr. Per A. Lothman, Head of Research, Foviatech GmbH, Germany

## **Abstracts of Session 1**

#### GNN1165 Carbon based energy storage and conversion materials

#### Muhammad Arshad

National Centre for Physics, Quaid-i-Azam University Camus, Islamabad, Pakistan

**Abstract.** The structural versatility and properties of carbonaceous allow to include them in devices and hybrid functional materials that hold promise for emerging technological developments. These materials offer a wide range of applications including energy storage and conversion devices. However, challenges remain in the controlled application-specific synthesis as well as in the robust integration of versatile carbon structures into hybrids, and in how their properties are influenced when they become building blocks of a composite material. Interface investigations of carbon-based hybrid structures are also critical to understand the structure-property relation to enhancing device performance. This presentation is aimed at shedding light on these prospects and challenges.

#### GNN1148

## Enhanced hydrophobic properties of zinc oxide rod coated cotton membrane for self-cleaning and oil/water separation

#### **Diptonil Banerjee**

Faculty of Engineering and Computing Sciences, Teerthanker Mahaveer University, India

Abstract. A very simple low-temperature deposition of zinc oxide (ZnO) nanorod for different times has been reported on commercially available cotton fabrics. Also large area deposition was taken for the lowest deposition time. Field emission scanning electron microscope was used to investigate the morphology evolution of the ZnO with deposition time. X-ray diffraction confirms the crystallinity of the sample. Fourier transformed infrared spectroscopic study analysed the different bonding present in the sample. The as synthesized samples showed good hydrophobic properties which got significantly worse for the sample synthesized for the highest time duration. The surface energies of the samples have been calculated using conventional Young's equation. The sample was further modified by simple stearic acid treatment in order to get a very small rolling angle thus capable of doing self-cleaning. Also it is seen that the samples, thus prepared partially allow oil over water to pass thus become a material of potential regarding oil-water separation. This work probably for the first time shows that such ZnO-cotton fabric can simultaneously have nearly super-hydrophobicity, self-cleaning property and at the same time can work as a partial separator of oil and water in a single platform. Here the effect of sample synthesis conditions on hydrophobicity has been discussed. Detail theoretical calculation has been done in order to find the surface energy and its effect on the observed hydrophobicity.

#### GNN1161 Nano carbon particle preparation and interface property control in supercritical water from waste plastic

#### Hui Jin and Bin Bai

State Key Laboratory of Multiphase Flow in Power Engineering (SKLMF), Xi'an Jiaotong University, Xi'an, Shaanxi 710049, China

**Abstract.** The global plastic production increased over years due to the vast applications of plastics in many sectors. The increasing consumption of plastics has led to a large amount of waste plastics being discarded in the natural environment, which contributed to the environmental problems. Now, plastic pollution has been one of the most important environmental problems faced today. And it is extremely urgent to dispose waste plastics rationally. As petroleum-based materials, waste plastics are potential hydrocarbon resources. Rational recycling of waste plastics has broad application prospects to cope with the energy crisis. Therefore, in this work, supercritical water gasification technology is employed to recycle waste plastics. With the excellent properties of supercritical water, such as high diffusivity, reactivity, and organic solubility, waste plastics have been successfully converted into clean fuels, and a batch of carbon spheres with excellent appearance have been prepared. Based on these carbon spheres, their formation conditions and mechanisms are also discussed. Moreover, the surface hydrophobic properties of these carbon spheres are also tested to find the relationship between the morphology of carbon spheres and their hydrophobic properties. Finally, in view of the particularity of this work, this method of plastics gasification in supercritical water is also expected to be applied to the drag reduction and anti-corrosion measures of small-size pipelines.

Keywords: Supercritical Water; Plastic; Gasification; Carbon Spheres

### GNN1151 Quantum phase transition in three dimensional Heisenberg antiferromagnet

Hamed Rezania Razi University, Kermanshah, Iran

Abstract. The field induced quantum critical properties of the three dimensional spin-1/2 anisotropic antiferromagnetic Heisenberg model has been studied. We have investigated the quantum phase transition between the spiral order and field induced ferromagnetic order by means of Bose-Einstein condensation of magnons in terms of a bosonic representation. The effect of in-plane anisotropy on the critical properties has been studied via the bosonic model by Green's function approach. We have found an analytic expression for the gap exponent in addition to numerical results for the critical magnetic field in terms of anisotropy parameter. The in-plane anisotropy breaks the U(1) symmetry explicitly which changes the universal behavior by a drastic change on the gap exponent. Moreover, the critical magnetic field depends strongly on the in-plane anisotropies. The divergence of the transverse structure factor at the antiferromagnetic wave vector confirms the onset of the magnetic order which scales with the negative value of gap exponent as the magnetic field approaches the critical one. The transverse staggered magnetization as an order parameter vanishes with exponent \$\beta=0.5\$ when the magnetic field reaches its critical value in low field region.

### GNN1153 Graphene based nanofluid applications in combustion engines as nano-fuel, nanocoolant and nano-lubricant

#### Mohammad Hatami

Associate Professor of Esfarayen University of Technology, North Khorasan, Iran

**Abstract.** Nanofluids have a wide application in different industries such as internal combustion engines (ICEs). The most usable criteria of nanofluids in ICEs are nano-fuels (as additives), Nanolubricants (as oils) and nano-coolants (such as radiator cooling). In this presentation, we will review and study all of the possible nanofluids in these three applications and try to find the best performance in each application using experimental and numerical methods. The effect of nanofluids on the wear, friction reductions, fuel efficiencies, thermal efficiency, emissions and etc. is discussed and suitable nanofluids are presented. For instance, Graphene oxide nanoparticles due to its high thermal conductivity and high surface area improves the combustion and increases the cylinder pressure.

### GNN1152 The study of thermodynamics of magnetic insulator Cs<sub>2</sub>CuCl<sub>4</sub>

Hamed Rezania Razi University, Kermanshah, Iran

Abstract. We have studied the effect of both axial and transverse anisotropy on the critical field and thermodynamic properties of the field induced three-dimensional antiferromagnetic Heisenberg model on the frustrated hexagonal lattice for  $Cs_2CuCl_4$  compound. The spin model is mapped to a bosonic one with the hard-core repulsion constraint and the Green's function approach has been implemented to get the low energy spectrum and the corresponding thermodynamic properties. To find the critical field (*Bc*) we have looked for the Bose-Einstein condensation of quasi-particles (magnons) which takes place when the magnon spectrum vanishes at the ordering spiral wave vector. We have also obtained the dispersion of magnon spectrum in the critical magnetic field for each anisotropy parameter to find the spiral wave vector where the spectrum gets its minimum. The magnon energies show a linear dispersion relation close to the quantum critical point. The effect of hard-core boson interaction on the single particle excitation energies leads to a temperature dependence of the magnon spectrum versus magnetic field. We have also studied the behavior of specific heat and static structure factor versus temperature and magnetic field.

### GNN1157 Characterization of InSb nanopillars for field emission applications

Filippo Giubileo<sup>1,\*</sup>, Enver Faella<sup>2</sup>, Aniello Pelella<sup>1,2</sup>, Alessandro Grillo<sup>1,2</sup>, Maurizio Passacantando<sup>3</sup>, Ray LaPierre<sup>4</sup>, Curtis Goosney<sup>4</sup> and Antonio Di Bartolomeo<sup>1,2</sup>

<sup>1</sup>CNR-SPIN Salerno, via Giovanni Paolo II n. 132, Italy

<sup>2</sup>Physics Department "E. R. Caianiello," University of Salerno, via Giovanni Paolo II n. 132, Italy <sup>3</sup>Department of Physical and Chemical Science, University of L'Aquila, and CNR-SPIN L'Aquila, via Vetoio, Italy

<sup>4</sup>Department of Engineering Physics, McMaster University, 1280 Main Street West, Canada

Abstract. A piezoelectrically driven metallic nanoprobe is installed inside a scanning electron microscope in order to perform local characterization of the field emission properties of InSb nanopillars. The tip-shaped anode can be precisely positioned at sub-micron distances from the

emitters, to collect electrons from areas as small as  $1\text{um}^2$  under the application of external bias up to 100 V. Current-voltage characteristics are measured for cathode-anode separation down to 500 nm and are analyzed in the framework of the Fowler-Nordheim theory. We give estimation of performance parameters such as the field enhancement factor and the turn-on field and their dependence on the cathode-anode separation distance. We demonstrate the time stability of the emitted current for several minutes. Finally, we perform a finite element electrostatic simulation to calculate the electric field in proximity of the nanopillars and we evaluate the effective emitting area as well as the screening effect due to presence of other pillars in close vicinity. In conclusion, we show that InSb nanopillars are very stable emitters, that allow current density as high as  $10^4 \text{ A/cm}^2$  and excellent time stability, crucial characteristics to envisage device exploitation.

**Keywords:** Indium Antimonide; Semiconducting Nanopillars; Field Emission; Field Enhancement Factors; Turn-On Field; Electric Field Simulations

#### **GNN1146**

## Fabrication, characterization of suspended graphene with attached masses and their application in ultra-small and sensitive NEMS accelerometers

#### Xuge Fan

Researcher, Division of Micro and Nanosystems, School of Electrical Engineering and Computer Science, KTH Royal Institute of Technology, Sweden

Abstract. Graphene, as an ultra-thin 2D membrane material, is very promising in applications of micro- and nanoelectromechanical system (MEMS and NEMS) due to its atomic thickness and unique mechanical, electrical and optical properties. Currently, studies have successfully shown the feasibility of using suspended graphene in resonators, pressure sensors, switches, loudspeakers, microphones and gas sensors, etc. Suspended graphene can be fabricated by transferring graphene from the original substrate to 1) a pre-fabricated substrate with trenches, cavities or membranes made of dielectric layers, or 2) a flat silicon dioxide (SiO<sub>2</sub>) or polymer substrate surface and then removing parts of the material underneath the graphene by sacrificial etching. However, fabrication of suspended graphene structures, especially suspended graphene with an attached proof mass is very challenging, such as collapse and rupture of the suspended graphene. We report a robust route for fabricating double-layer CVD graphene membranes and ribbons with attached SiO<sub>2</sub>/Si proof masses, which is compatible with waferscale MEMS and semiconductor manufacturing technologies. Graphene ribbons and membranes with attached SiO<sub>2</sub>/Si proof masses were demonstrated to be extremely robust and were able to withstand AFM tip indentation forces of up to ~7000 nN. Based on atomic force microscope (AFM) tip indentation experiments, the averaged Young's modulus of stacked double-layer CVD graphene films in our devices was extracted to be 0.22 TPa. The built-in stress of hundreds of MPa exist in the graphene ribbons and thereby cannot be ignored. The measured resonance frequencies of graphene ribbons and membranes with attached SiO<sub>2</sub>/Si proof masses ranged from tens to hundreds of kHz, with O between  $\sim 10^1$  and  $\sim 10^2$ . We demonstrate that the suspended graphene ribbons and membranes with attached SiO<sub>2</sub>/Si proof masses can be used as combined spring-mass and piezoresistive transducers in NEMS accelerometer. The graphene NEMS accelerometers occupy at least two orders of magnitude smaller die area than conventional state-of-the-art silicon accelerometers while keeping competitive sensitivities. These findings pave the way for a new class of extremely small and highly sensitive graphene NEMS devices and are an important step toward bringing ultra-small piezoresistive graphene NEMS closer toward deployment in emerging applications such as internet of things (IoT) devices.

## GNN1147 Fractal explanation of Meyer- Neldel Rule

Samy A. Elsayed Physics Department, Faculty of Sciences, Benisuef Universit 62514, Egypt

Abstract. The relation between Meyer–Neldel rule (MNR) and fractal is investigated. Using very simple and elementary mathematics, it is proved that the (MNR) is one of Mandelbrot sets form. The dc conductivity in temperature range 1.7 K-300 K of structural disordered germanium irradiated fast neutrons with fluencies  $10^{16} \text{ cm}^{-2} \le \Phi \le 1.2 \times 10^{17} \text{ cm}^{-2}$  is measured. From analysis, the dc conductivity results, the obtained EMN values is proportional with dc activation energies of each mechanisms of conduction. From the three values of EMN related to each mechanism of conduction the second stage of EMN is obtained. The second stage of EMN value is lower than EMN obtained from  $\Delta E1$  or  $\Delta E2$ . This result confirms the smaller replicas of self-similar distribution of impurity centers in germanium disordered fast neutrons irradiation. EMN is postulated as the loss of energy dissipated in formation certain fractal system in a medium

**Keywords:** Meyer-Neldel Rule, Mandelbrot sets, germanium irradiation disordered fast neutrons, electrical conductivity, hopping conduction,

### GNN1135

# Numerical modelling to asses synergistic wear-corrosion behaviour of nanocomposite coatings

#### Professor Zulfiqar A Khan

NanoCorr, Energy & Modelling Research Group, Department of Design & Engineering, Bournemouth University, United Kingdom

Abstract. This study has been conducted to analyse wear and corrosion performance of nanocomposite coating. Comparative analysis of their wear-corrosion with non-coated samples has been presented. An experimental study was conducted to compare wear-corrosion performance of Nickle-Graphene coatings and carbon steel, mainly deployed in hard wearing surfaces and lightly stressed gears. During this research mechanical properties, intrinsic grain size and coefficient of thermal elastic mismatch and have been taken as input parameters. Nanocomposite coating in contaminated and noncontaminated lubrication has been studied to assess their wear-corrosion performance. Nanocomposite coating performance has been compared with non-coated carbon steel in both lubricating conditions. Standalone corrosion and wear rates were studied for both nanocomposite coating and automotive steel. Wear-corrosion results demonstrated that Ni/GPL had superior performance comparing to carbon steel. Results from this study enabled the development of a novel 2-D synergetic wear-corrosion model to evaluate tribo-performance of nanocomposite coating and steel. Both experimental and analytical results are in close agreement in terms of higher performance of nanocoating as compared to automotive steel especially in contaminated lubrication.

#### GNN1156 The effect of metal doping/co-alloying on the synthesis of all-inorganic halide perovskite nanocrystals

#### Maning Liu, Anastasia Matuhina, and Paola Vivo<sup>\*</sup> Faculty of Engineering and Natural Sciences, Tampere University, Finland

**Abstract.** The doping of colloidal halide perovskite nanocrystals (PNCs) with manganese cations  $(Mn^{2+})$  has recently enabled enhanced stability and novel optical properties and charge carrier dynamics in PNCs. However, the influence of Mn-doping on the synthetic routes and the band structures of the host PNCs has still not been clearly elucidated. Herein, we prove that Mn-doping promotes a facile, less toxic, and less corrosive path toward the synthesis of all-inorganic bismuth-based PNCs (Cs<sub>3</sub>Bi<sub>2</sub>I<sub>9</sub>) by effectively suppressing the CsI by-product of the Cs<sub>3</sub>Bi<sub>16</sub> intermediate decomposition reaction. Furthermore, the energy levels of the as-formed Cs<sub>3</sub>Bi<sub>2</sub>I<sub>9</sub> PNCs can be tuned upon different Mn-doping amounts. This results in a higher open-circuit voltage of the corresponding PNCs-based solar cells compared to those employing the undoped Cs<sub>3</sub>Bi<sub>2</sub>I<sub>9</sub>.

The heterovalent co-alloying of the B-site of perovskites has been also proposed as effective strategy to tune the optoelectronic properties of perovskites both in bulk and nanocrystals. Here, we demonstrate for the first time the alloying of lead (Pb) with titanium (Ti) as a successful approach to reduce the toxicity of PNCs and engineer their morphology and optical properties.

Our work opens new insights on the role of doping and co-alloying in the synthetic route and optoelectronic properties of halide PNCs with reduced toxicity.

