

P LYMER CONNECT OCTOBER 23-25, 2024 | ATHENS, GREECE

# **ABSTRACT BOOK**

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### **Keynote Presentations**

#### **Gasification Processes for a Circular Economy**

Daniel Serrano<sup>a</sup>, Marcelo P. Calagu<sup>a</sup>, Alberto García-Peñas<sup>b\*</sup>, María L. Cerrada<sup>c</sup>, José M. Gómez-Elvira<sup>c</sup>

<sup>a</sup>Thermal and Fluid Engineering Department and IAAB, Carlos III University of Madrid, Leganés, Spain <sup>b</sup>Materials Science and Engineering and Chemical Engineering Department and IAAB, Carlos III University of Madrid, Leganés, Spain

°Polymer Science and Technology Institute (ICTP-CSIC), Madrid, Spain

#### Abstract:

New European regulations emphasize the critical role of circular economy in addressing the continent's limited natural resources. This approach aims to reduce waste and promote the efficient use of materials, ensuring sustainability for future generations. In this context, innovative techniques, such as pyrolysis and photocatalysis, have emerged as promising solutions for recovering raw materials, providing a new perspective on how to handle waste and contribute to the circular economy.

Our research group has focused on the importance of material microstructures in predicting their behavior, particularly in terms of thermal stability. Understanding of thermal stability is crucial, as it plays a significant role in determining performance and durability of materials in various applications. Moreover, this knowledge is key to assess the energy requirements for processes like chemical recycling, which is essential for sustainable practices in industries ranging from plastics to metals.

By analyzing microstructural features, we can better understand how materials will respond under different conditions, especially during high-temperature processes like pyrolysis. This insight allows us optimizing recycling methods, reducing energy consumption, and improving the overall efficiency of material recovery. As Europe moves toward a more sustainable future, the development and applications of these advanced techniques will be essential in minimizing resource depletion and creating a more resilient and environmentally friendly economy.

#### **Biography:**

Dr. Alberto García-Peñas is an assistant professor in Materials Science and Engineering at University Carlos III of Madrid, where he also directs the master's in Circular Engineering and serves as Secretary for Academic Affairs of the "Álvaro Alonso Barba" Institute. He has over 55 publications in JCR journals, such as Chemical Engineering Journal and Chemosphere, and has contributed to 5 book chapters. Dr. García-Peñas has received 10 awards, including the Borealis Student Innovation Award and recognition from the Spanish National Research Council for his PhD thesis on polypropylene microstructures and their properties.

#### Valorization of Biodegradable Fibers Adressed to The Biomedicical And Environmental Concerns: The Structural Characterization and The Transport Phenomena Evaluation

#### Alexey Iordanskii<sup>a</sup>\*, Valentina Siracusa<sup>b</sup>, Anatoliy Olkhov<sup>a,c</sup>, Anna Zhulkina<sup>a</sup>.

<sup>a</sup>Semenov Scientific Center of Chemical Physics, RAS Moscow, RF. <sup>b</sup>University of Catania Department of Chemical Science, Catania,Italy. <sup>c</sup>FSBI National Medical Research Center for Obstetrics, Gynecology and Perinatology n.a. V. I. Kulakov of the Ministry of Healthcare of the Russian Federation

#### Abstract:

Minimizing gas emissions to atmosphere, using sustainable bioresources for plastic productions, and eliminating polymer waste are the principal issues of world circular economy. As the direct solution of these concerns, the efficient industrial transfer from fossil-based to bio-based materials should be provided by the comprehensive academic exploration of biodegradable plastics. The latter are especially designated for the innovative implementations in biomedicine, active packaging design, and eco safety provision. Therefore, a number of biodegradable polyesters, namely PLA, PHB, PCL and chitosan, which are currently leading on the word's market, were thoroughly studied on the structural, crystalline and kinetic levels to present the multifaceted pattern of their behavior in such phenomena as controlled release, smart barrier features, oil recovery after disastrous spills, etc. The special attention was paid to ultrathin fibers fabricated by electrospinning via solute and melt formation. The evolution of the initial structure for the fibers due to blending, water diffusion, drug embedding, and the impact of external factors like temperature, hydrolysis and ozonolysis are inherently given as the topics of the presentation. The up-to-data powerful methods, namely Mössbauer and EPR spectroscopies, FTIR and SEM were appropriately employed to manage the drug release profiles and to control the structure hierarchy of the polymers during their exploitations in thermal and hydrothermal conditions. The multifarious analysis of the nanostructured fibers and their mats could provide the specialists to enhance the performance outlook for the development of drug vehicles and the smart food packaging design.

#### **Biography:**

Alexey Iordanskii, Prof., DSc (Polymer chemistry), is a Principal Investigator at Semenov Federal Research Center for Chemical Physics, RAS Moscow RF. His researches have focused on diffusion in nano- and microsystems, drug release and biodegradation in biopolymers with the emphasis on composites and nanofibers. He is internationally respected expert in the above areas with 340 publications. Fellowship at the Institute of Macromolecular Chemistry, Prague, Czech Republic and the Institute of Medical Polymer Chemistry. Wroclaw, Polish Republic. Academic lecturing in the "Rhone Poulenc Co" Lion-Paris France (1987) Earlier, he was nominated by the Gold medal for Artificial heart design. Nowadays, Alexey Iordanskii is the Editorial Board Member of Polymers MDPI Publishing, Switzerland, and Reviewer Board Member.

#### **Temperature Cycles limits of PCT-Based Smart Heaters from Conductive Polymers**

#### Petr Špatenka<sup>1\*</sup>, Josef Blažek<sup>2</sup>, Stanislav Krum<sup>1</sup>, Jan Sezemský<sup>1</sup>, Sumesh Keerthiveettil Ramakrishnan<sup>1</sup>

<sup>1</sup>Czech Technical University in Prague, Faculty of Mechanical Engineering, Department of Materials Engineering, Karlovo Namesti 13, CZ-12135 Prague, Czech Republic

<sup>2</sup>University of South Bohemia, Faculty of Education, Jeronýmova 10, 371 15 Ceské Budějovice, Czech Republic

#### Abstract:

Conductive composite polymers with PTC effect are promising material for simple and cheap production of smart self-regulating heaters. However, the poor electrical reproducibility after repeated temperature cycles is a limiting factor for their industrial application.

To address this problemm we performed number of experiments with samples made by injection molding from commercially available conductive HDPE composite material Sabic 8520. The square-form samples were equipped with sputtered cupper contacts and which were connected to a power supply. The time dependence of temperature was studied. To investigate the time stability the heating was repeated on selected samples. A decrease in the current with time was observed resulting in high irreproducibility leading to sample distortion after several cycles. Based on the experimental results combined with theoretical calculation we have found the reason for the decrease in the total current through the sample. We found that the reason was based in a small inhomogeneity in the sample conductivity. Due to a positive feedback an extention of this high resistivity area extended across the sample forming a line-like structure

parallel to the electrodes which hiders the heating effect of the sample. Microscopic investigation indicated that agglomeration of the conductive fillers was the reason for the conductivity decrease.

#### Short Biography:

Roland Petrény , Ádám Bezerédi , László Mészáros: Electrically conductive polymer composites: Today's most versatile materials? Express Polymer Letters Vol.18, No.7 (2024) 673–674

Hai-Ping Xua,b,c,\*, Hui-Jing Liua, Hua-Qing Xieb,c, Wei Yua,b,c, Dan-Dan Yanga: Excellent positive temperature coefficient behavior and electrical reproducibility of HDPE/(TiC-CB) composites. 3. Results and discussion European Polymer Journal 175 (2022) 11133\$

### Investigating the Properties of Polybutadiene and Styrene-Butadiene Copolymers: A Comparative Study Using Atomistic and Systematic Coarse-Grained Models

#### Anastassia Rissanou,<sup>a,\*</sup> Antonis Chazirakis,<sup>b,c</sup> Vagelis Harmandaris<sup>b,c,d</sup>

<sup>a</sup>Theoretical & Physical Chemistry Institute, National Hellenic Research Foundation, 48 Vassileos Constantinou Avenue, 11635 Athens, Greece.

<sup>b</sup>Institute of Applied and Computational Mathematics (IACM), Foundation for Research and Technology Hellas, (FORTH), IACM/FORTH, Heraklion, Greece.

<sup>o</sup>Department of Mathematics and Applied Mathematics, University of Crete, Heraklion, Greece.

<sup>d</sup>Computation-based Science and Technology Research Center, The Cyprus Institute, Nicosia 2121, Cyprus.

#### Abstract:

The systematic coarse graining of polymeric systems is a usual route in order to extend the range of spatiotemporal scales and systems accessible to molecular simulations. Here we present a hierarchical bottom-up methodology in order to obtain coarse-grained (CG) models for copolymers, derived from more than one species of monomers, via detailed atomistic simulations. In the proposed scheme each monomer type is represented as a different CG particle. The effective CG interactions are obtained via a dual stage multi-component iterative Boltzmann inversion optimization scheme, in which the same component terms of the CG model are obtained from homopolymer simulations, whereas the interactions between different CG type particle (mixed terms) from the simulation of a single copolymer, of symmetric composition of the different microstructures. As an example, the proposed optimization scheme is initially applied on polybutadiene (PB) copolymers consist of cis-1,4, trans-1,4 and vinyl-1,2 isomers. The resulting CG copolymer model is examined with respect to its molecular weight transferability and copolymer composition. Structural properties are presented via the detailed atomistic and the systematic CG simulations, as a function of monomeric concentrations. Moreover, dynamic properties of PB copolymers are calculated for various compositions. The effect of the vinyl-1,2 component in conformational properties of PB copolymer melts is particularly emphasized, due to the different local packing imposed by the side groups. In the following the same methodology is applied on styrene-butadiene (SBR) copolymers, examining the transferability of the CG model through its ability to explore the conformational phase space of such complex systems.

#### **Biography:**

Dr. Anastassia Rissanou is Assistant Researcher at the Theoretical and Physical Chemistry Institute, of the National Hellenic Research Foundation, Athens, Greece. She has basic education in Physics and long expertise in modeling of soft materials. Systems of interest are polymers, colloids, biological molecules such as peptides, proteins, RNA/DNA, as well as hybrid nanostructured materials of the aforementioned matrices with organic or inorganic nanofillers. She is skilled in various simulation methods in atomistic and coarse-grained level, as well as multi-scale simulation techniques. She has many publications in high-impact international journals and participations in many national and international conferences.

### **Featured Presentations**

#### **Polymer Nanocomposites: Structure, Dynamics and Properties**

#### Kiriaki Chrissopoulou

Institute of Electronic Structure and Laser, Foundation for Research and Technology-Hellas, Heraklion Crete, Greece

#### Abstract:

Polymer materials are often filled with inorganics to improve their properties. The cases in which the additive exists in a fine nm-sized dispersion within the polymeric matrix producing a nanocomposite allow the investigation of basic scientific problems. At the same time, the behavior of polymers restricted in space or close to surfaces/interfaces can be very different from that in the bulk. The investigation of the structure, morphology, chain conformations and dynamics of hydrophilic polymers in nanohybrids containing either layered materials or spherical nanoparticles will be presented. Mixing polymers with layered additives can lead to intercalated hybrids when the interactions between the constituents are appropriate; these can serve as model systems for the investigation of the static and dynamic properties of macromolecules in nano-confinement. On the other hand, using nanoparticles of largely different sizes provides the opportunity to vary the confining length as well the chain adsorption capacity. The polymer thermal and rheological properties are correlated with the obtained structure in an attempt to understand the relationship between the physicochemical attributes of the constituents and the final properties of the hybrids. Additionally, confined polymer dynamics is probed utilizing polymers with different hydrophillicity, functional groups and/or different architectures to investigate the influence of the interactions between the constituents and the geometry and size of the additive on both the local motion and the segmental relaxation. Acknowledgements: This work was supported by the Hellenic Foundation for Research and Innovation (H.F.R.I.) (Project SAXS-SOFT, Project Number: 3401).

#### Biography:

Dr Chrissopoulou is a Researcher B at the Institute of Electronic Structure and Laser of the Foundation for Research and Technology – Hellas. She is a Physicist and she holds a PhD in Polymer Science. During 2001-2002, she was Maître de Conférences at Collège de France, Paris, France. Her research interests are in the area of the structure and dynamics of multi-constituent polymer systems as well as polymer nanocomposites. She has published 44 papers in refereed journals, 8 in conference proceeding included in the citation index, 4 chapters in books and 1 editorial. Her h-index is 19.

#### Hybrid Polymeric Nanostructures from Synthetic Polymers and Biological Macromolecules

#### **Stergios Pispas\***

Theoretical and Physical Chemistry Institute, National Hellenic Research Foundation, Athens, Greece

#### Abstract:

The synthesis of novel polymeric nanomaterials based on synthetic, well-defined, responsive polymers and natural macromolecules (proteins, nucleic acids, polysaccharides) through covalent attachment or non-covalent interactions. Designed RAFT polymerization schemes are utilized to synthesize the functional polymers and facilitate the covalent attachment of functional synthetic polymer chains on biomacromolecules. Self-assembly processes, involving electrostatic and hydrophobic interactions, provide self-organized hybrid nano-assemblies with novel characteristics. Physicochemical studies in aqueous media, by application of a gamut of physical chemistry characterization techniques provide information on the structure and properties of the obtained nanostructures. The nano-assemblies are exploited as nanocarriers and/or nanocontainers for medical and environmental applications.

#### **Biography:**

Stergios Pispas is Director of Research at TPCI/NHRF. He studied Chemistry at the University of Athens, Greece and he obtained his PhD in Polymer Chemistry in 1994. He joined TPCI/NHRF in 2004. His research interests include the tailored synthesis of amphiphilic block copolymers and polyelectrolytes utilizing controlled polymerizations, physicochemical studies on block copolymer supramolecular assemblies and the development of hybrid, organic-inorganic and synthetic-biological, polymer-based nanostructures for applications in nanomedicine. He is currently serving as Deputy Director of TPCI/NHRF, Editor of Polymers and Member of the Editorial Advisory Board of the European Polymer Journal and Colloid and Polymer Science.

#### Self-Assembled Biopolymer Nanostructures for Applications in Food Technology and Biomedicine

#### Aristeidis Papagiannopoulos\*

Theoretical and Physical Chemistry Institute, National Hellenic Research Foundation Athens, Greece

#### Abstract:

Soft biomaterials based on the self-organization of natural macromolecules such as polysaccharides and proteins are attractive as nanocarriers of drugs, scaffolds and films for tissue engineering and wound healing. In addition, they receive great interest for food supplements, food stabilization and nutrient delivery. These materials are biocompatible and nontoxic and, in many cases, renewable. In this presentation our recent work on self-assembled biopolymer biomaterials will be discussed. The role of electrostatic interaction on the formation of the hierarchical nanostructures and the biocompatibility of the proposed preparation methods will be highlighted. Examples will include the preparation and optimization of protein/polysaccharide nanoparticles for the delivery of bioactive compounds, hybrid polysaccharide hydrogels for pharmaceutical and food science applications and protein/polysaccharide multilayers for cell culture. Characterization methods that will be illustrated include small angle neutron and X-ray scattering, light scattering, surface plasmon resonance and light spectroscopy. These studies demonstrate that proteins may act both as building blocks and nanocarriers inside multifunctional nanostructures while polysaccharides offer water holding capacity and hierarchical organization. The prepared nanoparticles, hydrogels and multilayers can be viewed as templates to design and develop other biomaterials based on polysaccharides and proteins tailor-made for targeted applications.