**Keywords:** Halide Perovskite Nanocrystals; Optoelectronic Devices; Colloidal Synthesis; Lead-Free; Doping; Co-Alloying

Acknowledgements: We acknowledge Jane & Aatos Erkko foundation (project 'ASPIRE') for financial support. This work is part of the Academy of Finland Flagship Programme, Photonics Research and Innovation (PREIN), Decision No. 320165.

## GNN1154 Ferroelectric domain walls – novel & reconfigurable 2DEGs

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**Abstract.** For the last 10 years, domain wall conductivity (DWC) in ferroelectrics has become a very prospective field of research, since allowing to engineer 2-dimensional electron gases (2DEGs) integrated into a robust solid state, practically at will. We intensively explore DWs in bulk and thin-film LiNbO<sub>3</sub> (TFLN) single crystals, a material that is known for its large bandgap of ~4 eV, optical endurance, and excellent CMOS compatibility. When engineering domains across such crystals, domain walls (DWs) i.e. the tiny region that separates adjacent areas of opposite polarization, show, to our great surprise, excellent metallic-like properties. Applying a small voltage of  $\pm 4$  V across such a wall, allows to drive/switch extremely large DWCs of up to  $\pm 1$  mA per DW, and this even at room temperature. Mandatory for this to happen, however, are low injection barriers as well as optimized electron (hopping) transport properties along such DWs, as is experimentally mediated through the slight inclination of DWs with respect to the polar LNO axes.

In this talk, I will provide clear proof for the existence of this 2DEG in these DWs by exploring Halltransport properties, excited both with and without external photo-illumination. In addition, I will show how to follow and track the effective trajectory of electrons when travelling along DWs by means of dedicated non-linear optical micro-spectroscopy. Lastly, our reconfigurable 2DEGs allow to fabricate nanoelectronic devices such as low-power memories that possess a high endurance and a large memory window.

**Keywords:** Ferroelectrics; Domain Walls; 2DEG, Hall Transport; Electron Hopping; 3D Trajectory; Second Harmonic Generation; Memory Device

Acknowledgements: German Science Foundation, ct.qmat

### GNN1169 Exfoliation mechanism of Graphene-like MoS<sub>2</sub> prepared by intercalationdetonation method and promising exfoliation for 2D materials

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**Abstract.** Graphene-like MoS<sub>2</sub> has attracted significant interest because of its unique electronic, optical, and catalytic properties with two-dimensional lamellar structure. In this work, a novel intercalation-detonation method was used to prepare monolayer and multilayer graphene-like MoS<sub>2</sub>. MoS<sub>2</sub> was first completely intercalated by abundant oxygen-containing functional groups bonded to the sulfur atom layer in basal planes of the MoS<sub>2</sub> structure, increasing the layer spacing and decreasing the Van-der-Waals' force between the layers. Then, the intercalated MoS<sub>2</sub> was rapid exfoliated by high energy of detonation. In addition, bulk WS<sub>2</sub> and h-BN powders were also exfoliated to single and few layers nanosheets successfully by detonation method, showing the promising wide range of application of exfoliation in two-dimensional materials. The further research on magnetic and electrocatalytic hydrogen evolution properties show that the exfoliated MoS<sub>2</sub> has excellent magnetic response and electrocatalytic efficiency, demonstrating promising potential for applications on diluted magnetic semiconductor and energy conversion.

**Keywords:** Graphene-like MoS<sub>2</sub>; Intercalation-detonation method; Exfoliation mechanism; 2D materials; Magnetic property; Electrocatalytic hydrogen evolution

**Acknowledgements:** This work was supported by the Youth Innovation Team of Shaanxi Universities (2019-2022), Outstanding Doctorate Dissertation Cultivation Fund of Xi'an University of Architecture and Technology (6040317013), Fok Ying Tung Education Foundation (171101) and top young talents project of "Special Support Program for High Level Talents" in Shaanxi Province (2018-2023).

#### PCM3057 Multiscale material's self-assembly

#### Per A. Löthman Foviatech GmbH, Hamburg, Germany

**Abstract.** Multiscale materials are ubiquitous in Nature and Engineering, sometimes they may be hierarchial, possibly self-similar, displaying various degrees of organisation at different scales.

Self-assembly is a truly multiscale phenomenon and it plays a role in so seemingly unrelated fields such as buildings and architecture as well as in nanotechnology, protein folding and plant leave's surface components (waxes) serving as a protection against plant pathogens, and it serves as a promising method for manufacture of novel advanced materials. Its fundamentals have been not entirely understood or implemented into materials synthesis. This gap may be filled by analogous experimentation at the macroscopic level. Self-assembly has been studied successfully using macroscopic magnetic self-assembly which can give insight into such seemingly unrelated aspects such as DNA-function as well as how to self-assemble true 3D materials. It reveals the underlying mechanisms of Self-assembly which can be exploited also at the micro- and the nanoscopic level. Herewith micro-, nano and macroscopic materials can be self-assembled and material's self-assembly as a phenomenon can be investigated.

The carbon nanomaterial Graphene can be self-assembled into various structures enabling its usage in several applications showing its feasability as future high-tech material. It has astonishing properties and is a promising candidate for flexible sensors and energy storage applications. To fully appreciate the properties of graphene and other nanomaterials and implement into applications it is necessary to understand the underlying principles of self-assembly.

The understanding coming from macroscopic self-assembly in several dimensions may be combined with experiments at the nano- as well as microlevel in order to achieve successful self-assembly of advanced graphene-based nanomaterials. We need multiscale Self-assembly for a variety of future advanced materials.

Keywords: Multiscale Material's Self-Assembly; Graphene; Sensors

## Session 2\_ Graphene and NanoMaterials (2)

Time: 08:30-12:25, November 3, 2020

**Session Chairs:** 

08:30-10:30 Prof. Gunther Andersson, Flinders University, Australia 10:40-12:40 Prof. Ishaq Ahmad, National Centre for Physics, Pakistan Session Room Link: http://www.academicconf.com/teamslink?confname=gnn2020

08:30-08:55	GNN1149	A novel carbon nanotube ink as a lubricant for extreme conditions Dr. Germán Prieto, IFISUR, CONICET, Argentina
08:55-09:10	GNN1140	A new-fashioned two-step strategy for high-yield preparation of few-layer graphene: resonance ball-milling and hydrothermal exfoliation Dr. Yang Qingfeng, Tsinghua University, China
09:10-09:35	GNN1144	Violet phosphorus and phosphorene Prof. Jinying Zhang, Xi'an Jiaotong University, China
09:35-09:50	GNN1139	Few-layer borophene prepared by mechanical method and its terahertz shielding performance Dr. Zhixun Zhang, Tsinghua University, China
09:50-10:15	GNN1166	Exploring the dynamics of molecular rotors in novel framework materials for renewable energy technology Dr. Naveed Zafar Ali, Quaid-i-Azam University Campus Islamabad, Pakistan
10:15-10:30	GNN1141	Preparation and radiation properties control of nano-sponge doped with graphene/carbon nanotubes Dr. Mingyang Yang, Tsinghua University, China
10:30-10:40		BREAK
10:40-11:05	GNN1158	Determining the electronic structure of the outermost layer of graphene and related materials Prof. Gunther Andersson, Flinders University, Australia
11:05-11:30	GNN1159	Metal oxides doped graphene oxide nanocomposites and their applications Assoc. Prof. Muhammad Akhyar Farrukh, Forman Christian College (A Chartered University), Pakistan
11:30-11:45	GNN1142	Borophene/graphene heterostructure as the anode of lithium-ion batteries with controlled interlayer spacing Dr. Jianwen Yu, Tsinghua University, China
11:45-12:00	GNN1167	Application of Graphene as transparent electrodes in PV solar cells Dr. Ali Abdolahzadeh Ziabari, Islamic Azad University, Lahijan, Iran
12:00-12:25	GNN1168	Graphene hetero structures and other 2D materials Dr. Rashid Jalila, University of Engineering & Technology, Pakistan
12:25-12:40	GNN1170	2-Dimensional transition metal dichalcogenides (TMD): next

## Abstracts of Session 2

#### GNN1149 A novel carbon nanotube ink as a lubricant for extreme conditions

Germán Prieto<sup>1,2\*</sup>, Bruno A. Pilotti<sup>2,3</sup>, Walter R. Tuckart<sup>1,2</sup> and Mariana Dennehy<sup>4</sup> <sup>1</sup>IFISUR, CONICET, Argentina <sup>2</sup>Engineering Department, Universidad Nacional del Sur, Argentina <sup>3</sup> PLAPIQUI, CONICET, Argentina <sup>4</sup> Chemistry Department, Universidad Nacional del Sur, Argentina

**Abstract.** In high demanding applications, such as oil extraction, mining equipment, or aerospace components, lubrication using oils or greases is sometimes not possible, due to the elevated contact stresses involved, high temperatures, low sliding speeds, high vacuum, and even radiation damage. In these kinds of environments, solid lubricants are often the only available choice for preventing excessive wear and reducing friction between sliding surfaces.

For this purpose, a novel and eco-friendly method for dispersing carbon nanotubes and metallic sulfide nanoparticles was developed. These dispersions were used to generate layers of nanoparticles in the form of soft coatings that prevented direct metal-to-metal contact and lowered the friction coefficient. The obtained soft coatings were evaluated in a reciprocating tribometer under different atmospheric conditions, to analyze the influence of ambient humidity on their frictional response and durability. Wear surfaces were examined using SEM-EDS and Raman microspectrometry.

The obtained results have shown that carbon nanotube coatings deposited with this method have excellent lubricant properties under a wide range of conditions, providing low friction coefficients and wear protection of steel substrates.

Keywords: Carbon Nanotubes; Bismuth Sulphide; Nanoparticles; Lubrication; Wear; Friction

Acknowledgements: The authors wish to express their appreciation for the support of the ANPCyT for the Grant PICT-2017-1316.

#### GNN1140

## A New-fashioned two-step strategy for high-yield preparation of few-layer graphene: resonance ball-milling and hydrothermal exfoliation

Qingfeng Yang<sup>1</sup>, Ming Zhou<sup>12\*</sup> Mingyang Yang<sup>1</sup>, Zhixun Zhang<sup>1</sup>, Jianwen Yu<sup>1</sup>, Yibo Zhang<sup>1</sup>, Wenjun Cheng<sup>1</sup>, Xuyin Li<sup>1</sup>

<sup>1</sup>State Key Laboratory of Tribology, School of Mechanical Engineering, Tsinghua University, China <sup>2</sup>Key Laboratory for Advanced Materials Processing Technology, Ministry of Education, China

**Abstract.** Graphene shows great potential applications in functional coating, electrodes, and ultrasensitive sensors, but high-yield and scalable preparation of few-layer graphene (FLG) by mechanical exfoliation method is still a formidable challenge. In this work, a simple newsfashioned two-step method for high-yield preparation of FLG is developed by combining resonance ball milling and hydrothermal treatment. During the resonance ball milling process, the utilization of magnetic Fe<sub>3</sub>O<sub>4</sub> nanoparticles as a new "particle wedge" resulted to facilitate fragment and delamination of graphitic layers. In addition, further hydrothermal treatment can enhance ball milling product (BMP) exfoliation, which is attribution to the shear force driven by the Brownian motion of various

intercalated molecules at high temperature and high pressure. As expected, the two-step method can have the high exfoliation efficiency up to 92% (less than or equal to 10 layers) without purification and high output rate up to 85.26% compared with the starting expanded graphite flakes, which is due to the synergistic mechanism of resonance ball milling and hydrothermal stripping. This work provides a new-fashioned strategy for mechanical large-scale production of graphene. Moreover, the FLG nanosheet ink can easily achieve the formation of FLG coatings on the surface of various substrates, resulting in good electrical conductivity (the lowest average sheet resistance of ~51.80  $\Omega$ /sq on PET film), which possesses potential applications in various fields including functional coating, energy storages, and electrochemical sensors, etc.

Keywords: Resonance Ball Milling; Hydrothermal Process; Few-Layer Graphene nanosheets

### GNN1144 Violet phosphorus and phosphorene

#### Jinying Zhang<sup>,\*</sup>, Lihui Zhang, Bo Zhang

State Key Laboratory of Electrical Insulation and Power Equipment, Center of Nanomaterials for Renewable Energy, School of Electrical Engineering, Xi'an Jiaotong University, China

Abstract. Violet phosphorus was first promoted by Hittorf in 1865 and structurally characterized by Thurn and Krebs in 1969. It was named 'violet phosphorus' due to its purple colour. However, no convincing experimental data has been obtained to for violet phosphorus since its promotion in 1865. It was even debated that whether violet phosphorus was even a stable allotrope or a metastable intermediate from red to black phosphorus. We have synthesized violet phosphorus single crystals with sizes of millimeter in lab. The single crystals are dark red transparent instead of purple. The lattice structure of the as-produced violet phosphorus has been determined to be monoclinic with a space group of P2/n (13), CSD-1935087. The interlayer distance of violet phosphorus was demonstrated to be 1.1 nm. The yield of violet phosphorus has been improved to be 80%. The decomposition temperature of bulk violet phosphorus (512 °C) is 52 °C higher than that of black phosphorus (460 °C), indicating that violet phosphorus is the most stable phosphorus allotrope. Violet phosphorene has for the first time been exfoliated by both mechanical and liquid methods under ambient conditions. The work function of violet phosphorene nanoflakes has been shown to decrease with the increase in layers from 5.16 eV to 4.79 eV and tends to be stable on a gold substrate. The work functions measured on a silicon oxide substrate are much higher due to charge accumulation. The band alignments of different layered violet phosphorene materials were also calculated to give a practical route for future applications.

Keywords: Violet Phosphorus; Violet Phosphorene; Lattice Structure; Yield; Work Function; Band Alignment

Acknowledgements: Financial support for this research is from the National Natural Science Foundation of China (21771143).

#### GNN1139

## Few-layer borophene prepared by mechanical method and its terahertz shielding performance

Zhixun Zhang,<sup>1</sup> Ming Zhou,<sup>\*1,2</sup> Taohong Zhang,<sup>3</sup> Mingyang Yang<sup>1</sup>, Qingfeng Yang<sup>1</sup>, Jianwen Yu<sup>1</sup>, Yibo Zhang<sup>1</sup>

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<sup>3</sup>Department of Computer, School of Computer and Communication Engineering University of Science and Technology Beijing (USTB), China

Abstract. Once two-dimensional boron based materials were forecasted, its excellent physical and chemical properties have realized the attractive application value in the field of material science. However, borophene couldn't exist independently and stably in nature. Molecular beam epitaxy (MBE) is the only way being used currently for preparation of borophene, which has low yield and harsh experimental installation conditions. Here, we propose the theory that few- layer borophene supported by silver nanoparticles can exist stably and perform large-scale preparation of few-layer borophene by mechanical resonance first. We have revealed the structure of prepared borophene is  $\alpha$ -sheet and the thickness of it is less than 4 nm. The oxidation rate of borophene from the experiment is about 0.19, which indicates that the few-layer borophene possesses good stability. We have also studied the stability of the borophene on silver nanoparticles by the first principle calculation. The calculation proves that few-layer borophene can exist stably supported with silver nanoparticles. Furthermore, the terahertz shielding and stealth performance of the few-layer borophene has been explored. The maximum terahertz shielding effectiveness value of the prepared material could reach up to 50 dB and 21.5 dB for the reflection loss value in the broadband range of 0.1-2.7 THz. The large-scale preparation of few-layer borophene through the mechanical method makes it possible to study the properties of borophene and to apply them on a large scale at a low cost. Such as the study of terahertz shielding and stealth performance in the article which facilitate the lightweight material design for terahertz shielding and stealth.

Keywords: Borophene; Few-Layer; Mechanical Resonance; Terahertz; First Principles

## GNN1166 Exploring the dynamics of molecular rotors in novel framework materials for renewable energy technology

#### Naveed Zafar Ali National Centre for Physics, Quaid-I-Azam University Campus, Islamabad, Pakistan

**Abstract.** Conceptual design of molecular rotors based framework materials is of great importance among energy storage and conversion technology applications. Research endeavours in the pursuit of next generation "super-protonic solid acids proton conductors" for Fuel Cell applications and as "solid state electrolyte (SSE)" for all solid state batteries has seen a huge research thrust in the recent decade. The basic concept rely solel on understanding the dynamics of ROTOR molecules ideally incorporated within the framework assembly that exhibits rapid reorientation of XO<sub>4</sub> anion groups as the mechanism of proton transport.

In the first round of the talk, I will be talking about the conceptual designing of new ROTOR molecules and their role in achieving high proton conductivity as a substituent to NAFION membrane for PEM(proton exchange membrane) Fuel Cells. The preliminary focus would be to spotify new kind of hybrid functional architecture materials for their application in fuel-cell-powered vehicles. Focus will be to highlight new phosphate and silicate analogue to known sulfate and selenate solid acids with high conductivity and subsequently discuss methodologies to incorporate these functional guest rotor molecules into potential framework architeture, that will facilitate proton conduction through well defined crystalline pores at wide-ranging temperature window.

In second phae of talk, I will focus on the screening of potent rotor molecules as superion conducting solid state electrolyte (SSE) materials that offers high ionic conductivity, good ductility and processability, as well as good compatibility with the electrode rendering their ideal use in the research and application of all solid state batteries(ASSBs). The typical structural feature of these SSE decorated with "rotatable polyanion" is that the high temperature-induced drastic increase in the atomic displacement parameters (ADPs) of cental atoms with huge thermal ellipsoids, in such a way that the atoms 'jump' in a quantum-like manner from a given well-defined orientation into a dynamically disordered framework with subsequent disordered phase transition triggered by polyanion rotation leading to a sharp increase of cationic conductivity. Therefore, it is of great significance to get in depth structural insight into the rotational dynamics of polyanions in order to further optimize the properties (ion conduction and interface compatibility) of novel solid electrolyte. I will briefly discuss how the operando/in-situ synchrotron powder X-ray and neutron diffraction can be concomitantly used to study the rotational dynamics of polyanions in novel solid state electrolyte materials. The role of precise doping of selected elements at corresponding lattice sites will also be highlighted besides quantifying and discussing strategies to circumvent the emerging amorphous phases responsible for creating large charge transfer resistance at the Solid Electrolyte Interface (SEI).

**Keywords:** Solid Electrolyte Materials; Rotating Dynamics of Polyanions; Synchrotron X-Ray & Neutron Powder Diffraction

## GNN1150 Bi-containing ferrite garnet type thin-film materials synthesis and characterization at ESRI, nano-fabrication lab during the last twelve years

Mohammad Nur-E-Alam<sup>\*</sup>, and Kamal Alameh Electron Science Research Institute, School of Science, Edith Cowan University, Australia

Abstract. Over the last twelve years at the Nano-fabrication laboratory in ESRI, Edith Cowan University, Australia, we have devoted research efforts to the synthesis, and characterization of Bismuth containing ferrite-garnet type thin-film magneto-optic (MO) materials of different compositions.

In this talk, we report on highly bismuth-substituted iron garnet thin films prepared on various substrates (glass, GGG, and Si) using radio frequency (RF) magnetron sputtering followed by high-temperature annealing crystallization. We study the process parameters associated with the RF magnetron sputter deposition technique and investigate the necessity of optimized process parameters including optimized annealing crystallization regimes for achieving the best MO properties. In order to improve the MO properties of Bi-containing iron garnets we implement several techniques including fabrication of co-sputtered nanocomposite films, all-garnet multilayer structures, implantation of oxygen plasma treatment on amorphous garnet layers just after the deposition process, and modification of the annealing crystallization process. We observe significant improvement in MO properties of Bi-containing ferrite type garnet thin-film materials, including record high MO figure of merit and improved conventional and un-conventional type hysteresis loops of Faraday rotation. The attractive optical, magnetic and magneto-optic properties obtained in highly bismuth-substituted iron garnet thin-film materials are relevant to the context of manufacturing next-generation ultra-fast

optoelectronic devices, such as light intensity switches and modulators, high-speed flat panel displays, and high-sensitivity sensors.

**Keywords:** Bi-Substituted; RF Magnetron; Sputtering; Annealing; Oxygen Plasma Treatment; Magneto-Optic; Faraday Rotation; Figure of Merit; Hysteresis Loop; Imaging, Sensing

## GNN1141 Preparation and radiation properties control of nano-sponge doped with graphene/carbon nanotubes

Mingyang Yang<sup>1</sup>, Ming Zhou<sup>1,2,\*</sup> Qingfeng Yang<sup>1</sup>, Zhixun Zhang<sup>1</sup>, Jianwen Yu<sup>1</sup>, Yibo Zhang<sup>1</sup>, Wenjun Cheng<sup>1</sup>, Xuyin Li<sup>1</sup>

<sup>1</sup> State Key Laboratory of Tribology, School of Mechanical Engineering, Tsinghua University, China <sup>2</sup> Key Laboratory for Advanced Materials Processing Technology, Ministry of Education, China

Abstract. Modern electronic reconnaissance equipment covers almost all available electromagnetic bands, which seriously threatens the survival of military facilities on the battlefield. The research of stealth materials compatible with multiple frequency bands is particularly important but remains a challenging issue. As a kind of thermal insulation material, nano-sponge has application prospects in infrared stealth. Graphene/carbon nanotubes have excellent absorbing properties in terahertz band. It is an effective way to achieve infrared and terahertz compatible stealth by combining them. Here, we use mechanical vibration and vacuum sintering methods to prepare carbonized nano-sponges doped with graphene/carbon nanotubes. SEM images show that the three-dimensional network structure of nano-sponges is well retained, the graphene/carbon nanotubes are bound to its skeleton. Infrared emissivity of the prepared material can be adjusted widely (from 0.3 to 0.9 in the 3-5  $\mu$ m and 8–14  $\mu$ m atmospheric window) by using magnetron sputtering film deposition system to deposit metal materials with different thickness on the surface. Since the prepared material remains three-dimensional network structure and high porosity, its thermal insulation performance is almost unaffected. The infrared stealth capability changes with emissivity. Photos of thermal imaging camera confirm that the infrared stealth performance improved when emissivity decreased. The results of terahertz time-domain spectrometer show that the prepared material has excellent absorption properties at 0.3-2.5 THz. This work may provide a new strategy for the preparation of infrared and terahertz compatible stealth materials.

Keywords: Nano-Sponge; Graphene; Carbon Nanotubes; Infrared and Terahertz Stealth

### GNN1158 Determining the electronic structure of the outermost layer of graphene and related materials

#### Gunther G. Andersson

Flinders Institute for NanoScale Science & Technology, Flinders University, Australia

**Abstract.** Two-dimensional carbon materials like graphene and carbon nanotubes have a unique electronic structure. Directly measuring the electronic structure of such materials can be challenging for various reasons. The most important of these reasons is being able to separate in the measurements the electronic state of the outermost layer of the carbon material from the rest of the sample. In case of graphene a monolayer of the material is deposited onto a substrate and the electronic structure of graphene needs to be separated from the underlying substrate. In the case of carbon nanotubes challenges are separating the outer wall electronic structure from the inner wall electronic structure

(double- or multiwall carbon nanotubes) or purifying a sample such that only a single chirality is present (single wall carbon nanotubes). In a number of cases it is also not necessarily given that the carbon material does not contain functional groups attached to the outermost layer. Metastable induced electron spectroscopy (MIES) is an ideal tool for determining the electronic structure of the outermost layer of carbon materials. The method relies on the interaction of metastable helium atoms (He\*) with substrates leading to the emission of valence electrons. The method is similar to UV-photoelectron spectroscopy (UPS). MIES in contrast to UPS is sensitive exclusively to the outermost layer because the He\* only interact with the outermost layer of a sample.

## GNN1159 Metal oxides doped graphene oxide nanocomposites and their applications

#### Muhammad Akhyar Farrukh

Department of Chemistry, Forman Christian College (A Chartered University), Pakistan

**Abstract.** Multiple approaches have been carried out to synthesize the rare earth-transition metal oxides nanocomposites as well as graphene oxide and reduced graphene oxide doped with metal oxides for the purpose to achieve enhanced activities for the degradations of textiles pollutants, pesticides, organic pollutants, explosive materials etc.

We have successfully synthesized more than 50 nanocompostes with variety of metals. Various factors e.g. change in precursors, pH, temperature, feed rate, surfactants, solvents, methods of preparation, concentration of precursors, were studied which change the efficiency of the nanocomposites. Our focus is to synthesize nanocomposites having band gap in the visible region so that they may be used for enhanced catalytic activity under sun light.

The structural investigation, thermal degradation, crystallite size, morphology, surface and photocatalytic properties of synthesized samples were studied by using different characterization techniques i.e. Thermogravimetric analysis (TGA), Differential scanning calorimetry (DSC) Fourier transform-infrared spectroscopy (FTIR), Particle Size Analyzer (PSA), Powder X-ray diffraction (XRD), Scanning electron microscopy (SEM), Transmission electron microscopy (TEM), and Ultraviolet-Visible spectrophotometer (UV-VIS). Applications of nano-materials in formulation of nanofiltration nano-medicines, solar cells, forensics, slow release fertilizers, photodegradation, and nanocatalysts for synthesis of organic reactions were also studied.

Keywords: Nanocomposite; Graphene Oxide; Reduced Graphene Oxide; Characterization; Applications

### GNN1142 Borophene/graphene heterostructure as the anode of lithium-ion batteries with controlled interlayer spacing

Jianwen Yu<sup>1</sup>, Ming Zhou<sup>1, 2, \*</sup>, Mingyang Yang<sup>1</sup>, Qingfeng Yang<sup>1</sup>, Zhixun Zhang<sup>1</sup>, Yibo Zhang<sup>1</sup> <sup>1</sup>State Key Laboratory of Tribology, School of Mechanical Engineering, Tsinghua University, China <sup>2</sup>Key Laboratory for Advanced Materials Processing Technology, Ministry of Education, China

Abstract. Borophene has been predicted to be a potential anode material of lithium-ion batteries (LIBs) because of its high specific capacity, high mechanical strength and low diffusion barrier. However, borophene cannot be stable without metal substrates, impeding the industrial applications. Hence, we proposed to form van der Waals heterostructures to improve the stability of monocomponent

borophene, and by calculation found graphene to be an alternative substrate for stabilizing borophene as borophene/graphene (B/G) heterostructure. The graphene was considered as a framework with high conductivity, easy to fabricate, high chemical stability and mechanical strength, compared with other 2D materials, stabilizing borophene instead of the Ag(111) substrate and forming network structures, while borophene was designed for storing Li in anode of LIBs. We find that B/G has high adsorption energy of Li (-2.959eV), high theoretical specific capacity (1469.35mAh/g) and low diffusion barrier (0.613eV). And these properties change with the interlayer distance of B/G, theoretical specific capacity increasing from 1469.35 to 1763.22mAh/g and diffusion barrier decreasing to 0.353eV, benefitting for quick charge/discharge performance. Thus, the B/G heterostructure can be a perfect candidate as anode material for LIBs. Also, it will give us a new theoretical strategy to adjust properties of heterostructures anode by changing the morphotype of it.

**Keywords:** Borophene, Graphene Heterostructure, First-Principles, Interlayer Distance, Lithium-Ion Batteries

### GNN1167 Application of Graphene as transparent electrodes in PV solar cells

#### Ali Abdolahzadeh Ziabari

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Abstract. Using photovoltaic (PV) solar cells is one of the easiest and cheapest ways to generate clean renewable energy. Therefore, the need for efficient solar cells becomes more crucial. Generally, the solar cells are not that efficient. However, recent progresses in graphene-based solar cells have shown the reflectance of solar rays reduced by 20%, which provides a potential efficiency increase up to 20%. Currently, there are different variations of graphene-based solar cells being investigated. This article gives a comprehensive overview into the different types that are being investigated by academic and corporate researchers worldwide. The relation between optical transparency, sheet resistance, and the number of layers can be determined by a proportional decrease in both the optical transparency and the sheet resistance, with an increasing number of graphene layers. A single layer of graphene displays an optical transparency of 97.7%. A 3-layered graphene stack shows around 90.8% optical transparency and the addition of each layer corresponds to a 2.3% decrease in optical transparency. A single sheet of graphene produces a sheet resistance of 2.1 k $\Omega$ sq<sup>-1</sup> and 350  $\Omega$ sq<sup>-1</sup>, while retaining 90% optical transparency. The quenching effect of multiple graphene layers can be up to 11% greater than monolayer graphene, due to a higher hole accepting density of state. Altogether, compared to the conventional transparent conducting oxide (TCO) electrodes such as ITO and FTO, the graphene-based electrodes are very promising and efficient. In this presentation, in addition to a brief review of PV solar cells, the application of Graphene as transparent electrodes is studied.

Keywords: Solar Cells; Graphene; TCO; Photovoltaics; Renewable Energy

### GNN1168 Graphene hetero structures and other 2D materials

#### Rashid Jalila

Nanotechnology Research Center, Department of Physics, University of Engineering & Technology, Pakistan

Abstract. The isolation of two-dimensional graphene from the layered material graphite by using the simple and unusual method of repeated mechanical peeling by scotch tape has stunned the scientific

world. Rapid progress in graphene research and demonstration of proof-of-principle applications in short time has forced R&D organizations and industries to strongly focus on graphene in variety of areas. An attractive feature of graphene is its very high electronic quality that is generally expressed by the mobility of its charge carriers. Transport measurements revealed graphene's charge carrier mobility on usual Si/SiO2 ~ 5000-15,000 cm2V-1s-1, which is far less than graphene's predicted intrinsic mobility (in suspended graphene samples). Efforts to utilize electronic properties of new material graphene in the world of electronics and device technology have so far been achieved in the form of certain graphene-based transistors. High frequency graphene-based transistors have been shown to be applicable for applications in imaging, radar, data communication and high frequency spectroscope. However, in the strongest industrial area of digital applications, the use of graphene for device electronics still needs much more advancement since the absence of an intrinsic band gap in graphene's electronic structure composes an as yet not overcome hurdle. Aside from technological applications, many phenomena of quantum physics can be probed and studied in detail in the excellent quality electronic system of graphene. The superior carrier mobility of graphene compared to other semiconductor materials is a quite attractive electronic feature. The work presented here include the electrical measurements of graphene-based field effect transistors FET's. Cross sectional view of graphene hetero structures and investigation of Coulomb's drag and ballistic transport in graphene.

Keywords: Graphene; Mobility; Boron nitride

#### GNN1170

# 2-Dimensional transition metal dichalcogenides (TMD): next generation of saturable absorber material for pulsed laser generation

#### Harith Ahmad, Rizal Ramli, Ooi Shok Ing, Norazriena Yusoff, Siti Aisyah Reduan and Muhamad Zharif Samion

**Abstract.** Transition metal dichalcogenides (TMD) are highly desirable 2-Dimensional (2D) materials that have become the focus of intense investigative efforts over the last decade. The desirable properties of TMD arise from the many possible combinations of a transition metal atom with two chalcogen atoms to form the 2D TMD material, thus giving it different electronic and optical properties and remarkable optoelectronic properties. In the development of 2D materials for photonics application, TMD materials have been widely used as saturable absorbers (SA) to induce Q-switching and modelocking within fiber laser cavities. The generated pulsed laser is highly desired for potential applications, ranging from medicine, environmental sensing, telecommunication, industrial, and material processing. Researchers have a great interest towards optical fiber laser due to its advantages of being compact and robust system as well as cost-effective operation compared to their conventional bulk laser counterparts. In the past few years, we have successfully producing the Q-switched and mode-locked fiber laser operating at various wavelength regions with the assistance of different type of TMD materials which acts as a passive optical switch to modulate intracavity loss and enables access to a wide space of pulse parameters. Our finding has revealed the great potential of the 2D TMD materials for the ultrafast photonics community.