#### **Biography:**

Dr. Aristeidis Papagiannopoulos has a BSc in Physics (University of Patras, GR), an MSc in Polymer Science and Technology (Universities of Patras and Ioannina, GR) and a PhD in Physics (University of Leeds, UK). He is a Senior Researcher at the Theoretical and Physical Chemistry Institute of the National Hellenic Research Foundation. He is a member of the Hellenic Society of Biomaterials, the Hellenic Society of Polymers, and the Hellenic Colloids and Interface Society. His research is focused on nanostructured biomaterials e.g., protein/polysaccharide nanoparticles for the delivery of drugs and nutrients, biointerfaces for cell culture and biopolymer hydrogels.

# Synthesis and Characterization of Statistical and Block Copolymers of Various Isocyanates via Coordination Polymerization

Marinos Pitsikalis\*, Aikaterini Katara, Dimitra Mantzara, Maria Panteli, Maria latrou, Ioannis Choinopoulos

Industrial Chemistry Laboratory/National and Kapodistrian University of Athens, Athens, Greece

#### Abstract:

Coordination polymerization techniques were employed using the half-titanocene complex  $[(\eta^5-C_5H_5)](S)-$ 

2-Bu-O)TiCl<sub>2</sub>] as initiator for the synthesis of statistical and block copolymers of *n*-hexyl isocyanate, HIC, with 2-chloroethyl isocyanate, ClEtIC, 2-phenylethyl isocyanate, PEIC, and 3-(triethoxysilyl)propyl isocyanate, TESPI. In addition, statistical and block copolymers of n-dodecyl isocyanate and allyl isocyanate were also synthesized via the same polymerization methodology. The copolymers were characterized by NMR and IR spectroscopy, Size Exclusion Chromatography, SEC, and circular dichroism, while their thermal properties were investigated through Differential Scanning Calorimetry, DSC, and Thermogravimetric Analysis, TGA. In the case of the statistical copolymers the monomer reactivity ratios were calculated employing various graphical methods, as well as the COPOINT program, in the frame of the terminal copolymerization model. Structural parameters, such as the dyad monomer sequences and the mean sequence lengths were investigated as well. The kinetics of the thermal degradation of the statistical copolymers was studied, and the activation energies of the thermal decomposition were examined through the Kissinger, Ozawa-Flynn-Wall, OFW and Kissinger-Akahira-Sunose, KAS approaches. The block copolymers were synthesized by sequential addition of monomers. SEC, IR and NMR measurements confirmed the synthesis of well-defined products. The copolymers containing allyl isocyanate units were employed as scaffolds to conduct thiol-ene click reactions leading to functionalized polymers or more complex macromolecular architectures.

#### **Biography**:

**M. Pitsikalis** received his B.Sc. (1989) and Ph.D. (1994) in Chemistry from the National and Kapodistrian University of Athens, NKUA, Greece. He worked as a Postdoctoral Fellow at the University of Alabama at Birmingham, USA (1995-1996). He was elected Lecturer (1998), Assistant (2002), Associate (2009) and Full Professor (2014) at the Dept. of Chemistry of the NKUA. He worked as a Visiting Scientist at several institutions. His research interests include the synthesis and characterization of complex macromolecular architectures and the study of their solid and solution properties in common good and selective solvents.

### Facile Design of Libraries of Multi-Functional Copolymers Based on Dialkylamino-Derivatives

# Zacharoula latridi<sup>a,\*</sup>, Ioanna Tzoumani<sup>b</sup>, Maria Filomeni Koutsougera<sup>b</sup>, Dionisia Druvari<sup>b</sup> and Georgios Bokias<sup>b,c</sup>

<sup>a</sup>Department of Materials Science, University of Patras, GR-26504 Patras, Greece <sup>b</sup>Department of Chemistry, University of Patras, GR-26504 Patras, Greece <sup>c</sup>Foundation for Research and Technology Hellas (FORTH), Institute of Chemical Engineering and High Temperature Chemical Processes, GR-26504 Patras, Greece

#### Abstract:

Aiming at "smart" multifunctional materials, significant emphasis has been given in recent decades on polymeric materials exhibiting responsive characteristics to external stimuli, such as temperature, pH,  $CO_2$  etc. Tertiary amine methacrylate (or methacrylamide) derivatives have attracted particular attention, especially those derived from 2-(dimethylamino)ethyl methacrylate (DMAEMA), 2-(diethylamino)ethyl methacrylate (DEAEMA) or N-[3-(dimethylamino) propyl] methacrylamide (DMAPMA). Beyond their inherent temperature and pH sensitivity, these materials can undergo alkylation to form cationic derivatives, thereby expanding their potential applications, including self-organization, surface modification, and the introduction of biocidal properties.

Herein, homopolymers, as well as copolymers of DMAEMA and DMAPMA with hydrophilic monomers like 2-Hydroxyethyl methacrylate (HEMA) or hydrophobic ones such as methyl methacrylate (MMA), were successfully synthesized though free radical polymerization (FRP). Depending on the comonomer, the final products form amphiphilic self-assemblies in aqueous media (at room temperature). The critical aggregation concentration (cac) of these assemblies is controlled by pH and hydrophilic/hydrophobic balance, as revealed by Nile Red probing. Moreover, these systems allow the design of polymer libraries exhibiting a Lower Critical Solution Temperature (LCST) phase separation behavior in water within the whole accessible temperature range for liquid water, covering a wide pH range in the alkaline region, from pH=14 down to pH~8. Additionally,  $CO_2$ -responsiveness is investigated for some systems. Alkylation of

the aforementioned copolymers with propyl-, dodecyl- or hexadecyl-derivatives affects decisively selfassembly behavior and responsive properties, while it leads to materials with promising antimicrobial performance.

#### **Biography:**

Zacharoula latridi is an Assistant Professor in the Department of Materials Science at University of Patras since 2024. Previously, she has been a Post Doctoral researcher at Greek Universities as well as in the Institute of Chemical Engineering Sciences (ICE-HT) in Patras. Her research activities focus on the development of functional polymeric materials, stimuli-responsive polymers, polymer hydrogels, injectable hydrogels, study of drug release from polyampholyte self-assemblies, fabrication of polymer-coated nanoor micro-particles (e.g.  $SiO_2$ ,  $Fe_3O_4$  nanoparticles).

### Polyethylene-*co*-norbornene Polyolefins Characterization and Chemical Recycling: A Starting Point Towards Photocatalytic Upgrade

#### Daniel Serrano<sup>a\*</sup>, Marcelo P. Calagua, Alberto García-Peñas<sup>b</sup>, María L. Cerrada<sup>c</sup>, José M. Gómez-Elvira<sup>c</sup>

<sup>a</sup>Thermal and Fluid Engineering Department and IAAB, Carlos III University of Madrid, Leganés, Spain <sup>b</sup>Materials Science and Engineering and Chemical Engineering Department and IAAB, Carlos III University of Madrid, Leganés, Spain

°Polymer Science and Technology Institute (ICTP-CSIC), Madrid, Spain

#### Abstract:

New production processes should focus on circular strategies rather than linear economy. This will lead to improve energy efficiency and optimize the use of raw materials, avoiding to employ new ones. Implementation of the circular economy will bring the option not only to recycle materials for new products but also to deal with the high amounts of wastes accumulated in landfills. In this context, plastics are goods of great interest due to the high use in everyday activities. The recycling mechanism for high consumption plastics, mostly polyolefins, has traditionally been mechanical, consisting of separating, washing and drying the waste for subsequent agglutination and further extrusion into new products. This process may lead into materials with not enough quality as its predecessors.

The purpose of this work is to study the chemical recycling of novel polyolefins consisting of ethylene and norbonene to recover the raw monomers initially used in the polyolefins production. The recovered monomers could be employed to produce again polyolefins with similar properties to those prepared from raw monomers. Prior to the chemical recycling by pyrolysis, thermogravimetric experiments must be carried out to determine the degradation kinetics and thermal stability, as well as semicrystalline morphology as a function of norbornene content. Then, pyrolysis technique is employed to recycle the polyolefins, as a starting point for further photocatalytic upgrade of the products.