# Session 3\_ Polymers and Composite Materials: Synthesis, Structure and Characterization

Time: 14:00-18:55, November 3, 2020

**Session Chairs:** 

14:00-16:10Prof. Jamil Akhtar, Manipal University Jaipur, Rajasthan India16:45-18:55Dr. Bo Lin, Huizhou University, China

Session Room Link: http://www.academicconf.com/teamslink?confname=pcm2020

14:00-14:25	PCM2949	Characterization and application of superhydrophobic and superoleophilic OTS-LDH/melamine sponge Dr. Bo Lin, Huizhou University, China
14:25-14:40	PCM3030 (Video)	Fabrication of micro-pattern on polypropylene sheet using hot embossing technique for packaging applications Dr. Charinee Winotapun, National Metal and Materials Technology Center, National Science and Technology Development Agency, Thailand
14:40-14:55	PCM3042	The dynamic behavior of water droplets on superhydrophobic surface with nanoscale roughness <i>Ms. Hyae Rim Hong, Seoul National University, Republic of Korea</i>
14:55-15:10	PCM3052 (Video)	Development of multifunctional additives for highly strength and biodegradable nitrile butadiene composites Dr. Nurhidayatullaili Muhd Julkapli, Universiti Malaya, Malaysia
15:10-15:25	PCM2966	Features of amplitude frequency characteristics of abs plastic 3-d printed metamaterial sample Dr. Natalia Shirgina, Lomonosov Moscow State University, Russia
15:25-15:50	PCM3024 (Video)	Diamond magnetometry for detecting polymer degradation Prof. Romana Schirhagl, Groningen University, the Netherlands
15:50-16:10	PCM3043	Analysis of toxic products during the burning of chemically set plastics Ms. Kamila Mizera, Central Institute for Labour Protection - National Research Institute, Poland
16:10-16:45		BREAK
16:45-17:10	PCM3063	Hybrid coagents and ionic liquids applied to support the peroxide crosslinking of saturated elastomers Assoc. Prof. Magdalena Maciejewska, Lodz University of Technology, Poland
17:10-17:25	PCM3045	The effect of electron irradiation and thermal treatment on the surface of carbon materials Dr. Beata Lesiak-Orlowska, Institute of Physical Chemistry Polish Academy of Sciences, Poland
17:25-17:40	PCM3018 (Video)	Machine learning algorithms for the prediction of the mechanical properties of railways' rail pads <i>Dr. Jose A. Sainz-Aja, University of Cantabria, Spain.</i>
17:40-17:55	PCM3038	Flammability of PIR based sandwich panels Dr. Maciej Celinski, Central Institute for Labour Protection - National Research Institute, Poland

17:55-18:10	PCM3074 (Video)	Characterization of additive manufactured aerospace-grade
		thermoplastic composites
		Dr. Audrey Diouf-Lewis, École Polytechnique de Montreal, Canada
18:10-18:25	PCM3076	SOI, Diffused and Polysilicon versions in the fabrication of
		piezoresistive MEMS pressure sensor: A qualitative process
		analysis
		Prof. Jamil Akhtar, Manipal University Jaipur, Rajasthan India
10.25 10.40	PCM2970	Wet-spun biodegradable fibers modified with bioactive agents
18:23-18:40		Dr. Natália C. Homem, University of Minho, Portugal
18:40-18:55	PCM3069	Experimental study on polymer/graphene oxide composite as a fluid
		loss agent for water-based drilling fluids
		Ms. Ma Jingyuan, China University of Geosciences (Beijing), China

## **Abstracts of Session 3**

#### PCM2949 Characterization and application of superhydrophobic and superoleophilic OTS-LDH/melamine sponge

#### Bo Lin

School of Chemistry and Materials Engineering, Huizhou University, China

**Abstract.** The *n*-octadecyltrichlorosilane (OTS) had been coated onto the layered double hydroxides (LDH), and the resultant composite of OTS-LDH was further loaded on the surface of melamine sponge by a soaking method to obtain the OTS-LDH/melamine sponge for efficient oil absorption in this work. The surface chemical compositions of the OTS-LDH/sponge and its precursors were characterized by EDS, XPS, and FTIR. The results from EDS, XPS, and FTIR showed that the OTS had been successfully coated on LDH. The surface morphologies from SEM for the the melamine sponge before and after modification illuminated that the surface skeleton of the OTS-LDH/sponge took a rough micro-nanostructure and the surface had been loaded with the low surface energy material of OTS, which made the OTS-LDH/sponge display the superhydrophobic properties. The experiments of oil-water separation proved that the OTS-LDH/sponge took an excellent oil-water efficiency and the modified sponge still took the better oil-water separation performance with an oil absorption capacity of 13.7–21.1 times of the mass of the pristine sponge even after undergoing repeated extrusion for 60 times during the repeated cycle test.

**Keywords:** Melamine Sponge; Layered Double Hydroxides; *N*-Octadecyltrichlorosilane; Superhydrophobic; Oil-Water Separation

#### PCM3030

## Fabrication of micro-pattern on polypropylene sheet using hot embossing technique for packaging applications

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Abstract. The micro-patterns on polypropylene (PP) surface were fabricated using a hot embossing technique at various temperatures and applied forces. To evaluate the replication quality of the hot

embossing process, an effective filling ratio was calculated from a volume of formed pattern divided by a volume of mold cavity. In this research, it was found that the effective filling ratio increased with increasing embossing temperature. For instance, under a constant force of 100 N, filling ratio increased from 0.11 to 0.32 when the embossing temperature was increased from 160 to 175 °C. With increasing applied force, the filling ratio also increased. The filling ratio increased and reached the maximum value of 0.94 at the embossing temperature of 175°C under the force of 300 N. In order to study the effect of easy-opening property for packaging applications such as tray and lidding film package system, two sets of PP sheets including micro-patterned PP sheet and PP sheet without micropattern were heat-sealed with commercial biaxially oriented polypropylene (BOPP) films at various temperatures. Sealing pressure, dwell time and the full sealing contact area between the BOPP and PP sheet was constant. The micro-patterned PP sheet showed the reduction of seal strength compared to PP sheet without micro-pattern owning to its low contact area. At the sealing temperature of 150 °C, the micro-patterned PP sheet with the sealing contact area of only  $5.44 \times 10^6 \,\mu\text{m}^2$  (~ 10% of full sealing contact area) revealed the easy peel property and the seal strength was around 1.18 N/50 mm<sup>2</sup> which was acceptable for the easy peel criteria (0.9-2.7 N/50 mm<sup>2</sup>). Overall results are beneficial for understanding the important key conditions of the hot-embossing technology for the fabricating micropattern on polymeric surface. Moreover, the results clearly demonstrated that micro-pattern on PP sheet films can be applied for easy-peel property for packaging applications.

Keywords: Hot Embossing; Polypropylene; Easy-Open Packaging

**Acknowledgements:** The authors gratefully acknowledge financial support of this study from National Metal and Materials Technology Center (MTEC), Thailand. We are thankful to Prof. Hiroshi Ito from Yamagata University, Japan, for hot embossing equipment support.

## PCM3042 The dynamic behavior of water droplets on superhydrophobic surface with nanoscale roughness

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Department of Textiles, Merchandising and Fashion Design, Seoul National University, Republic of Korea

Abstract. The effects of the nanoscale roughness of superhydrophobic surface on the dynamic behavior of water droplets were analysed. For this, polyvinylidene fluoride (PVDF) nanowebs with different surface structures and wettability were fabricated by electrospinning at various concentrations. Nanoscale roughness was controlled by the CF<sub>4</sub> plasma etching treatment time, and the boundary treatment conditions where the dynamic behavior of the water droplets transit from pinning to rolling down were investigated. After introducing nanoscale roughness, static contact angles of the electrospun PVDF nanowebs increased and the water droplets rolled off easier than before. As a result, the water droplets on the surface of PVDF nanoweb with 20 wt% concentration showed a pinning phenomenon, but after the plasma treatment for more than 5 min, the static contact angle increased to  $160^{\circ}$  or more, and water droplets were easily rolled off, demonstrating the lotus effect. In addition, the lotus effect was observed for the plasma treatment over 10 min of 15 wt% nanoweb. Thus, it was confirmed that when the three-phase contact line formed by the water droplet on the surface is discontinuous and the contact area is reduced between the surface and the droplet, containing air layers on the interface coming in contact with the droplets. This leads to the decrease in adhesive force and the impact of negative pressure, easier to exhibit lotus effect. This finding can contribute to the application of the droplet manipulation in microfluidic devices or self-cleaning, thereby producing surfaces fitting to practical purposes.

**Keywords:** Superhydrophobicity; Nanoscale Roughness; Dynamic Behavior of The Water Droplets; Pinning; Lotus Effect

**Acknowledgements:** This work was supported by the National Research Foundation of Korea (NRF) grant funded by the Korea government (Ministry of Science and ICT; Grant No. NRF-2016M3A7B4910940 and the Ministry of Education; Grant No. NRF-2019R1A6A3A13095712); by Korea Institute for Advancement of Technology (KIAT) grant funded by the Korea Government (MOTIE) (P0012770, Professional Human Resources Training Project).

#### PCM3052

# Development of multifunctional additives for highly strength and biodegradable nitrile butadiene composites

Erfan Suryani abd Rashid and Nurhidayatullaili Muhd Julkapli

Nanotechnology and Catalysis Research Center (NANOCAT), Institute for Advanced Studies (IAS), Universiti Malaya, Malaysia

Abstract. Nitrile butadiene (NBR) gloves have limitation on its mechanical, biodegradability and free radical stability which makes its commercial and industrial application being restricted. NBR gloves has lower strength, flexibility and puncture-resistance than natural rubber, instable for chemical agents and natural disposal problem. With that in mind, sulfonated-nanocystalcellulose-antioxidant has been designed and applied in this project as multifunctional nanomaterial served as additive not only to improve the mechanical and stability properties of NBR gloves but also induced some degree on biodegradability properties. Indeed, the carbon content and natural derivatives on nanocellulose provides NBR gloves with bio-disposal characteristics. Sulfonated-nanocrystal cellulose has been synthesized with different aspect ratio to investigate the mechanical and thermal properties of the NCC/NBR composites with defined optimal loading. The production of sulfonated-nanocrystal cellulose using hydrolysis acid method and NBR composites has been prepared using dipping method to simulate the real condition of glove production. The addition of 2 phr sulfonated-nanocrystal cellulose has increased thermal stability and activation energy of NBR up to 75%. Meanwhile, the storage modulus of composites increased by 12 GPa at the 3 phr loading of additive. Tensile strength also shows increasing at 3phr loading with the value 18GPa. Surface modification of nanocellulose using Gallic Acid (GA) is prepared, namely sulfonated-nanocrystal cellulose-antioxidant. The attachment of GA is not causing any changes in morphology, but the crystallinity of the additive reduces significantly with the highest GA. The chemical bonds were confirmed using Fourier Transmission Infra-Red (FTIR) at 1645cm<sup>-1</sup>. DPPH test was performed to study the effectiveness of GA in non-modified nanocellulose and sulfonated-nanocrystal cellulose-antioxidant with ratio 1:4 gives the lowest IC<sub>50</sub> value which is less than 3mg. From the FTIR, FESEM, TEM, AFM analysis, it has been revelaed that, sulfonated-nanocrystalcellulose-antioxidant obtained a good interfacial bonds and hydrogen bonds with NBR polymeric chains which contribute to the above-mentioned results. Furthermore, the highly crystalline and nanosized of additives played important role to improve the flexibility and strength of NBR composites.

Keywords: Nanocellulose; Surface functionalization; Compatibility; Rubber Compounds

**PCM2966** To avoid repeatability issue, this abstract will be available after the full paper is published in the conference proceedings.

## PCM3024 Diamond magnetometry for detecting polymer degradation

Runrun Li, Sandeep Padamati, Aryan Morita, Aldona Mzyk and Romana Schirhag<sup>\*</sup> Department of Biomedical Engineering, Groningen University, University Medical Center Groningen, the Netherlands

**Abstract.** Diamond magnetometry is a new technology, which allows nanoscale MRI. It is based on a fluorescent defect in diamond, which changes its optical properties based on its magnetic surrounding. Since optical signals are much easier to detect this method offers unprecedented sensitivity, which is orders of magnitude better than conventional magnetic resonance techniques. Here we apply diamond magnetometry to follow the degradation of a polymer. More specifically, we chose to investigate polylactic acid for our proof of principle study due to its relevance as a biodegradable polymer. To study the degradation process, we embedded fluorescent nanodiamonds, which function as sensors. We further added gadolinium to the degradation medium. Since gadolinium is an MRI contrast agent it can be detected via its spin noise. When the polymer degrades, and the gadolinium can get closer to the sensors. Thus, we are able to follow the process in real time.

Keywords: Diamond; Polymer; NV Center; Magnetometry; Degradation

## PCM3043 Analysis of toxic products during the burning of chemically set plastics

Kamila Mizera<sup>\*</sup>, Kamila Sałasińska, Maciej Celiński and Agnieszka Gajek Department of Chemical, Aerosol and Biological Hazards, Central Institute for Labour Protection -National Research Institute, Poland

**Abstract.** The thermal decomposition and combustion of plastics used in construction and means of transport may occur during major industrial accidents, road accidents, or fires in households. Some experimental procedures can be used to test the products of combustion, mainly relying on laboratory scale test methods which have been developed in an attempt to recreate the decomposition conditions of products released during fires.

Burning plastics is a process that requires many physical and chemical transformations, during which a mixture of chemical substances with a complex composition is created. Every fire, regardless of where it occurs, is characterized by the production of smoke, consisting of a mixture of air and gases with solid and liquid particles resulting from incomplete combustion. The products of combustion or thermal decomposition (pyrolysis) occurring in the fire environment create a complex mixture of gases and suspended particles, which poses many threats to humans. During the combustion of polymers, a large amount of thermal energy and exhaust gases are released, which are suspended in the air in the form of heated soot and ash particles, as well as gaseous products.

Chemically set plastics are polymers that form a cross-linked structure under the influence of chemical factors. They cure at room temperature under the action of special substances. This reaction is faster at elevated temperatures. Epoxy resins (EP), unsaturated polyester resins (UP) and polyisocyanurate foams (PIR) are among the most commonly used chemically hardening materials in construction and transport.

At this stage of the project, we focused on the assessment of toxic combustion products by examining commercially available PIR foams, EP and UP systems to verify the connection of the Purser furnace with a system of selective analyzers based on the operation of FT-IR infrared spectrometry.

Keywords: Chemically Set Plastics; Purser Furnace; FT-IR Spectroscopy; Toxic Products

Acknowledgements: This paper has been based on the results of a research task carried out within the scope of the fifth stage of the National Programme "Improvement of safety and working conditions" partly supported in 2020–2022 — within the scope of research and development — by the Ministry of Science and Higher Education/National Centre for Research and Development. The Central Institute for Labour Protection – National Research Institute is the Programme's main coordinator.

### PCM3063 Hybrid coagents and ionic liquids applied to support the peroxide crosslinking of saturated elastomers

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Abstract. The vulcanization of rubber is one of the most important processes in elastomer technology. During this process, crosslinking reactions occur, resulting in useful materials that possess the required performance. The most popular curing agents for saturated polymers are organic peroxides. Peroxide vulcanizates are resistant to thermal aging and ozone, but their poor mechanical and dynamic properties compared to sulfur-crosslinked elastomers limit their industrial applications. In order to enhance the mechanical properties, crosslink density, and vulcanization efficiency of rubber compounds cured with peroxides, coagents are commonly used, like triallyl cyanurate, triallyl isocyanurate, and diallyl phthalate. In this work, nanosized CaO with its surface grafted with an unsaturated acid, such as allylmalonic acid (ALA), was applied as a coagent for the peroxide crosslinking of an ethylene-propylene copolymer (EPM). A hybrid coagent consisting of an inorganic core and an organic shell was achieved in this way. 1-Butyl-3-methylimidazolium ionic liquids (ILs) with different anions were applied to improve the dispersion of CaO/ALA in the elastomer matrix, as well as to catalyze the interfacial crosslinking reactions. The CaO/ALA with ILs reduced the vulcanization time of the rubber compounds. Their application resulted in an increased vulcanizate crosslink density and improved tensile strength compared to the pure peroxide system. The influence of 1-butyl-3-methylimidazolium ILs on EPM vulcanization and performance depended on the ionic liquid's anion. The most active IL seemed to be that with the tetrafluoroborate anion.

Keywords: Coagent; Ionic Liquid; Peroxide Crosslinking; Elastomer; Calcium Oxide

#### PCM3045 The effect of electron irradiation and thermal treatment on the surface of carbon materials

#### B. Lesiak\*

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**Abstract.** The chemical properties of surfaces of carbon materials submitted to electron irradiation (to 300 C cm<sup>-2</sup>) and thermal treatment were studied by electron spectroscopic methods, i.e. X-ray photoelectron spectroscopy (XPS), X-ray induced Auger electron spectroscopy (XAES) and reflection electron energy loss spectroscopy (REELS), revealing different in-depth information. The studies concern selected polymers and multiwall carbon nanotubes (MWCNTs). The approaches of evaluating

the electron spectroscopic methods spectra include: (i) the fitting of XPS C 1s spectrum, (ii) analysis of the width of XAES C KLL spectrum (parameter D), (iii) analysis of the REELS spectrum surface and bulk components, (iv) spectra line shape analysis by the pattern recognition method using the fuzzy k-nearest neighbors rule and (v) evaluation of the hydrogen content using the effect of electron "recoil" on atom.

Results obtained from analysis by the same electron transition are in agreement. Otherwise, an inhomogeneous in-depth distribution of C  $sp^3/sp^2$  bonds is observed under electron irradiation and temperature. Graphitization proceeds with a higher rate at the surface. The highest stability exhibits polyethylene of ultra-high density. The surface degradation due to X-ray irradiation is negligible in comparison to electron beam irradiation.

**Keywords:** Polymers; MWCNTs; Surface; Electron Spectroscopic Methods; Electron Irradiation; Temperature Treatment

**PCM3018** To avoid repeatability issue, this abstract will be available after the full paper is published in the conference proceedings.

## PCM3038 Flammability of PIR based sandwitch panels

Maciej Celiński<sup>1\*</sup>, Kamila Sałasińska<sup>1</sup>, Kamila Mizera<sup>1</sup> and Agnieszka Gajek<sup>1</sup> Department of Chemical, Aerosol and Biological Hazards, Central Institute for Labour Protection -National Research Institute, Poland

**Abstract.** A standard sandwich panel consists of: two external layers (responsible for the panel's bending strength) and an internal thermal insulation layer (thermal insulation core) ensuring appropriate thermal and acoustic insulation parameters of the entire barrier. The most important structural element of a sandwich panel is its core.

The materials used as a thermal insulation core are a commonly used and easily accessible panels:

- EPS (made of expanded polystyrene foam with apparent density of about 16 kg/m3 and reaction to fire class E),

- mineral wool (made with fibre pulled out of melted magma rock, thanks to which they are practically non-flammable, but much heavier, which often does not allow for their use on structural elements such as: the wall, the wall and the wall. This is why they are practically non-flammable and much heavier, which often does not allow for their application on structural elements, e.g. roofing elements),

- polyurethane and polyisocyanurate foams (PUR and PIR - closed cell foams, characterized by low weight and good insulating properties).

Polyurethane and polyisocyanurate foams differ in the amount of isocyanate in relation to the polyol used in the production process. PIR foams typically has isocyanate/polyol ratio higher than 180 (200-300), while PUR indices are normally around 100. Such a large excess of one component results in additional reactions between its molecules. In PIR foams, a very important and desirable reaction is the trimming reaction (three isocyanate molecules undergo a cyclization reaction with between C=N groups leading to a six-part ring called an isocyanurate trimmer. Such a change in composition translates into the functional properties of the foam, especially its flammability. Apart from isocyanate/polyol ratio, the type of used compounds also influences the flammability of polyurethane foams. In our work we plan to develop PIR foam containing non-halogen flame retardants to be used

in sandwich panels. At this stage of the project we focused on the comparison of PIR foams produced on the basis of various types of polyols and isocyanates and comparing them to commercially used materials that constitute the core of sandwich panels.

Keywords: Sandwich Panels; Polyisocyanurate Foams; Halogen-Free Flame Retardants; Heat Release Rate

Acknowledgements: This paper has been based on the results of a research task carried out within the scope of the fifth stage of the National Programme "Improvement of safety and working conditions" partly supported in 2020–2022 — within the scope of research and development — by the Ministry of Science and Higher Education/National Centre for Research and Development. The Central Institute for Labour Protection – National Research Institute is the Programme's main coordinator.

## PCM3074 Characterization of additive manufactured aerospace-grade thermoplastics composite

Audrey Diouf-Lewis<sup>1,\*</sup>, Loic Mastromatteo<sup>1</sup>, Rouhollah D. Farahani<sup>1</sup>, Nicola Piccirelli<sup>2</sup>, and Daniel Therriault<sup>1</sup>

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Abstract. Additive manufacturing (AM), or 3D printing has demonstrated a great potential for the fabrication of complex shape polymer parts. As one of the most popular AM methods, Fused Filament Fabrication (FFF) is easy-to-use with common printable materials like Poly-lactic acid (PLA) and Acrylonitrile-butadiene-styrene (ABS). Regarding aerospace-grade thermoplastics, Poly-ether-etherketone (PEEK) is one of the most interesting materials to be used as 3D printing feedstock for advanced engineering applications. However, PEEK material is particularly challenging to process by FFF due to its high processing temperature (e.g., 380°C) that may cause several structural defects such as warpage, delamination, etc. The objective of this project is to formulate a reinforced PEEK material featuring high mechanical properties while printable in FFF printers for the manufacturing of parts with complex shapes. Here, we formulated PEEK composite materials by mixing PEEK and chopped carbon fiber (CF) at 5 different concentrations of 5%wt., 10%wt., 15%wt. 20%wt., 25%wt. and 30%wt in order to investigate the effect of CF concentration on the mechanical properties of the resulting composite materials. The mechanical test was performed on 0.6 mm-diameter filaments fabricated with a commercial 3D printer (AON-M2 3D printer). With the help of µ-CT tomography, we explored the composite microstructural features such as the CFs dispersion, adhesion to the PEEK matrix, and the quantity of porosity present in the 3D printed filament. Our developed material exhibits a significant improvement of the Young's modulus which proves that PEEK composite could be promising for the AM of non-structural parts in advanced engineering applications.

**Keywords:** Poly-Ether-Ether-Ketone (PEEK); Additive Manufacturing; Carbon Fiber; µ-CT Tomography; Thermoplastics Composite

#### PCM3076 SOI, Diffused and Polysilicon versions in the fabrication of piezoresistive MEMS pressure sensor: A qualitative process analysis

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**Abstract.** Piezoresistive Micro-Electro-Mechanical-Systems (MEMS) pressure sensor is in high demand owing to its versatile applications almost in all sectors of modern development and the fabrication process compatibility with silicon technology. Piezoresistors are configured in Wheatstone's bridge configuration over a movable diaphragm subjected to the pressure. A controlled realization of silicon diaphragm by employing anisotropic etching of crystalline silicon whereas assists in accurate placement of piezoresistors, the silicon being a piezoresistive material further adds for resistors realization with desired accuracy, repeatability and stability. The fabrication technology of the piezoresistive pressure sensors is driven by the way silicon piezoresistors are realized and their subsequent functional behavior in real time working environment (1). Three technology routes; Silicon on Insulator (SOI), Crystalline doped and Doped polysilicon, are discussed in this work for their respective process qualitative analysis. Technology of MEMS piezoresistive pressure sensors for low pressure to high pressure applications at elevated operating temperature is shown for the three versions.

## PCM2970 Wet-spun biodegradable fibers modified with bioactive agents

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Aims: Chronic wounds (CW) are characterized by a defective cell matrix, high numbers of bacteria (colonies) and moisture imbalance. Current treatments include a set of costly therapies which are inefficient in many cases, due to increased antimicrobial drug resistance. Antimicrobial therapies combining dressing and antimicrobial peptides (AMPs), which exhibit both antimicrobial and regenerative characteristics, have been suggested as potential alternatives for treating CW. Among these we can cite the Tiger 17, derived from tigerinine, which is relatively new but has shown significant effects in three stages of wound healing, and the 22-amino-acid peptide pexiganan, which has exhibited a broad-spectrum of antibacterial activity against both Gram-negative and Gram-positive bacteria. Also, recent studies have demonstrated that biomaterial functionalization with essential oils, namely the cinnamon leaf oil and the niaouli oil, have significant antimicrobial potential against multidrug-resistant pathogens. In this study, we report the production of polymeric dressings with fibrous, biocompatible and biodegradable 3D structures, functionalized with immunoregulatory AMPs and essential oils for the treatment of CW. Fibers were successfully produced by different combinations of natural and/or synthetic polymers (e.g. cellulose, poly(vinyl alcohol) and polycaprolactone) and AMPs and essential oils, using the wet-spinning technique. Fibers were then arranged in 3D structures using industrial-like looms. The resultant dressings showed great potential for applications in CW healing by protecting against infection while accelerating tissue healing and regeneration.

Keywords: Fibrous Dressings; Antimicrobial Peptides; Essential Oils; Wound Healing

Acknowledgements: This work was funded by FEDER and FCT funds, under the scope of the project PEPTEX with reference POCI-01-0145-FEDER-007136 and project UID/CTM/00264/2019 of Centre for Textile Science and Technology (2C2T), funded by national funds through FCT/MCTES.

#### PCM3069

## Experimental study on polymer/graphene oxide composite as a fluid loss agent for water-based drilling fluids

#### Ma Jingyuan

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**Abstract.** The wellbore instability caused by the penetration of drilling fluid into the formation is a vital problem in the drilling process. In this study, we synthesized a polymer/graphene oxide composite (PAAN-G) by aqueous free radical polymerization as a fluid loss additive in water-based drilling fluids. The polymer (PAAN) is a terpolymer of acrylamide (AM), 2-acrylamide-2-methyl-propane sulfonic acid (AMPS), and N-Vinylpyrrolidone (NVP). The composition, micro-morphology and thermal stability properties of PAAN-G were characterized by Fourier transform infrared spectroscopy (FT-IR), transmission electron microscopy (TEM) and thermal gravity analysis (TGA). According to the American Petroleum Institute (API) standards, the influence of PAAN-G on the rheological and filtration properties of bentonite-based mud was evaluated. Experimental results show that even at high temperatures, PAAN-G can still significantly improve the rheology and filtration properties of bentonite-based mud containing salt ion contamination. The fluid loss control performance in bentonite-based through particle size distribution and scanning electron microscope (SEM). PAAN-G can effectively improve the quality of drilling fluid filter cake, making it thinner and denser.

Keywords: Polymer/graphene oxide composite; Drilling fluid; Fluid loss; Rheology

# Session 4\_ Fibers, Multi-Functional Composites and Novel Applications

Time: 08:30-12:40, November 4, 2020

**Session Chairs:** 

08:30-10:50Dr. Wong King Jye, Universiti Teknologi Malaysia, Malaysia11:00-12:55Assoc. Prof. Ning Li, Xingzhi College of Zhejiang Normal University, China

Session Room Link: http://www.academicconf.com/teamslink?confname=pcm2020

08:30-08:55	PCM3072	Nanocomposites of PBAT and cellulose nanocrystals Prof. Carolina Morelli, Federal University of Pernambuco, Brazil
08:55-09:10	DCM2046	Quantitative approaches to characterization of nanoparticle mixing
	(Video)	in polymer nanocomposites
	(video)	Dr. Jayadurga Iyer Ganapathi, Stevens Institute of Technology, USA
09:10-09:35	PCM3055	A composite material for interconnections in advanced electronics Prof. Cher Ming Tan, Chang Gung University
09:35-10:00	PCM3059 (Video)	Lightning induced damage of carbon fiber reinforced polymer composites based on its dynamic electric conductive model
	( ,	Prof. Xueling Yao, Xi'an Jiaotong University, China
10:00-10:25	PCM3062 (Video)	Near-infrared absorbing phosphate ester copper complex containing resin material for window application <i>Mr. Nacki Hayashi, Kuraha Corporation, Japan</i>
		Progress of structural manipulation for producing high performance
10:25-10:50	PCM3061	Nd <sub>2</sub> Fe <sub>14</sub> B/Fe(Co) nanocomposite permanent magnets Dr. Fengqing Wang, Ningbo Institute of Material Technology and Engineering, Chinase Academy of Sciences (CAS). China
10.20-11.00		BREAK
10.50 11.00		Electrospinning and in-situ hierarchical thermal treatment to tailor
11:00-11:15	PCM3065	$C-NiCo_2O_4$ nanofibers for tunable microwave absorption
		Dr. Min Zhang, Beijing Institute of Technology, China
11:15-11:30	PCM3040	A new method for mixed-mode I/II/III delamination test Dr. Wong King Jye, Universiti Teknologi Malaysia, Malaysia
		Spherical and sub-micron scale lignin particles as multifunctional
11.30-11.45	PCM2973	fillers for PVA composite films
11.30-11.45		<i>Ms.</i> Bongkot Hararak, National Science and Technology Development Agency, Thailand
		Effect of mixing ratio on the superhydrophobicity of
11.45-12.00	PCM3036	polyester/cotton fabric treated with alkaline hydrolysis and thermal
11.45-12.00		aging
		Ms. Hyewon Kim, Seoul National University, Korea
		Exploration of new applications of metal matrix
12:00-12:25	PCM3073	composites/nanocomposites manufactured by stir casting and
12100 12120		powder metallurgy
		Dr. Pallav Gupta, Amity University Uttar Pradesh, India
		Characterization of brominated natural rubber by solution state 2D
12:25-12:40	PCM3077	NMR spectroscopy Dr. Nuorn Choothong, Rajamangala University of Technology Rattanakosin, Thailand
12:40-12:55	PCM3011	Surface modification of h-BN and its influence on PVA properties Dr. Xiaodong Wang, University of Science and Technology of China, China

## **Abstracts of Session 4**

#### PCM3072 Nanocomposites of PBAT and cellulose nanocrystals

#### Carolina Morelli

#### Federal University of Pernambuco, Brazil

Abstract. Polybutylene adipate-co-terephthalate (PBAT) is a biodegradable polymer which properties could be improved with the incorporation of renewable and biodegradable reinforcements as cellulose nanocrystals (CNC). Nonetheless, CNC high polarity difficults its dispersion and compatibility with less polar polymers. Superficial chemical modifications in CNC aim to circumvent this problem. This presentation intend to present results regarding CNC grafted with an aliphatic and an aromatic isocyanate and incorporated in PBAT matrix through solvent casting and melt extrusion. The treated-CNC reinforced composites displayed improved mechanical properties, with an increase up to 120% and 40% in elastic modulus and tensile strength, respectively. Rheological analysis confirmed the achievement of a percolated network in the composite with 10wt% of the treated-CNC. The best results were obtained with CNC grafted with the aromatic isocyanate, probably due to the  $\pi$ - $\pi$  interactions between the phenyl rings grafted onto the CNC molecules and the aromatic rings of the polymeric chain, as indicated by Raman spectroscopy.