#### **Biography:**

Daniel is an Associate Professor at University Carlos III of Madrid. He has worked on gasification and pyrolysis field for energy purposes, including chemical characterization of reaction products. Nowadays, his current research is focused on photocatalysis processes to reduce the CO<sub>2</sub> produced in industrial processes. Additionally, he continues working on the chemical recycling of waste, especially to recover the polyolefins from the original monomers and synthesize new polyolefins. Along with that Daniel is lecturing courses on heat transfer, thermal engineering, and environmental technology.

#### Thermoresponsive and Biodegradable Poly(Oligoethylene Glycol Methyl Ether Methacrylate) Nanogels for Targeted Drug Model Release

#### **Mazrina Mazlan\* and Tom O. Mcdonald**

<sup>a</sup>Department of Chemistry, The University of Manchester, Oxford Road, Manchester, UK <sup>b</sup>Department of Materials, Henry Royce Institute, The University of Manchester, Oxford Road, Manchester, UK

#### Abstract:

In situ forming implants offer the potential to avoid complications associated with the poor medication adherence of patients. Poly(N-isopropylacrylamide) (PNIPAM) nanogels have been demonstrated as a thermoresponsive that can be used to form in situ implants. One concern regarding PNIPAM is the nature of the acrylamide monomers used. An alternative to PNIPAM is poly(oligoethylene glycol methyl ether methacrylate) (POEGMA), which avoids the use of acrylamides and their associated toxicity concerns. In this work, we present the development of a biodegradable POEGMA nanogels as in-situ forming implants.

The POEGMA nanogels were polymerised by dispersion polymerisation, resulting nanogels with the size of 85-183 nm. Two types of crosslinkers were used: degradable cross-linker bis(acryloyl)cystamine (BAC) and non-degradable crosslinker N,N-methylenebis acrylamide (MBA). BAC possesses thiols that allow the nanogels to degrade in the presence of the reducing agents dithiothreitol (DTT) and glutathione (GSH). These nanogels aggregate to form an implant when heated to body temperature at the physiological ionic strength. This temperature for aggregation can be tuned by varying the monomer ratio of 2-(2methoxyethoxy) ethyl methacrylate (MEO\_MA) and oligo(ethylene glycol) (OEGMA) monomers. The POEGMA nanogel sample demonstrated time-dependent degradation at pH 7, using concentrations of 20 mM DTT and 40 mM GSH. The ability for the implants release model water-soluble compounds was then investigated with a focus on understanding how the charge on the model compound influenced the release behaviour. Ultimately the nanogels were used to control the model release behaviour of different charges : Acid Orange 7 (negatively-charged), Rhodamine B (positively-charged) and Bromophenol Blue (neutral) and the release were fitted to Korsmeyers-Peppas model. All dye releases showed Fickian diffusion. Among these dyes, Acid Orange 7 demonstrated the most favourable release characteristics for POEGMA nanogel as part of an in-situ forming implant application, with correlation coefficient of 0.9961. In contrast, Rhodamine B had a correlation coefficient of 0.9741, while Bromophenol Blue exhibited a correlation coefficient of 0.9311.

#### **Biography:**

Mazrina joined the Polymer Chemistry Group at the University of Malaya, Malaysia, in 2018 to pursue her master's project. Her research, titled "The Impact of Substitution of Two Hydrophobic Moieties on the Properties of Guar Gum-Based Hydrogel," was subsequently published in Pigment Resin and Technology. In 2022, Mazrina continued her PhD studies in Polymer Chemistry by joining the McDonald Group at the University of Manchester. Her current research focuses on "Thermoresponsive and Degradable Poly(oligoethylene glycol methyl ether methacrylate) for Targeted Drug Model Release."

#### Thermoresponsive Polymer Drug Conjugates for Precision Oncology

#### George Pasparakis\* and Dimitra Toumpa

Department of chemical engineering, University of Patras, Greece 265 04, Greece

#### Abstract:

We report on thermoresponsive polymer-drug conjugates bearing camptothecin and gemcitabine as frontline drugs against model pancreatic cancer cells. Copolymers with a lower critical solution temperature (LCST at ca. 42°C) based on poly(ethylene glycol) methacrylate were chain-extended with polymerizable drug-monomers using reversible addition fragmentation chain transfer (RAFT) polymerization. Welldefined block copolymer drug conjugates were synthesized that could form self-assembled micelles with thermoresponsive coronae. Our synthetic methodology enabled fine control of the drug content, which could be precisely adjusted during the polymerization reactions, hence affording well-defined PDCs. The micelles were found to exert comparable or even more potent cytotoxicity against cancer cell lines, which was further augmented above the LCST due to the hydrophobic collapse of the micelles, favoring their cellular uptake into the cytoplasm. The cytotoxicity profile of these nanomedicinal formulations was dependent on the size of the micelles, the drug type and content, as well as the hydrolysis rate of their respective linker (i.e., ester, disulfide, etc.). Additional steps to further enhance the cytotoxicity profile were considered by inserting sonosensitizers as reactive oxygen species generators activated by ultrasound to induce synergistic apoptotic pathways. Our proposed strategy constitutes a relatively simple nanomedicinal formulation platform that can combine sonothermal and sonochemical triggering as stimulation mechanisms to maximize therapeutic potency at the site of ultrasound treatment.

**Acknowledgments:** This project is funded by the Hellenic Foundation for Research and Innovation (grand No. 81439, ULTRAMED).

#### **Biography:**

George Pasparakis is an Associate Professor of advanced materials at the University of Patras, Greece. From 2013 to 2015, he was an independent Research Associate under an Excellence Fellowship, and from 2015 to 2019, an EPSRC Early Career Fellow at the UCL School of Pharmacy; he previously researched laser phototherapies at IESL-FORTH. He earned a PhD from the University of Nottingham in 2009 and holds a Ptychion in Materials Science from the University of Patras. His research interests include nanomedicinal cancer therapies, drug delivery systems, as well as controlled polymerization methods, and precision polymers for bioapplications.

### Thermoresponsive Polymer Particles with Both LCST and USCT-Type Behaviours Produced via RAFT Mediated Pisa

#### Beth A. Jordan<sup>1\*</sup>, Amanda Pearce<sup>2</sup>, Helen Willcock<sup>1</sup>, and Fiona L. Hatton<sup>1</sup>

<sup>1</sup>Department of Materials, Loughborough University, Loughborough, LE11 3TU <sup>2</sup>Department of Chemistry, Loughborough University, Loughborough, LE11 3TU

#### Abstract:

Polymerisation induced self-assembly (PISA) is a way to create polymer particles with a range of morphologies. The polymers produced by PISA can exhibit a wide range of properties including thermoresponsive behaviour this is where the polymers exhibit changes in their physical properties with temperature. These polymers can exhibit lower critical solution temperatures (LCST) and upper critical solution temperatures (UCST) caused by the solvation of the polymer chains at various temperatures. The combination of UCST and LCST behaviours into one polymer may lead to a complex dissolution behaviour and switchable nanostructures. PISA was utilised to create a variety of diblock copolymers nanoparticles that showed a variety of thermoresponsive behaviours based on the polymer types and solvents used. This behaviour was studied using a variety of techniques to determine the cause of this behaviour.

#### **Biography:**

Beth Jordan is a 3rd year PhD student at Loughborough University under the supervision of Dr Fiona Hatton and Dr Helen Willcock in the Department of Materials Engineering. Her research currently focuses on RAFT mediated polymerisation induced self-assembly of polymer particles and resultant thermoresponsive behaviour of the particles. Previously She studied at the University of Nottingham where she completed a BSc and MRes in Chemistry.

# Numerical Study of the Mechanical Behavior of a Conceptual Polymeric Modular Design System for Hydroponics

#### André Gomes<sup>a</sup>\*, Bruno Sousa<sup>a</sup>, Joel Antunes<sup>a</sup>, Filipa Carneiro<sup>a</sup>, Ana Fonseca<sup>b</sup> and Joel Prior<sup>b</sup>

<sup>a</sup>PIEP - Centre for Innovation in Polymer Engineering, Universidade do Minho Campus de Azurém, Guimarães, Braga, Portugal

<sup>b</sup>J. Prior - Plastic Injection Company, Vagos, Aveiro, Portugal

#### Abstract:

Hydroponics is an increasingly attractive alternative to traditional farming solutions, but challenges remain in developing eco-friendly systems, such as the using sustainable materials and processes during production, optimization of the structures, and lifetime extension with these materials. Following worldwide concerns about sustainability, this work is engaged in study, and develop a new conceptual design solution to test, and place on the market a new/more eco-friendly system for hydroponics which, when compared to the one currently produced with metallic materials. Polymeric materials (e.g. ABS, PVC, HDPE, etc.) are the most promising ones to give the answer to develop a lightweight modular hydroponic system with higher recyclability and performance.