## PCM3046 Quantitative approaches to characterization of nanoparticle mixing in polymer nanocomposites

Jayadurga Iyer Ganapathi<sup>1</sup>, Dilhan M. Kalyon<sup>2, 3</sup> and Frank T. Fisher<sup>1</sup> <sup>1</sup>Department of Mechanical Engineering, Stevens Institute of Technology, USA <sup>2</sup>Department of Chemical Engineering and Materials Science, Stevens Institute of Technology, USA

<sup>3</sup>Department of Biomedical Engineering, Stevens Institute of Technology, USA

Abstract. Polymer nanocomposites are of tremendous interest in the pursuit of light-weight multifunctional materials with outstanding physical properties. However, obtaining a uniform nanoparticle dispersion during manufacturing is a known technological challenge as most studies regarding CNT dispersion and distribution are still qualitative in nature. Here a systematic study was conducted to incorporate carbon nanotubes (CNTs) in polycaprolactone (PCL) using a multi-stage sonication process, with Stage 1 sonication of CNT/solvent followed by Stage 2 sonication of the preprocessed CNT/solvent with the polymer. Characterization techniques such as optical microscopy, image analysis, thermogravimetric analysis, and DSC were used to quantitatively characterize the CNT dispersion and distribution within the polymer nanocomposite using Mixing Indices. In addition, the shear induced crystallization (SIC) behavior of the nanocomposite was used as an indirect measure to characterize the dispersion and distribution of CNT aggregates. Shear-induced crystallization has been demonstrated to be highly sensitive to crystal nucleation initiated by the tremendous surface area provided by the embedded nanoparticle. In particular, shear-induced crystallization occurred at a faster rate when the nanocomposites exhibited greater homogeneity (as characterized by the Mixing Indices) and was found to be a more sensitive indicator of the mixing states of the CNTs in comparison to the more commonly used linear viscoelastic rheological material functions. In this manner the coupled use of these characterization techniques was able to reveal subtle differences between different dispersion states. Specifically, here it was shown that Stage 1 sonication plays a critical role in the dispersion of nanoparticles in the polymer matrix while, on the other hand, Stage 2 sonication was only minimally effective in further enhancing the nanoparticle dispersion.

## PCM3055 A composite material for interconnections in advanced electronics

Cher Ming Tan<sup>1,2</sup>

<sup>1</sup>Center for Reliability Science and Technologies, Chang Gung University <sup>2</sup>Center for Reliability Engineering, Ming Chi University of Technology

**Abstract.** VLSI Interconnects are essential as billions of transistors in an IC are interconnected to form a working circuit specific to achieve certain functions. With the advent of IC technology, the line-width of VLSI interconnects is shrinking and hence their reliability is deteriorating significantly. Copper (Cu) has remain a prime choice for an interconnection material in Semiconductor Industries for years owing to its best balance of conductivity and performance. However, Cu interconnects are running out of steam, but complete replacement of Cu is not trivial due to many considerations to be considered. There has been proposal of using Carbon Nanotubes, 2D materials like Graphene, etc. as alternatives but these proposals presented difficult challenges to be answered. Scalability, manufacturability, ability to be integrated in current semiconductor process are some of the major challenges.

Owing to the excellent properties of Graphene, including electrical and thermal conductivities, high current density tolerance and high electromigration reliability on Graphene Interconnects, Graphene is likely to be the most suitable candidate for future interconnections. This work presents our proposal on the novel composite material which is a copper interconnect with Graphene sandwiched in between. The synthesis method and its performance as well as reliability are proven experimentally by our group and will be presented. With such a composite material as interconnections, the VLSI-IC industry and even printed circuit board industry can enjoy high performance and highly reliable interconnections.

## PCM3059 Lightning induced damage of carbon fiber reinforced polymer composites based on its dynamic electric conductive model

Xueling Yao<sup>1\*</sup>, Jinru Sun<sup>1, 2</sup>, and Jingliang Chen<sup>1</sup>

<sup>1</sup>State Key Laboratory of Electrical Insulation and Power Equipment, Xi'an Jiaotong University, China

<sup>2</sup>Institute of Polymer Materials and Plastics Engineering, Clausthal University of Technology, German

**Abstract.** As a natural discharge phenomenon with high voltage and high current, lightning strike seriously affects the safe operation of aircrafts. The proportion of the carbon fibre reinforced polymer (CFRP) composite continues to grow in commercial aircraft, military aircraft, unmanned aircraft and stealth aircraft due to its mechanical advantages of superior static strength, low density, high durability and excellent workability. The lightning damage effect of advanced CFRP composite is a key factor restricting its wide application in aerospace field due to its poor electrical and thermal conductivity.

This study aims to reveal the damage properties and mechanism of carbon fiber-reinforced polymer (CFRP) composites subjected to lightning components by artificial lightning tests. The damage behavior of CFRP composite was deduced and the damage regions were quantitively analyzed by detecting the surface morphology and microstructural changes and analyzing the lightning strike process. The results indicated that the lightning-induced damage included lightning attachment damage due to direct contact with the lightning arc, laminate peeled-off damage caused by the explosive gas impact, and internal delamination induced by expanding pyrolysis gas.

The distribution and conduction path of lightning current inside CFRP laminate subjected to lightning strike are determined by its dynamic conductive model, which directly affect the lightning damage of CFRPs. In this work, via experimental and circuit simulations, the equivalent circuit and dynamic conductivity parameters of CFRP materials were quantitatively analyzed. A coupled thermal-electrical CFRP model, which first introduces the dynamic conductivity of CFRP materials, was established. The comparison results indicated that the Joule heating-based numerical model can simulate the evolution of thermal damage well, although the laminate peeled-off damage resulting from the mechanical impact was not included in the simulation scope. The dynamic conductivity simulation model can reduce the deviation of lightning damage areas and damage depths between the simulated calculation and experimental results from +304% and -39.2% (DC static conduction model) to -4.9% and +2.9%, respectively.

This research is helpful for understanding the lightning damage mechanism of CFRP material, and can provide experimental and theoretical support for the optimization in lightning damage numerical model and the improvement in the lightning protection structure design.

### PCM3062 Near-infrared absorbing phosphate ester copper complex containing resin material for window application

Naoki Hayashi<sup>1,2</sup>

<sup>1</sup> Process Development Department 1, Kureha Corporation, Japan

<sup>2</sup> Department of Applied Chemistry and Biotechnology Faculty of Engineering, Chiba University, Japan

Abstract. With the recent increase in environmental and energy saving awareness, improvement of cooling efficiency in many pieces of equipment and various facilities is being promoted. In order to enhance the cooling efficiency, it is required to provide windows with a heat shielding efficiency. Absorption of near-infrared (NIR) rays, which have high thermal energies even in sunlight, can greatly contribute to improvement of the heat shielding. Furthermore, for keeping brightness, high transparency in visible region should be maintained. The window material is required to have both brightness and heat shielding function. Our research team developed the alkyl phosphate ester copper complexes as a NIR absorbing dye. The properties of these complexes and the performances of a resin composite containing the preferable compound for NIR absorbing dye were evaluated. 2-Ethylhexyl phosphate copper complex showed decomposition temperatures above 250 °C and broad absorption in the NIR region with weak absorption in the visible region. Poly (2-Ethyhexyl methacrylate) involving a similar structure of the ligand showed high compatibility with the phosphate ester copper complex. By using this polymer as a polymer matrix, a transparent NIR-absorbing resin plate could be made. This resin plate has >80% visible light transmittance and <50% solar direct transmittance. Thus, this resin composite is suitable as a window material that requires heat-shielding properties and brightness.

**Keywords:** Near-Infrared; Phosphate Ester Copper Complex; Resin Material; Solar Direct Transmittance; Solubility; Thermal Stability; Visible Light Transmittance

Acknowledgements: This work was funded by Kureha Corporation.

#### PCM3061

## Progress of structural manipulation for producing high performance Nd<sub>2</sub>Fe<sub>14</sub>B/Fe(Co) nanocomposite permanent magnets

Fengqing Wang, Jinkui Fan, Weichuang Shen and Lulu Yao

CAS Key Laboratory of Magnetic Materials and Devices, Ningbo Institute of Material Technology and Engineering, Chinese Academy of Sciences (CAS), China

Abstract. Hard/soft nanocomposite magnets have attracted great interests for their potentials in developing strong permanent magnets containing less Rare-earth elements. However, existing nanocomposite magnets exhibit limited energy products because it is challenging to control synchronically the desired structures with nanoscale grain size, strong grain orientation (texture), and tailored phase volume. By using varied Co-substituted soft-phase precursors in the mechanical alloying process, our study demonstrated a structural synchrony between the grain size and tailored soft-phase volume. The best energy product of 17.4 MGOe shows 26% enhancement as compared to the case with Co-free precursor. Effective directional atomic diffusion is explained as the main mechanism for the structural and magnetic improvements. More importantly, by using slow strain rate and low temperatures during the bulk plastic deformation process, our study achieved a synchrony of the nanoscale grain size and strong texture in the bulk Nd-Fe-B magnets. The degree of the grain orientation can reach high levels of above >90%, giving the nanograin magnets record high energy products up to 49 MGOe. Grain boundary mediated creep-like deformation is thought as the mechanism for the high-degree nanoscale grain alignment under the deformation conditions without liquid phase. The controlled atomic interdiffusion and grain boundary mediated deformation are promising methods for structural manipulation of advanced nanostructures including the permanent magnets.

Keywords: Permanent Magnets; Nanocomposites; Plastic Deformation; Grain Size; Texture

## PCM3065 Electrospinning and in-situ hierarchical thermal treatment to tailor C-NiCo<sub>2</sub>O<sub>4</sub> nanofibers for tunable microwave absorption

Min Zhang and Mao-Sheng Cao\*

School of Materials Science and Engineering, Beijing Institute of Technology, China

**Abstract.** The available efficient electromagnetic energy absorbing materials in different frequency bands is expected to satisfy the need of national defence especially active camouflage and real-time communication in the information era. Herein, C modified nickel cobalt oxide porous nanofiber (C-NiCo<sub>2</sub>O<sub>4</sub>) is successfully constructed by electrospinning and hierarchical thermal treatment engineering. The thermal treatment temperature enables tailoring of the carbon content of C-NiCo<sub>2</sub>O<sub>4</sub> so as to modulate the conduction loss and dielectric loss. More importantly, the absorption frequency can be tuned from Ku band to X band and even to C band with a red shift. The synergy of conduction loss, relaxation loss, eddy current and natural magnetic resonance is responsible for the tunable absorption peak by matching the impedance of each composite at different microwave bands. And the maximum reflection loss of three different C-NiCo<sub>2</sub>O<sub>4</sub> samples reach -52.7 dB at 15.6 GHz, -51 dB at 8.56 GHz, and -18.7 dB at 5.12 GHz. Since low reflection loss suggests efficient energy conversion and heat generation, the high electromagnetic absorption makes the material extremely potential for application in multifunctional nano-micro electromagnetic devices. This working opens new horizons for frequency selective materials, and has potential in multifunctional electromagnetic heaters or even electromagnetically driven sensors.

Keywords: C-NiCo<sub>2</sub>O<sub>4</sub> Nanofiber; Electrospinning; Thermal Treatment; Microwave Absorption

## PCM3040 A new method for mixed-mode I/II/III delamination test

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<sup>1</sup> School of Mechanical Engineering, Universiti Teknologi Malaysia, Malaysia <sup>2</sup> Faculty of Engineering and Science, Curtin University Malaysia, Malaysia

Abstract. Delamination is one of the earliest damages occurred in laminated composite structures. In addition, as the loadings in real life applications are generally complex, it is essential to study the mixed-mode delamination behaviour of the composites. In the present work, a new method is proposed to characterise the mixed-mode I/II/III delamination of carbon/epoxy composites. A new jig is developed to perform the respective experiment through ten-point bending plate (10PBP) test. Mode I, mode II and mode III delamination are induced through the bending of the specimen about different axes, respectively. The material used in this study was a carbon/epoxy composite with a nominal ply thickness of 0.15 mm. A 26-ply composite plate with the dimension of 500 mm  $\times$  400 mm was fabricated at the stacking sequence of  $[(90/0)_{3S}/0]_{S}$ . In addition, a 15 µm Teflon film was placed at the mid-thickness of the composite plate to induce pre-crack. The cured carbon/epoxy composite using hot-press technique has an average thickness of 3.9 mm. The composite plate was cut into four specimens with the size of 180 mm  $\times$  144 mm. Results reveal that the force increases linearly with the displacement until the first drop in the force, which signifies the initiation of the crack propagation. Subsequent loading leads to the increment in the force, which is postulated to be attributed to fibre bridging. Finite element modelling is required to estimate the mode ratio and crack propagation behaviour of the composite.

Keywords: Carbon/Epoxy Composites; Delamination; Mixed-Mode I/II/II; Ten-Point Bending Plate

Acknowledgements: This work is supported by Universiti Teknologi Malaysia through UTMShine Grant No. 09G16 and Collaborative Research Grant (08G01).

## PCM2973 Spherical and sub-micron scale lignin particles as multifunctional fillers for PVA composite films

B. Hararak\*, C. Winotapun, J. Inyai, W. Daud and C. Prahsarn

National Metal and Materials Technology Center (MTEC), National Science and Technology Development Agency, Thailand

Abstract. Approximately 90% of an industrial-waste lignin from Kraft pulping process has been burned for energy. In this work, we purposed the utilization of waste lignin for high value-added applications by purification and conversion into spherical particles. The spherical lignin particles with an average diameter of  $736 \pm 39$  nm were produced and used as multifunctional and renewable fillers for polyvinyl alcohol (PVA) films. The PVA/spherical lignin composite films were fabricated by solution casting. An enhancement in thermal and mechanical properties and UV-shielding ability of the PVA/spherical lignin composite films was demonstrated. With only 0.2 wt% incorporation of spherical lignin particles, the PVA composite films exhibited a melting temperature of  $176.6 \pm 2.6$  °C which was approximately 14 °C higher than that of pristine PVA films. The crystallinity of composite films containing 0.2 wt% lignin particles increased by 80% compared with neat PVA. Mechanical performance of PVA/ spherical lignin composite films was enhanced such that the modulus increased significantly from  $1.7 \pm 0.1$  GPa to  $2.0 \pm 0.1$  Gpa with 0.2 wt% loading of lignin particles. The yield stress reached the maximum value of  $44.5 \pm 0.17$  Mpa when the content of lignin particles was 0.5 wt%. The UV transmittance in the composite films with 0.2 wt% lignin particles was significantly reduced in both UVA and UVB spectrum while a satisfactory visible light transmittance was retained. With an increase of spherical lignin content to 1.0 wt%, the composite films showed better UV-shielding performance, which was observed by a decrease in UV light transmittance. The transmittances at 300 nm (UVB) and 400 nm (UVA) of the 1.0 wt% composite films were 4% and 44%, respectively, while those of the pristine PVA films were 84% and 91%. This work provides a simple process for producing spherical lignin particles, which can be used as UV-shielding materials with enhance thermal and mechanical properties for PVA films. Moreover, a meaningful approach for fully biodegradable films with potential applications in UV protection was also demonstrated.

Keywords: Lignin; Lignocellulosic; PVA; UV-Shielding

#### PCM3036

## Effect of mixing ratio on the superhydrophobicity of polyester/cotton fabric treated with alkaline hydrolysis and thermal aging

Hyewon Kim, Somin Lee, Chung Hee Park\*

Department of Textiles, Merchandising and Fashion Design, Seoul National University, Republic of Korea

Abstract. Superhydrophobic fabrics composed of polyester and cotton yarns were developed in this study. The fabric samples were alkali hydrolysed for making nano structure and then thermal-aged to lower surface energy. After treatment, superhydrophobicity, changes in the tensile strength, vapor/air permeability and function durability were evaluated. By the alkaline treatment, nano-roughness was formed on the polyester fibers, and micro-roughness also increased due to differences in the thicknesses of the two yarns, thinner polyester yarns and swollen cotton yarns. The superhydrophobicity, with a static contact angle of 155.8  $\pm$  3.2 ° and shedding angle of 11.1  $\pm$  0.8 °, was achieved with 90 % polyester/ 10 % cotton fabric treated with 20 % alkali concentration for 20 min with tension, then followed by 24 h of thermal aging at 130 °C. The tensile strength of the superhydrophobic polyester/cotton fabric (28.7 Mpa) was higher than that of 100 % polyester fabric (20.1 Mpa). Fabric usual strength loss due to the alkali treatment in polyester fabrics was not shown in this study, by mixing with cotton varns. The water vapour transmission rate and air permeability of the superhydrophobic polyester/cotton fabric were also improved compared with 100 % polyester fabric. After five times of tape tests, static contact angles higher than 150 ° were shown. This study has a strength in that superhydrophobic fabric mixed with polyester and cotton yarns was developed without fabric strength loss and with the enhanced the vapor/air permeability by thermal ageing after common alkali treatment, which usually causes strength loss.

Keywords: Superhydrophobic; Polyester; Cotton; Alkaline hydrolysis; Mercerization; Thermal Aging

**Acknowledgements**: This work was supported by the National Research Foundation of Korea (NRF) grant funded by the Korea government (Ministry of Science and ICT; Grant No. NRF-2016M3A7B4910940 and NRF-2018R1A2B6003526); by Korea Institute for Advancement of Technology (KIAT) grant funded by the Korea Government (MOTIE) (P0012770, Professional Human Resources Training Project).

#### PCM3073

## Exploration of new applications of metal matrix composites/nanocomposites manufactured by stir casting and powder metallurgy

#### Pallav Gupta

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Abstract. New technology in current global world has propelled the researcher's to look for new and advanced class of materials. Metal Matrix Composite (MMC) is such a new class of material in which ductile metallic matrix is added with hard ceramic reinforcement. Moreover, advancement in MMCs has led to the development of Metal Matrix Nanocomposites (MMNCs) which has the particle size of final product less than 100 nm. Among various processing techniques, stir casting and powder metallurgy are the two major routes for fabricating large scale MMC/MMNC products. The present talk will focus on the fabrication and characterization of metal matrix composites/nanocomposites using Aluminium, Copper and Iron as the matrix material with the use of wide range of ceramic reinforcements. Aluminium and Copper based composites were fabricated using Stir Casting whereas Iron based nanocomposites were fabricated using Powder Metallurgy. Property evaluation has been done in respect of structural, mechanical and corrosion behavior for the fabricated specimens. Apart from this an attempt has also been made to use the metal matrix composite as an efficient coating material. It is expected that developed MMCs/MMNCs will explore a new era for wide range of engineering applications.

**Keywords:** Metal Matrix Composites/Nanocomposites; Stir Casting; Powder Metallurgy; Coatings; Property Evaluation

## PCM3077 Characterization of brominated natural rubber by solution state 2D NMR spectroscopy

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<sup>1</sup>Deapartment of Materials science, Faculty of Engineering, Rajamangala University of Technology Rattanakosin, Thailand

<sup>2</sup>Department of Materials science and Technology, Faculty of Engineering, Nagaoka University of Technology, Nagaoka, Niigata 940-2188, Japan

**Abstract.** Nuclear magnetic resonance (NMR) spectroscopy is one of the most powerful technique for characterize the primary structure of polymer. Essentially, solution state NMR spectroscopy is recognized to be indispensable for the characterization, which the signal are assigned to a chemical shift, coupling constant and intensity ratio as well as spin coupling between homo- and hetero-nuclei. For example, two-dimension (2D) NMR measurement such as HETCOR, HMBC and COSY enables to assign the complicated signals, which were difficult to assign with one dimension (1D) NMR measurement. <sup>1</sup>H and <sup>13</sup>C signals of brominated natural rubber (BrDPNR), which brominated by *N*-bromosuccinimide at allylic position, is assigned with 1D-and 2D-NMR spectroscopy. The *cis*- and *trans*- isomerization of BrDPNR was proved by the different signal of methyl and methylene proton. The signals at 21.8 and 20.5 ppm were assign to methyl proton of *cis*- and *trans*- isomerization, respectively. This result indicated that the signal assignment of BrDPNR was carried out by 1D- and 2D-NMR measurements to establish the new plausible structure of BrDPNR.

## PCM3011 Surface modification of h-BN and its influence on PVA properties

Xiaodong Wang<sup>1,2</sup> and Yuan Hu<sup>2</sup>

<sup>1</sup>State Key Laboratory of Fire Science, University of Science and Technology of China, China <sup>2</sup> School of Chemistry and Material Engineering, Chaohu University, China

**Abstract.** In this study, the efficient preparation method of h-BN nanosheets was first explored from the point of view of the design and preparation of high performance thermal conductivity and flame retardant PVA composites. Then, the biomimetic polydopamine (PDA) was used to organically treat the surface of the h-BN sheet and construct an interface compatible coating to enhance the mechanical enhancement effect of the h-BN sheet on PVA. On the basis of organic modification, transition metal oxides was grown in situ on the surface of h-BN nanosheet by using the active site provided by the organic layer to prepare the core-shell type multifunctional hybrid sheet material, and its comprehensive influence on the mechanical properties, thermal conductivity and flame retardancy of PVA composites was studied.

## Session 5\_ Applications in Energy, Biomaerials, Medicine, and Food Industry

Time: 14:00-18:55, November 4, 2020

Session Chair:

14:00-16:10 Prof. Ishaq Ahmad, National Centre for Physics, Pakistan 16:35-18:55 Dr. Alina Vladescu, National Institute of Research and Development for Optoelectronics-INOE2000, Romania

Session Room Link: http://www.academicconf.com/teamslink?confname=pcm2020

14:00-14:15	PCM3023 (Video)	Cellulose as oxygen barrier in nanocellulose/polymer composites for food packaging Dr. Jinwu Wang, U.S. Forest Service Forest Products Laboratory, USDA Forest Service, USA
14:15-14:30	PCM3058 (Video)	Designing of multi-responsive hybrid hydrogel as a controlled drug release carrier Dr. Nafisa Gull, University of the Punjab, Pakistan
14:30-14:45	PCM3060	Reversing and non-reversing effects of PEEK-HA composites on tuning cooling rate during crystallization Dr. Sujoy Kumar Dey, Sikkim Manipal University, India
14:45-15:00	PCM3066	Reactive cathodic arc deposition of protective biocompatible carbide coatings used for medical applications Dr. Iulian Pana, National Institute of Research and Development for Optoelectronics-INOE2000, Romania
15:00-15:15	PCM3022	Fabrication of chitosan hydrogels in the presence of bio-based graphene oxide Dr. Zhaoxuan Feng, China University of Petroleum, China
15:15-15:40	PCM3050	Sputtered hydroxyapatite coatings used in medicine Dr. Alina Vladescu, National Institute of Research and Development for Optoelectronics-INOE2000, Romania
15:40-15:55	PCM3035	Biocomposites based on natural rubber and modified nano- crystaline cellulose Dr. Emad Saad Faheem, Polymer & Pigments department, National Research Centre, Egypt
15:55-16:10	PCM3008	Biodegradable wet-spun fibers modified with antimicrobial agents for potential applications in biomedical engineering Dr. Helena Prado Felgueiras, University of Minho, Portugal
16:10-16:35		BREAK
16:35-16:50	PCM3070	Synthesis of β-1,3-glucan mimics with Immunostimulant Activity Dr. Atsushi Miyagawa, Nagoya Institute of Technology, Japan
16:50-17:05	GNN1160 (Video)	Deciphering the Relationship between MicroRNAs and Nanoparticles in Clinical Research Prof. Durairaj Sekar, Saveetha University, India

17:05-17:30	GNN1155	Advanced materials for new generation energy storage devices Dr. Shahab Ahmad, Indian Institute of Technology Jodhpur, India
17:30-17:55	GNN1163	Ultrafast photobehavior of MOFs and related composites: relevance to photonic applications <i>Prof. Abderrazzak Douhal, University of Castilla La Mancha, Spain</i>
17:55-18:10	PCM3078	Exposure of heavy metals in Pakistani population and their association with risk factors of metabolic disorders Assoc. Prof. Muhammad Sajid Hamid Akash, Government College University Faisalabad, Pakistan
18:10-18:25	PCM2963 (Video)	Antibacterial chitosan-based films against wound chronicity Dr. Joana C. Antunes, University of Minho, Portugal
18:25-18:40	PCM3079 (Video)	Green optimization of the crosslinking process with glutaraldeide vapor in PVA based electrospun membranes for applications in wound dressings Dr. Marta A. Teixeira, University of Minho, Portugal
18:40-18:55	PCM3080	Enhanced antimetastatic activity of the ruthenium anticancer drug RAPTA-C delivered in fructose-coated micelles Dr. Mingxia Lu, University of Shanghai for Science and Technology, China

## **Abstracts of Session 5**

#### PCM3023

#### cellulose as oxygen barrier in nanocellulose/polymer composites for food packaging

#### Jinwu Wang<sup>1,2</sup>

<sup>1</sup> U.S. Forest Service Forest Products Laboratory, USDA Forest Service, USA

<sup>2</sup> School of Forest Resources, Advanced Structures and Composites Center, University of Maine, USA

**Abstract.** Cellulose emerges as a potential versatile biopolymer to make hydrogels for absorbents, aerogels for insulation, membranes for filters, films for packaging, and fibers for textiles and reinforcements. Wood cellulose is increasingly perceived by relevant stakeholders to be renewable, biodegradable, and sustainable. Can the properties of cellulose-based materials be competitive with conventional materials? This presentation surveys packaging properties of cellulose-based materials and visualize the data contrastively with other competitive materials and provides some insights into the potential and challenges of cellulose-based products to replace polymers and other materials for packaging applications.

Keywords: Cellulose; Nanocrystals; Fibers; Polymers; Composites; Barrier; Oxygen Permeation

## PCM3058 Designing of multi-responsive hybrid hydrogel as a controlled drug release carrier

Nafisa Gull<sup>1,\*</sup>, Shahzad Maqsood Khan<sup>1</sup>, Rafi Ullah Khan<sup>1</sup>, and Muhammad Taqi Zahid Butt<sup>2</sup> <sup>1</sup>Department of Polymer Engineering and Technology, University of the Punjab, Pakistan <sup>2</sup>College of Engineering and Emerging Technology, University of the Punjab, Pakistan

**Abstract.** Hydrogels (network of hydrophilic polymers) have capability of absorbing large amount of water, without losing their three-dimensional structure. They are of special interest in controlled drug release applications because of their soft tissue biocompatibility. One of the extensively studied approaches for controlling medicament delivery is the encapsulation of drug within polymer chains which sluggish the release on the basis of its crosslinked network. Discontinuous volume variations in hydrogels upon changes of environmental parameters, like polymer composition, temperature, pH, etc., are named multi-responsive hydrogels.

Multi-responsive hybrid hydrogels were designed using chitosan and polyvinyl pyrrolidone as base polymers by varying the amount of crosslinker (tetraethyl orthosilicate) via solution casting protocol. Swelling indices of these prepared hydrogels was determined in distilled water, buffer and electrolyte solutions of different concentration. FTIR, WAXRD and TGA were conducted to investigate the structures, crystallinity and thermal stability of these multi-responsive hydrogels, respectively. Extensively, mechanical properties, biodegradation, antimicrobial activity, cytotoxicity and drug release profile were also conducted. The above insights obviate the successful designing of non-toxic, hybrid-controlled drug deliverable hydrogels.

#### PCM3060

# Reversing and non-reversing effects of PEEK-HA composites on tuning cooling rate during crystallization

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Abstract. The development of bio-compatible materials for bone implants bone healing is one of the key research areas in biomaterials. In this paper, composites of polyether-ether-ketone (PEEK) (a biocompatible polymer) and hydroxyapatite (HA) were synthesized using thermal process, The qualities of the composites were analyzed with X-ray diffraction (XRD), Fourier-transform infrared spectroscopy (FTIR) for characterizing the nature of stress and bonding. The morphological study of the PEEK-HA composites were studied through scanning electron microscopy. The compressive nature of the composites as well as raw materials was observed based on XRD data with internal lattice-strain analysis. The temperature-modulated differential scanning calorimetry (TM-DSC) and conventional differential scanning calorimetry (DSC) were performed for analyzing the crystallization process. The TM-DSC showed that both reversing and non-reversing processes were active during the crystallization between 160 °C–330 °C. However, a higher residual time of PEEK at elevated temperatures tends to facilitate polymer degradation and spread the crystallization process over a broader temperature range. Addition of HA particles provided heterogeneous nucleation sites for crystallization but also reduced the mobility of polymer chains. The combination of enhanced nucleation rate, reduced chain mobility and polymer degradation processes together lead to a wide range of crystallinity in PEEK-HA composites.

## PCM3066 Reactive cathodic arc deposition of protective biocompatible carbide coatings used for medical applications

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**Abstract.** Load bearing implants are some of the most popular joint replacements specific to the human body. For load bearing applications, biomaterials are representing an efficient and practical solution against aseptic loosening, corrosion processes or to the leachable behaviour which occurs in the human body fluids. In order to withstand the body conditions, the present study aims to obtain protective biocompatible carbide coatings with a high corrosion resistance, good tribocorrosion resistance and a high hardness and adhesion strength. The reactive cathodic arc deposition technique was used to produce TiC, ZrC and TiNbC coatings on 316L stainless steel substrates. The coatings were investigated in terms of corrosion resistance, microstructural and mechanical properties. The corrosion resistance results proved an enhanced functionality of 316L stainless steel substrates by covering with TiNbC (lowest i<sub>corr</sub> = 0.55  $\mu$ A/cm<sup>2</sup>, highest R<sub>p</sub> = 81.27 kΩ, highest protective efficiency = 57.7 %), ZrC (i<sub>corr</sub> = 0.59  $\mu$ A/cm<sup>2</sup>, R<sub>p</sub> = 73.61 kΩ, protective efficiency = 54.6 %) or TiC (i<sub>corr</sub> = 0.70  $\mu$ A/cm<sup>2</sup>, R<sub>p</sub> = 62.7 kΩ, protective efficiency = 46.2 %) coatings. Meanwhile, the TiC coating exhibited a (111) preferred orientation and a higher porosity as compared to all coated samples. TiNbC showed the best tribocorrosive performance in 0.9 % NaCl at 37 ± 0.5 °C and the lowest friction coefficient (1.6) and wear rate (0.99 × 10<sup>-5</sup> mm<sup>3</sup> ·N<sup>-1</sup> ·m<sup>-1</sup>).