This study has a baseline metallic solution and proposes a polymeric alternative. A promising polymeric material was selected based on its mechanical performance, cost-effectiveness, and availability from the supplier (J.Prior). Various additives were analyzed to enhance the material's mechanical performance and chemical resistance to nutritive solutions, aiming to create a more sustainable and suitable option for hydroponics. To ensure these requirements were met, a numerical simulation study using Abaqus was conducted to evaluate the mechanical behavior of the proposed system with PVC.

The results indicated that the selected material could serve as a sustainable alternative for modular hydroponic systems. Consequently, a new conceptual design for the polymeric material was developed in comparison to the metallic solution. Future work will focus on optimizing the product and support geometry to further enhance mechanical performance and reduce system weight.

#### **Biography:**

Graduate in Product Design and current Master's student in Product Engineering at the University of Minho. Proficient in 3D modeling using various software, with skills in both manual and digital sketching, as well as additive manufacturing (FDM and LCD). Comprehensive knowledge in product development, from ideation to final execution. Strong ability to generate and develop innovative concepts, always focused on creative and functional solutions.

#### Biocompatible Drug Delivery Systems Able to Co-Deliver Antimicrobial and Anticancer Agents

#### Daniela Ailincai<sup>a</sup>\* and Luminita Marin<sup>a</sup>

<sup>a</sup>Petru Poni Institute of Macromolecular Chemistry, Iasi, Romania

#### Abstract:

The aim of the study was to develop formulations with suitable and promising properties to be used as temporary implants in the postsurgical treatment of breast cancer. At first, hydrogels containing safe and biocompatible materials were synthesized, with adequate properties to help maintain the shape of the breast by tissue expansion during the healing process. The hydrogels were characterized from structural, morphological and supramolecular points of view, as well as for their intended applications: biodegradability, biocompatibility, and antimicrobial activity. Furthermore, the hydrogels' biological properties were enhanced by encapsulating a natural antimicrobial agent and a commercial anticancer drug to create formulations capable of preventing infections and cancer recurrence. The morphology of the formulations revealed a uniform encapsulation of the drug into the hydrogel matrix, while FTIR and WXRD analyses demonstrated strong interactions between the drugs and the polymeric matrix. Moreover, the obtained systems were shown to be biocompatible, biodegradable, and to exhibit antimicrobial and anticancer properties. The *in vitro* release kinetics of the antimicrobial agent and anticancer drug indicated that the formulations could release them in a sustained manner over multiple days through a complex mechanism involving diffusion, matrix swelling, and erosion, suggesting these materials as promising candidates for use as temporary implants in postsurgical cancer treatment.

#### **Biography:**

Daniela Ailincăi is chemical engineer and scientific researcher at "Petru Poni" Institute of Macromolecular Chemistry in Iasi, Romania. In 2016, she defended the PhD thesis: Complex supramolecular architectures with potential bioapplications. She has experience in the synthesis and characterization of polymeric materials: hydrogels, nanoparticles, and composite films. Her fields of interest include supramolecular hydrogels based on chitosan, dynamic imino-chitosan films with antimicrobial properties, dendrimer-like supramolecular architectures for gene therapy and biomaterials based on chitooligosaccharides. She is co-author of 36 papers in 10 years of activity and in 2023 she was one of the L'oreal Unesco FWIS Young Talents in Romania.

**Acknowledgements:** This work was funded by the national fellowship program L'oreal – Unesco "For women in Science".

#### Application of Flexible Tools in Magnesia Sector: The Case of Grecian Magnesite

#### Christos Evaggelou<sup>1</sup>\*, Nikolaos Margaritis<sup>1</sup>, Panagiotis Grammelis<sup>1</sup>, Roberto Arévalo<sup>2, 3</sup>, Haris Yiannoulakis<sup>4</sup> and Polykarpos Papageorgiou<sup>5</sup>

<sup>1</sup>Centre for Research & Technology Hellas, Chemical Process and Energy Resources Institute (CERTH/ CPERI), 4th km. N.R. Ptolemais-Mpodosakeio, 50200 Ptolemais, Greece;

<sup>2</sup>CIRCE—Research Center, Industrial Park Dinamiza 3D, 1st Floor, 50018 Zaragoza, Spain;

<sup>3</sup>School of Architecture & Polytechnic, University Europea de Valencia, Paseo de la Alameda 7, 46010 Valencia, Spain

<sup>4</sup>Research and Development Center, Grecian Magnesite S.A., 57006 Thessaloniki, Greece;

<sup>5</sup>Yerakini Mines and Works, Grecian Magnesite S.A. (GM), 63100 Chalkidiki, Greece;

#### Abstract:

Two of the main challenges that the global community must face are climate change and the energy crisis, which are the results of reckless energy consumption and the continuous increase of environmental pollution. A highly important factor related to the above problem and its solution, is the operation of the Energy Intensive Industries (EIIs), as on the one hand consume more than 25% of the energy produced by fossil fuels, on the other hand are the main responsible for the emissions of carbon dioxide and other greenhouse gases. The following study focuses on an EEI, the Greek mining and production company of magnesium products, Grecian Magnesite (GM). Aiming to estimate the efficiency of using biomass as fuel in the production process at a technical, environmental and economic level, two flexible model tools were developed that simulate the production process on the GM demo site, which can prove to be key in decision making regarding the proper operation of the facilities. The first tool calculates the total production cost and CO<sub>2</sub> emissions when substituting different percentages of the pet coke energy with biomass. The second (CFD tool), simulating the operation of rotary kilns, delineates the operating conditions and estimates how they can be affected by the use of biomass. The utilization of the tools proved that the higher the percentage of biomass substitution, the higher the gains, both in CO, emissions and cost reduction. A proposed and feasible solution is the substitution with sunflower husk pellets by 50%, which will result in a 25% reduction in  $CO_2$  emissions and almost 10% in production costs.

#### **Biography:**

Christos Evaggelou is an Environmental Engineer, graduated from the Democritus University of Xanthi in 2014. He has a master's degree in Energy Resource Technologies and Management at the University of Western Macedonia, Department of Mechanical Engineering. He has worked as an Environmental Engineer in both private and public sector, while he is now a Scientific Associate at the Chemical Processes and Energy Resources Institute (CPERI) of the Centre for Research and Technology - Hellas (CERTH). In addition, he is a PhD candidate at the University of the Western Macedonia, in the Department of Mechanical Engineering. He possesses expertise in the utilization of alternative and renewable energy technologies and in the energy behaviour and upgrading of building infrastructures.

#### Introducing the Tailored Design of Polymers

#### Marianna Yiannourakou<sup>a\*</sup>, David Rigby<sup>a</sup>, Boris Belin<sup>a</sup> and Clive Freeman<sup>a</sup>

<sup>a</sup>Materials Design Montrouge, France & San Diego, California, USA

#### Abstract:

Polymers, the powerful building blocks of modern materials, possess a remarkable diversity of properties. This presentation focuses on the capabilities of molecular modeling and data science for predicting and identifying polymers with targeted functionalities.

We begin by exploring the power of model-building tools to construct realistic models of complex systems (thermosets, micelles and lipids, semi-crystalline polymers, reinforced polymer composites, etc.). Subsequent application of molecular dynamics (MD) and Monte Carlo (MC) simulations, leveraging classical forcefields, enables the prediction of a range of properties (mechanical behavior, solubility, gas transport phenomena, and swelling characteristics).