Keywords: Cathodic Arc Evaporation; Carbides; Corrosion Resistance; Tribocorrosion

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### PCM3022 Fabrication of chitosan hydrogels in the presence of bio-based graphene oxide

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**Abstract.** Water pollution, as a severe environmental issue, has caused great public attention. Among many treatment methods, adsorption is regarded as an effective approach to remove pollutants from water. In this context, we developed an eco-friendly bio-based chitosan-graphene oxide (CS-GO) hydrogel with genipin (GP) as crosslinking agent for wastewater purification application. Different from modified Hummer's method for GO preparation, we converted biopolymers, such as cellulose, starch and chitosan, to nano-GO by virtue of microwave-assisted hydrothermal carbonization process. This process has unique benefits such as 1) high yields 2) high efficiency with lower energy consumption 3) green solvents without toxic catalysts. The CS-GO hydrogels showed a honeycomb three-dimension networking structure as an indication of successful crosslinking. As explored, the CS-GO hydrogels were expected to be tunable in their properties, such as swelling behaviour, mechanical performance, and thermal stability with the variation of GO and GP content. Meanwhile, GO was found to play a role in the crosslinking reaction by GP resulting in the formation of darker and more homogenous chitosan hydrogel system.

Keywords: Chitosan; Genipin; Hydrogel; Graphene Oxide

## PCM3050 Sputtered hydroxyapatite coatings used in medicine

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**Abstract.** Implants made of metallic biomaterials have been used for over 100 years and it will continue to be central to medical applications because of their unique properties compared to those of other classes of materials. However, a major worry with metallic materials is their susceptibility to corrosion, wear and low osseointegration capabilities. Thus, the common solution was to coat the surface of metallic implants by biocompatible coatings such as hydroxyapatite. The coating followed only for a very thin layer and it did not affect the original mechanical properties of the metallic biomaterials. Usually, the hydroxyapatite should offer sufficient mechanical strength until the completion of the healing process. Hydroxyapatite possesses many advantages as biomaterials with outstanding osseoconductivity and bioactivity, and faster integration with host bone tissues. Thus, the aim of the present paper is the show a part of the group results about the preparation of hydroxyapatite coatings using RF magnetron sputtering. We have also proposed to improve the mechanical properties by the SiC addition and antibacterial abilities by Ag addition into hydroxyapatite matrix.

Keywords: Coatings; Hydroxyapatite; Magnetron Sputtering; Hardness; Bioactivity

Acknowledgements: The work was supported by the grant of the Romanian National Authority for Scientific Research and Innovation, CCCDI–UEFISCDI, Project no. COFUND-ERANET-RUS-PLUS-CoatDegraBac no.68/2018, within PNCDI III, as well the PROINSTITUTIO Project no. 19PFE/17.10.2018.

### PCM3035 Biocomposites based on natural rubber and modified nano-crystaline cellulose

#### Emad S. Shafik

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Abstract. There is a great awareness in developing biocomposites in manufacturing and technological areas due to their appreciated properties such as biodegradability, and ecological friendliness. In this study, nano-crystalline cellulose (NCC) was prepared from microcrystalline cellulose (MCC) through acid hydrolysis. Modification of nano-crystaline cellulose was achieved using cetyltrimethyl ammonium bromide as a cationic surfactant. The prepared NCC and modified NCC were characterized through fourier transformed infrared (FTIR) spectroscopy and X-ray diffraction (XRD). The biocomposites were prepared by incorporating NCC and modified NCC as reinforcing fillers at 2.5, 5 and 10 phr to natural rubber using two-roll mill mixer. The rheometric, physico-mechanical, electrical and thermo-oxidative properties were evaluated. Furthermore, the distribution of the fillers in the prepared composites was investigated by scanning electron microscope (SEM). The results showed that the tensile strength increased gradually with increasing NCC and modified NCC up to 5phr and then decreased with increase filler content up to 10 phr. On the other hand, the elongation at break values decreased with increasing the filler content. The modification of NCC led to a noticeable decrease in the curing time, confirming that modified NCC could accelerate the vulcanization process. The NR biocomposites containing cellulosic filler show good resistance to thermal aging rather than natural rubber.

Keywords: Nanocrystaline Cellulose; Acid Hydrolysis; Mechanical Properties

**PCM3008** To avoid repeatability issue, this abstract will be available after the full paper is published in the conference proceedings.

## PCM3070 Synthesis of β-1,3-glucan mimics with Immunostimulant Activity

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Abstract.  $\beta$ -1,3-Glucans are important as immunostimulant agents in living organisms. The multivalent binding of  $\beta$ -1,3-glucans to dectin-1, a cell surface receptor, activates immunological responses. To research the synthesis of artificial immunostimulant agents and the immunological mechanism, polymers carrying  $\beta$ -1,3-glucan trisaccharides as ligands for dectin-1 were synthesized. The  $\beta$ -1,3-glucan trisaccharide, defined as an active unit of  $\beta$ -1,3-glucan, was constructed from p-glucose by glycosylation. A norbornene group was introduced as a polymerizable group into the aglycone of the trisaccharide derivative. First, the glucose monomer as a model compound was synthesized. The acetyl glucosyl imidate was glycosidated with the prepared alcohol having endo and exo norbornenes. The stereoisomers of glucosyl monomers could be separated by silica gel chromatography and identified by NMR spectroscopy. While, the trisaccharide monomers were synthesized by glycosidation with each the separated alcohols having endo or exo norbornene. The synthesized glycosyl monomers were polymerized and copolymerized with norbornene using 2nd generation Hoveyda-Grubbs catalyst, deprotected, and purified by gel filtration to prepare watersoluble polymers of varied compositions and high molecular weights. These polymers will have the

potential for multivalent binding to dectin-1 to activate immune response and facilitate studies to understand the binding mechanisms of  $\beta$ -1,3-glucans with dectin-1.

**Keywords:** β-1,3-Glucan, Dectin-1, Glycopolymer, ROMP, Ruthenium Catalyst

### GNN1160 Deciphering the relationship between micrornas and nanoparticles in clinical research

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Abstract. MicroRNAs (miRNAs) are non-coding RNAs that play key role in the regulation of various important cellular functions such as cell proliferation, apoptosis and gene expressions. Mature miRNA is generated through two-step cleavage of primary miRNA (pri-miRNA), which incorporates into the effectors complex RNA-induced silencing complex (RISC). The miRNA functions as a guide by base-pairing with target mRNA to negatively regulate its expression. Hence delivering miRNA to target specific sites will be an effective system to treat various diseases. In this perspective, nanoparticles, which possess characteristic colors and properties with the variation in size and shape, can be utilized as a delivery vehicle. Nanoparticle delivery systems will be the key to bringing miRNA to the clinic level. Although nanoparticles are proposed for various biological and commercial applications, there are a limited number of literatures to display the role of microRNAs with the combination of nanoparticles. The present study highlights the importance of miRNAs and also nanoparticles as a delivery system to treat some important human diseases based on recent findings in clinical research.

**Keywords:** miRNAs; Nanoparticles; RISC; siRNAs; RNAi; Gene; mRNA; RNA Polymerase; Biomarkers; Delivery System

## GNN1155 Advanced materials for new generation energy storage devices

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Abstract. With several recent advancements in rechargeable battery technology the new generation energy storage systems are comprised of electrodes with multi-functionalities for unconventional device applications. For instance, Li-ion batteries are made flexible and shape conformal to power fully flexible consumer electronic devices such as wearable electronics, flexible displays etc. Design of highly flexible battery requires judicious engineering of electrodes to mitigate stress concentration and crack formation. We demonstrated ultra-flexible Li-ion batteries by designing CNT microstructures, loaded with nanocrystals, which decouple the stress induced during bending between the collector electrode and energy-storage material. These unique light weight electrodes not only alleviate stress, but also bring the active particles outside of the binder, which dramatically enhances the device performance. Emerging autonomous electronic devices require increasingly compact energy generation and storage solutions. Merging these two functionalities in a single device would significantly increase their volumetric performance, however this is challenging due to material and manufacturing incompatibilities between energy harvesting and storage materials. We recently demonstrated highly versatile and hybrid *photo-rechargeable* energy storage devices where the functionality of rechargeable battery and solar cell are merged together in a single optoelectronic device termed as *photo-battery* to avail advantages of both technologies simultaneously.

## GNN1163 Ultrafast photobehavior of MOFs and related composites: relevance to photonic applications

#### Abderrazzak Douhal

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**Abstract.** Metal-organic frameworks (MOFs) are being used for several applications such as gas separation and storage, chemical sensing, bioimaging, drug delivery, optoelectronic devices, and catalysis. They are created from the connection of metal ions or clusters with organic or organometallic linkers through coordination bonds, and provide flexible cages making them accessible to several potential guests, which can interact with the inoganic/organic parts. Therefore, upon photonic excitation a vast number of fast (ps) and ultrafast (fs) processes occur within the cavities of their composites. The development of ultrafast (spectroscopy and imaging) tools has allowed to investigate the photodynamics of these composites at intimate levels. In this lecture, I will show results on the state-of-the using fast and ultrafast techniques to decipher the photodynamics of MOFs and related composites. I will show cases where we observed upon photoexcitation, events such as: excimer formation, energy- and electron/charge- and proton-transfer, LMCT, MLCT, and interparticles interaction. I will also summarize the relevant applications of MOFs and related composites in modern science and technology using light.

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#### PCM3078

## Exposure of heavy metals in Pakistani population and their association with risk factors of metabolic disorders

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**Abstract.** Metabolic disorders (MDs) are rapidly aggregating in the increasing population globally. This is greatly affecting the social and financial status of the individuals particularly of developing countries. Among various environmental contaminants (ECs), we have focused on the occupational exposure of arsenic (As) and cadmium (Cd) in Pakistani population and their association with sociodemographic features, and risk factors for pathogenesis of MDs. Urinary concentrations of heavy metals (As and Cd) were determined by ICP-OES method. Pearson correlation coefficient was used to determine the urinary concentrations of heavy metals and risk factors of MDs. Sociodemographic data showed that urinary concentrations of heavy metals was significantly higher (P< 0.05) in study participants living in semi-urban and industrial areas where, heavy metals was found to be higher in diabetic participants when compared with that of non-diabetics. A significant correlation was also observed between the exposure of heavy metals in study participants and risk factors of metabolic disorders.

This emphasizes the urge to better understand the mechanisms of diseased progression, which will not only help to eradicate the exposure of ECs along with these underneath causative factors but may also propose targeted therapy for the treatment of MDs caused by ECs.

## **PCM2963** Antibacterial chitosan-based films against wound chronicity

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Abstract. Chronic wounds (CW) have numerous entry ways for pathogen invasion and prosperity, damaging host tissue and hindering tissue remodeling. Essential oils (EOs) exert quick and efficient antimicrobial (AM) action, unlikely to induce bacterial resistance. Cajeput oil (CJO) has strong AM properties, namely against Staphylococcus aureus and Pseudomonas aeruginosa, as previously established by the team (DOI: 10.3390/antibiotics9060314). Chitosan (CS) is a natural and biodegradable cationic polysaccharide, widely known for its AM features. CS (100-300 kDa; DA of 9.6±1.4%) and PVA (72 kDa, 88% hydrolyzed) films (ratio 30/70; 9%wt) were prepared by solvent casting and phase inversion method (similarly as in DOI: 10.1002/app.48626). Films thermal stability and chemical composition and reinforce the achievement of blended films. CJO-supplemented films contained a loading amount of 1 and 10wt% in relation to total polymeric mass. Loaded films with  $0.89 \pm 0.05$  and  $1.14 \pm 0.10$  mm in thickness were obtained, respectively, 23 and 57% thicker than the unloaded films. Degree of swelling (%) and porosity also increased, particularly with CJO at 10wt%. Tested AM activity revealed that CS films alone showed an outstanding AM activity against both bacteria, eradicating all P. aeruginosa colony traces within the hour (\*\*\*p<0.001). Still, loaded CS/PVA films showed improved AM traits, being more efficient than unloaded films right after 2h of contact (\*p<0.05 and \*\*p<0.005 for CS/CJO/PVA at 1 and 10% EO, respectively, against S. aureus; \*p<0.05 for CS/CJO/PVA at 10% EO, against *P. aeruginosa*). This study is a first proof of concept that CJO can be dispersed into CS/PVA films and show bactericidal effects, particularly against P. aeruginosa, this way opening new avenues for CW therapeutics.

Keywords: Bactericidal; Marine-Derived Polymers; Natural Bioactive Agents; Drug Delivery Systems; Blended Films

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#### **PCM3079**

## Green optimization of the crosslinking process with glutaraldehyde vapor in PVA based electrospun membranes for applications in wound dressings

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Abstract. In the last years, chronic wounds have become more prevalent, leading to a huge burden on the healthcare and social systems by requiring specialized protection. Indeed, wound dressings capable of assisting in the healing process are in urgent need. To that effect, nanofibrous dressings with a structure resembling the extracellular matrix have been engineered by electrospinning from combinations of poly(vinyl alcohol) (PVA) and cellulose acetate (CA) and optimized to endure physiological media contact and mechanical stress after crosslinking.

Mats were prepared at different PVA/CA ratios, 100/0, 90/10 and 80/20 v/v%, at 10w/v% concentration in acetic acid and water in a 75/25v/v% proportion and processed via electrospinning. Processing conditions were optimized to obtain uniform, continuous, bead free mats, with a flexible structure. The instant solubilization of the PVA portion of the mat in aqueous media was surpassed via crosslinking. Even though there are many chemical agents available to accomplish such task, glutaraldehyde (GA) is by far the most common due to its efficiency, ease of access and processing, and low cost. Further, in its vapor form, GA has demonstrated reduced or no cytotoxic effects. The amount of GA, crosslinking time, temperature, and drying procedure were optimized to guarantee mechanically resilient mats by means of the greenest methodology possible. Indeed, it was determined that GA vapor at 25% in water could be applied for 7 h at 60°C, using 6 mL of solution, in a 130×120 mm<sup>2</sup> mat with optimal results. All traces of GA were then eliminated from the mats in a controlled environment (41% relative-humidity and 19°C) and confirmed by FTIR. In the end, it was seen that the mechanical resilience and thermal stability of the mats were improved after the applied of the modified, green GAbased crosslinking, revealing the engineered methodology potential for applications in biomedical devices.

**Keywords:** Bio-Based Polymers; Wound Protection; Nanofibrous Electrospun Mats; Green Crosslinking Process; Glutaraldehyde Vapor; Mechanical Resilience

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#### PCM3080

## Enhanced antimetastatic activity of the ruthenium anticancer drug RAPTA-C delivered in fructose-coated micelles

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Abstract. The ruthenium complexdichlororuthenium (II) (p-cymene) (1,3,5-triaza-7phosphaadaman-tane) (RAPTA-C) - has shown to be remarkably effective at suppressing the growth of solid tumor metastases. However, poor delivery efficacy and the lack of targeting ability of the common drug delivery system pose significant obstacles to maximize the therapeutic benefit of RAPTA-C. Inspired by the overexpression of GLUT5 transporter on the surface of breast cancer tissues but not the healthy mammary tissues,<sup>1</sup> the use of D-fructose as the targeting moiety of the drug carrier can significantly improve the cellular uptake



**Figure 1.** Scheme of polymeric micc......, cellular uptake and inhibitory effect of different micelles.

of nanoparticles, thus further enhancing the therapeutic efficiency of RAPTA-C. In this work, fructosemicelles and 2-hydroxyethyl acrylate (HEA)-micelles are prepared to investigate the difference in cellular uptake. It is found that glycopolymer leads to an increased uptake by breast cancer cells, while the HEA-micelles show less uptake. This behavior is also reflected by the slightly faster movement of fructose-coated micelles in MCF-7 tumor spheroid models using light sheet microscopy as analytical tool. The incorporation of RAPTA-C into micelles can enhance the inhibitory effect of the ruthenium drug demonstrated using invasion, chemotaxis, and haptotaxis assays. As a result, fructose-coated nanoparticles can be a promising drug delivery platform of RAPTA-C for the treatment of metastatic breast cancer.

**Keywords:** Fructose polymer; Ruthenium; Drug delivery

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