Next, we introduce the Bicerano methodology [1], a QSPR approach that leverages established correlations between molecular structure and polymer properties. This method facilitates rapid property prediction based only on structural characteristics.

Finally, we bridge the gap between prediction and discovery by introducing access to a comprehensive precomputed polymer database (containing more than 1.1 million entries spanning diverse chemical variants) [2]. This powerful resource allows researchers to efficiently identify polymers with desired properties, accelerating the design and development of novel materials, including identifying and designing polymers derived from biobased starting points.

This presentation fosters a comprehensive overview of the prediction of polymer properties by highlighting the complementary strengths of the different methods. It paves the way for researchers to harness the combined power of molecular modeling and data science to tailor polymers for specific applications.

[1] Jozef Bicerano, Prediction of Polymer Properties, Third Edition (New York: Marcel Dekker, Inc., 2002)

[2] J. Bicerano, D. Rigby, C. Freeman, B. Leblanc, and J. Aubry, Polymer Expert - A Software Tool for De Novo Polymer Design, Computational Materials Science, 235, p 112810 (2024).

#### **Biography:**

Dr. Marianna Yiannourakou leads product management at Materials Design, Sarl, leveraging her expertise in fluid and soft matter simulations to develop innovative, high-performance software for property prediction. Marianna holds a Chemical Engineering PhD from the National Technical University of Athens and is widely published in fluid and condensed matter simulation.

#### From Single Molecule to Molecular Aggregate

#### Zhen Li\*

<sup>a</sup>Department of Chemistry, Wuhan University, Wuhan, Hubei, China

#### Abstract:

To construct p-molecules with different structures is one of the key points in the research field of optoelectronic materials. In many cases, the molecular structure not only affects the intramolecular-conjugation, but also the intermolecular p-p stacking, to result in the different functionalities. In this talk, some typical examples will be presented to partially demonstrate the interesting different properties with minor or even ignorable structural difference.

#### **Biography:**

Zhen Li received his BSc and PhD degrees from Wuhan University (WHU) in China in 1997 and 2002, respectively, under the supervision of Prof. Jingui Qin. In 2003-2004, he worked at the Hong Kong University of Science and Technology in the group of Prof. Ben Zhong Tang. In 2010, he worked at the Georgia Institute of Technology in the group of Prof. Seth Marder. He has been a full professor at WHU since 2006. His research interests are in the development of organic molecules and polymers with new structures and new functions for organic electronics and photonics.

#### Hierarchical Multiscale Modelling Schemes for Polymer Systems and Molecular Simulation Methods for the Study of Gas Sorption and Diffusion in Polymer Matrices

#### Niki Vergadou

Institute of Nanoscience and Nanotechnology, National Centre for Scientific Research "Demokritos", Athens, Greece

#### Abstract:

Molecular modeling methods provide a unique means for shedding light onto the microscopic mechanisms that are responsible for the materials end-use performance and the prediction of their properties, forming the basis for the molecular design of next generation tailor-made materials. The broad spectra of lengthand time-scales present in macromolecular systems necessitate the implementation of systematic hierarchical approaches for their computational study. Multiscale schemes are required for the study of small molecule diffusion in inflexible amorphous polymer matrices. Hierarchical methods are also necessary for the generation of realistic structures of polymers with complex chemical constitution that are based on coarsegraining (CG) strategies. Currently, CG Machine Learning-based (ML) approaches for complex chemical systems are also investigated and opportunities and challenges are to be presented. Systematic molecular simulation methods have been also developed and implemented for the study of gas sorption in polymeric matrices.

#### **Biography:**

Niki Vergadou is a Researcher at the Institute of Nanoscience and Nanotechnology of the National Centre for Scientific Research "Demokritos" in Athens, Greece. She holds a Diploma in Physics from the University of Ioannina, Greece, an MSc in Polymer Science and a PhD (2006), both granted from the Chemistry Department of the University of Athens. Her research involves the development and implementation of computational methods for the molecular simulation of materials and the prediction of a wide range of properties. Her research interests include the study of complex chemical systems such as polymers, complex fluids, ionic liquids and composite materials using a multitude of methodologies at various length and time-scales. Currently, her research activities also focus on the integration of machine learning techniques in materials modeling.

#### **Connectivity-altering Monte Carlo in Polymer Melts: An Overview and Perspective**

#### Loukas D. Peristeras\*

Institute of Nanoscience and Nanotechnology, National Center for Scientific Research "Demokritos", GR-15310 Aghia Paraskevi, Attikis, Greece

#### Abstract:

Understanding the behavior of polymers under various conditions is essential to developing innovative, novel materials. In this respect, in addition to the experiments, molecular modeling of polymeric melts is also challenging due to the large relaxation times that characterize the mechanisms underlying their properties. Molecular modeling of polymeric melts is challenging due to the large relaxation times that characterize the mechanisms underlying their properties. Molecular modeling of polymeric melts is challenging due to the large relaxation times that characterize the mechanisms underlying their properties. Connectivity-altering Monte Carlo (CAMC) stands out from a plethora of methods developed in this respect. This is due to its unique ability to equilibrate the conformational characteristics of high-molecular-weight polymeric systems, whose relaxation times are out of reach for conventional techniques like equilibrium molecular dynamics (MD). However, contrary to the MD-based method, CAMC is not part of the every-day modeling routine due to its difficulty in being implemented independently of the specific molecular features of the system at hand. Here the latest developments of CAMC will be presented and discussed.

#### **Biography:**

Dr. Loukas Peristeras is a researcher in the Molecular Thermodynamics and Modelling of Materials Laboratory (MTMML) at the National Center for Scientific Research "Demokritos" in Athens, Greece. His main scientific interest is the application of available schemes, their improvement, and the development of new approaches for the calculation of material properties by means of molecular and thermodynamic modelling. Among others, he created "Amorphous Builder," a software for the creation of initial configurations for molecular modeling, and contributed to Chameleon, a MC simulator for the calculation of realistic polymer structural properties, integrated into Sienomics MAPS<sup>®</sup> commercial software.

### Smart Nanostructured Materials as Drug Delivery Carriers to Treat Cancer, Kidney and Cardiovascular Diseases Title

### Hermis latrou<sup>\*,</sup><sup>a</sup>, Foteini Arfara<sup>a</sup>, Iro Kyroglou<sup>a</sup>, Pandora Thimi<sup>a</sup>, Dimitrios Skourtis<sup>a</sup>, Maria Kasimatis<sup>a</sup>, Konstantinos Dimas<sup>b</sup>, Dimitris Vlassopoulos<sup>c</sup>, Henrich Frielinghaus<sup>d</sup>

<sup>a</sup>National and Kapodistrian University of Athens, Department of Chemistry, Panepistimiopolis, Zografou, 15771, Athens, Greece

<sup>b</sup>Department of Pharmacology, Faculty of Medicine, University of Thessaly, Larissa, Greece

<sup>c</sup>FORTH, Institute for Electronic Structure and Laser, Heraklion 71110, Greece and Department of Materials Science & Technology, University of Crete, Heraklion 71003, Greece

<sup>d</sup>Jülich Centre for Neutron Science JCNS at Heinz Maier-Leibnitz Zentrum (MLZ), Forschungszentrum Jülich GmbH, Lichtenbergstraße 1, 85748 Garching, Germany

#### Abstract:

Novel, multifunctional nanoparticles and hydrogels that exhibit a unique set of properties for the effective treatment of cancer, kidney and cardiovascular diseases are presented. The materials are comprised of non-cytotoxic polypeptidic and polyethylene oxide polymers. The amphiphilic hybrid materials assemble in aqueous media to form micelles or vesicles, comprised of an outer hydrophilic corona of PEO chains, and a pH- and redox- responsive hydrophobic layer. Excessive characterization was performed to obtain the structure of the NPs. Moreover, the pH- and redox-responsiveness was investigated at the empty as well as the loaded NPs. Anticancer drugs was efficiently encapsulated in the hydrophobic core of the nanostructures and released under pH- and redox- conditions that simulate the healthy and cancer tissue

environment. Finally, in vitro and in vivo cytotoxicity assay of the loaded NPs against three different breast cancer cell lines showed that the nanocarriers exhibited better activity as compared to the free drug, rendering these novel NPs very promising materials for drug delivery applications.

Hybrid-polypeptidic materials formed injectable in situ forming quickly self-healing hydrogels, responsive to alteration of pH and increase of temperature. The connection between the alteration of secondary structure of the polypeptides with the viscoelastic behavior was revealed by means of Rheology and Circular Dichroism. Small-Angle Neutron Scattering and Scanning Electron Microscopy were employed to shed light to the structure of the polymers and how it affects their rheological properties. The results suggest that these biomaterials have the potential to be used in a number of bioapplications like drug delivery.

#### **Biography:**

Bachelor of Chemistry in 1989 from the Chemistry Department of NKUA, PhD from the Chemistry Department of NKUA in 1993. Post-Doc Fellow, Marie-Curie project at the Institute fur Festkoperforschungs" Forschungszentrum Juelich, Germany from 1994-1995. Director of the Analysis Laboratory of Aviation fuels for the Northern Greek Army Air Force Installations 1995-1997. Second post-doc at the University of Alabama at Birmingham, USA, 1997-1998. Research Fellow of Prof. Nikos Hadjichristidis at the NKUA, Chemistry Department, 1998-2002. Assistant professor of the Chemistry Department of NKUA, 2002, Associate Professor on 2009 and Professor on 2015 and Director of industrial Chemistry lab. His research interests are Polymer Chemistry, synthesis of biomaterials for drug and gene delivery, synthesis of nanostructured materials for biological applications, "smart" responsive nanomaterials for targeted drug delivery applications. He has published more than 150 papers.

#### Hydrogels and Nanogels for Biomedical Applications

#### Nikolaos Politakos<sup>a\*</sup> and Christos Chochos<sup>a,b</sup>

<sup>a</sup>Institute of Chemical Biology, National Hellenic Research Foundation, Athens, Greece <sup>b</sup>Advent Technologies SA., Patra, Greece

#### Abstract:

Biomedical applications can take a different approach regarding materials and the properties they use to achieve their goal. Some of the most well-known applications can be tissue engineering/regenerative medicine, drug delivery, medical devices, personalized medicine, and others. Two of the most important ones are considered drug delivery and tissue engineering. Therapeutics can be delivered to the human body in many ways. On the other hand, tissue engineering and regenerative medicine focus on the repair and restoration of tissues. Research is conducted in many biomedical applications, especially drug delivery. Pulmonary drug delivery is one promising way of delivering active compounds, pharmaceutical proteins, drugs, and vaccines. The respiratory tract and lungs specifically are promising in delivering compounds since local and systemic delivery can occur for many diseases. The delivery of drugs through the lung is limited but is under investigation and on the rise of inquiry. Formulations based on nanogels incorporated in microgels can be a solution in delivering drugs by increasing their size due to hydrophilicity to avoid macrophages and deal with the lung microenvironment. Hydrogels and nanogels are essential materials in biomedical applications. Hydrogels of any form can deliver active compounds, be biocompatible and have good physicochemical properties. Adding responsiveness, such as pH or others, can give an extra property and transform the formulations from passive materials to active ones.

#### **Biography:**

ABSTRACT BOOK

Dr. Politakos obtained his Ph.D. (2010) in Materials Engineering (University of Ioannina) in polymer synthesis. 2010 he moved to the University of the Basque Country, working with chemical modifications and composites. 2014, he worked in CICbiomaGUNE, preparing responsive copolymer brushes for biomedical applications. 2017, he started working on graphene oxide for CO2 capture in POLYMAT. 2020, he joined

the Responsive Polymer Therapeutics Group, preparing hydrogels for wound healing. 2024, he started at the NHRF as Fellow of HORIZON-WIDERA-2022-TALENTS, working with inhaled formulations to target lung cancer. His research interests include the synthesis of materials for biomedical and environmental applications.

#### Multiphase materials for 3D printing technology

#### Jan Sezemský, Petr Špatenka

Czech Technical University in Prague, Faculty of Mechanical Engineering, Department of Materials Engineering, Karlovo namesti 13, Praha 2, 120 00

#### Abstract:

The 3D printing technology allows production of complex and structural parts which would be difficult or ineffective to fabricate by conventional techniques such as injection and compression molding. However, one of the biggest limitation is the lack of materials suitable for the processing by this method. Moreover, significant external forces are not applied on the material during 3D printing, so it is complicated to achieve sufficient interfacial adhesion. Inadequate adhesion causes incomplete use of the potential reinforcement effect because there is no effective transfer of stress from the matrix to the fibres. Our research is focused on the adhesion improvement by plasma modification of the thermoplastic matrix in composite materials. New functional polar groups were bonded on the matrix surface during the treatment which enhanced its reactivity. By including plasma treatment on the powdery polymer matrix in the preparation procedure of initial mixture, the resulting mechanical properties of composite were substantially improved. This effect is attributed to enhanced specific adhesion between plasma modified polymer and the used secondary phase.

#### **Biography:**

Jan Sezemský has obtained the master 's degree in materials and production engineering at the Czech Technical University in Prague in 2019. He is currently enrolled in PhD program in Materials engineering and works as a researcher in the Department of Materials Engineering in the field of non-metallic materials. His major research focus is on sandwich materials produced by rotational molding and composite 3D printing.

#### Plasma-Synthesized Pyrrole-Derived Polymer Evolution Implanted in Rhesus Monkey Spinal Cord Transection Model

Axayacatl Morales-Guadarrama<sup>a,b,\*</sup>, Hermelinda Salgado-Ceballos<sup>c</sup>, Israel Grijalva<sup>c</sup>, Juan Morales-Corona<sup>d</sup>, Braulio Hernández-Godínez<sup>e</sup>, Alejandra Ibáñez-Contreras<sup>e</sup>, Camilo Ríos<sup>f</sup>, Araceli Diaz-Ruiz<sup>f</sup>, Guillermo Jesus Cruz<sup>b</sup>, María Guadalupe Olayo<sup>b</sup>, Stephanie Sánchez-Torres<sup>c</sup>, Rodrigo Mondragón-Lozano<sup>c</sup>, Laura Alvarez-Mejia<sup>d</sup>, Omar Fabela-Sánchez <sup>g</sup> and Roberto Olayo<sup>d</sup>

<sup>a</sup>Centro Nacional de Investigación en Imagenología e Instrumentación Médica, Departamento de Ingeniería Eléctrica, Universidad Autónoma Metropolitana Iztapalapa, CDMX, Mexico.

<sup>b</sup>Departamento de Física, Instituto Nacional de Investigaciones Nucleares, Axapusco, Mexico;

<sup>c</sup>Instituto Mexicano del Seguro Social, Unidad de Investigación Médica en Enfermedades Neurológicas, Hospital de Especialidades Centro Médico Nacional Siglo XXI, CDMX, Mexico;

<sup>d</sup>Departamento de Física, Universidad Autónoma Metropolitana Iztapalapa, CDMX, Mexico;

eInvestigación Biomédica Aplicada S.A.S. de C.V., CDMX, Mexico;

<sup>f</sup>Departamento de Neuroquímica, Instituto Nacional de Neurología y Neurocirugía Manuel Velasco Suárez S.S.A., CDMX, Mexico;

<sup>g</sup>Departamento de Química Macromoléculas y Nanomateriales, Centro de Investigación en Química Aplicada, Saltillo, Mexico.

#### Abstract:

In a spinal cord injury (SCI), nerve tissue is injured, giving rise to paraplegia or tetraplegia depending on the level in which the injury occurred. Currently, there is no effective therapeutic strategy for recovery derived from the injury. Several studies have demonstrated the growth of neurons in cell culture on plasma-synthesized pyrrole-derived polymers (PPPy), as well as a recovery of motor function after PPPy implantation in SCI in rats. In the process of transferring these advances to the clinic, it has been recommended to test in larger species, such as non-human primates, prioritizing the use of non-invasive techniques to evaluate the progression of the lesion. The magnetic resonance imaging (MRI) studies commonly used in SCI are gualitative, limited only to determining the morphology of the lesion, so the use of diffusion tensor imaging (DTI) in the clinic could be an important tool to evaluate and monitoring SCI. This work shows the follow-up by standard magnetic resonance imaging (T1W and T2W) and DTI of the evolution of the SCI transection in non-human primates by means of volumetric analysis (VA), fractional anisotropy (FA) and tractography calculation by diffusion tensor (DTT) around injury and the PPPy. Injury progression and PPPy status were analyzed up to three months after the day of injury using VA, FA, and DTT. VA preservation, FA recovery, and DTT restabilization were observed in the experimental subject implanted with PPPy, in contrast to the non-implanted subject. MRI-derived parameters are consistent with histology as well as demonstrated recovery of motor function.

#### **Biography:**

Dr. Axayacatl is a professor-researcher of biomedical engineering and a member of the scientific committee of the CI3M of the Universidad Autonoma Metropolitana-Iztapalapa. He has a doctorate in Biomedical Engineering, and a specialty at the National Institute of Nuclear Research. He is author of more than 20 scientific publications and 7 national and international patents. He has collaborated closely with various universities and health institutes for the generation of new knowledge. He has received awards for his scientific activity from prestigious organizations such as the Society of Engineering in Medicine and Biology (EMBS), the Mexican Society of Biomedical Engineering (SOMIB).

#### **Development of Planctomycetota Cell Factory Utilizing Cryogel-Based Bioreactor**

#### Yafang Guo<sup>a</sup>\*, Kumar Gaurav<sup>b</sup>, Nicolai Kallscheuer<sup>b</sup>, Ivo Nischang<sup>a</sup>, Christian Jogler<sup>b</sup>, Ulrich S. Schubert<sup>a</sup>

<sup>a</sup>Laboratory of Organic and Macromolecular Chemistry (IOMC), Friedrich Schiller University Jena, Jena, Germany

<sup>b</sup>Department of Microbial Interactions, Friedrich Schiller University, Jena, Germany.

#### Abstract:

In the pursuit of sustainable and efficient biotechnological processes, bacterial cell factories have emerged as a promising solution for the production of a wide array of bio-based products. However, optimizing operational conditions to maximize yield and productivity remains a significant challenge. The innovative application of cryogels as a novel support matrix for the development of bacterial cell factories offers a potential solution. Cryogels, with their unique macroporous structure, provide an ideal environment for bacterial immobilization, ensuring high cell density and enhanced mass transfer rates. This presentation details the synthesis and characterization of these cryogel matrices and their integration with planctomycetota strains that are widely prevalent and possess a high potential for producing active biomolecules. Additionally, a cryogel-based bioreactor was developed to facilitate the production of active biomolecules. The findings underscore the potential of cryogels to revolutionize the field of biotechnology by providing a robust platform for efficient bioproduction.

Keywords: Planctomycetota, cryogel, bioreactor, cell factory, biomolecules

#### **Biography:**

Yafang Guo is currently conducting postdoctoral research at the University of Jena in Germany with Professor Ulrich S. Schubert. She is developing biocompatible cryogels to immobilize bacteria, aiming to establish a bacterial factory for revolutionizing biomedicine discovery and production. After earning her Ph.D. from the University of Bologna, where she pioneered research on natural antioxidant mechanisms, she worked as a scientific editor at Wiley. In that role, she bridged the gap between research and publication, enhancing her scientific communication skills. This unique blend of academic, editorial, and research experience allows Guo to bring a unique perspective to polymer science and biotechnology.

#### **Wound Sealing Polymers**

#### Ashrit Nair<sup>a</sup>\*, Pooja Yadav<sup>b</sup>, Navneet Sharma<sup>c</sup> and Bhupendra Singh Butola<sup>a</sup>

<sup>a</sup>Department of Textile and Fibre Engineering, Indian Institute of Technology, Hauz Khas, Delhi, India <sup>b</sup>Department of Medical Elementology and Toxicology, Jamia Hamdard University, Mehrauli-Badarpur Road, Delhi, India

°Amity Institute of Pharmacy, Amity University, Sector 125, Noida, Uttar Pradesh, India

#### Abstract:

Haemorrhage accounts for 65% of preventable deaths with half the deaths occurring within first (golden) hour. In spite of enormous research, most of the commercialized haemostatic agents such as HemConTM, TissealTM, FlowsealTM etc. are targeted towards medical mishaps, and only a few active agents, sealants and absorbents such as QuikClot ACS+TM, XSTATTM etc. address bleeding injuries in uncontrolled environments such as battlefields, jungles, roads etc. However, the problem with these haemostatic agents is low benefit v/s burden ratio, due to decreased efficacy and applicability in noncompressible junctional wounds, secondary toxicological manifestations, requirement of a buddy, minimal tolerance against mean arterial pressure, minimal wet adhesive ability and short shelf-life. This highlights the requirement of a self-applicable wet tissue adhesive sealant that addresses these challenges. The development of a wet adhesive sealant requires a synergistic combination of different polymers, wherein, certain chemico-biological interactions can be targeted by various biomimetic and natural polymers to achieve enhanced wet tissue adhesion. Similarly, the synthetic polymers can be tuned to achieve the desired rheological and structural behaviour for selfapplication, flowability and tolerance to burst pressure. Further, the multi-functionality of certain polymers can be used to achieve additional characteristics such as active haemostasis and wound sterility. The selected lead materials and their combination parameters are crucial for establishing efficacy, stability and determining toxicity. Thus, understanding and fine-tuning of material, tissue and environmental interactions are important for the development of a high efficacy wound sealant for application in pre-hospital casualties.

#### **Biography:**

My area of research is focused on biomaterial sciences, combat casualty management and biotechnology. Currently, I am pursuing my PhD from the Department of Textile and Fibre Engineering, Indian Institute of Technology, Delhi, India, in collaboration with the Institute of Nuclear Medicine and Allied Sciences, DRDO, Delhi, India. My research, in the field of biomaterial sciences, is inclined towards the management of combat bleeding injuries.

I have a total of 8 publications, 2 best oral presentation awards in international conferences and 1 patent (granted) for the development of an antimicrobial spray (CovDecon), which has been successfully transferred to the industry.

#### Graphene Oxide Concentration Effect on in-situ PANI Polymerization

#### S. Djelamda<sup>\*a,b</sup>, F. Djefaflia<sup>a,b</sup>, A. Nait-Merzoug<sup>a,b</sup>, A. Harat<sup>2</sup>, El-Haskouri<sup>c</sup> and O. Guellati <sup>a,b</sup>

<sup>a</sup>Mohamed Chérif Messaadia University of Souk-Ahras, BP. 1553, Souk-Ahras 41000, ALGERIA. <sup>b</sup>LEREC Laboratory, Physic Department, Badji Mokhtar University of Annaba, BP. 12, 23000, Annaba ALGERIA. <sup>c</sup>Instituto de Ciencias de los Materiales de la Universitat de Val`encia, C/ Catedratico Jose Beltran, 2, 46980 Paterna, Valencia, Spain

#### Abstract:

Graphene oxide (GO) and polymer such Polyaniline (PANI) based Nanocomposite are widely used especially in energy conversion and storage as an electrode of supercapacitor due to their excellent physic-chemical properties.

In this investigation, we have prepared PANI/GO nanocomposite using in-situ polymerization method with different GO concentration in the presence of APS under acid conditions in low temperature less than 2 degrees. We report the identification of nanostructured products by using different techniques, such as: XRD, Raman spectroscopy, FESEM, UV- vis and electrochemical measurements. They show clearly excellent electrochemical properties, fast reversible Faradic reaction and especially interesting specific capacity due to both mechanic stabilities and high electric conductivity of GO as well as the PANI nanofibers conductivity.

Keywords: Graphene oxide (GO), Polyaniline (PANI), supercapacitor, electrochemical measurements, nanofiber.

#### **Biography:**

Sara Djelamda holds a Ph.D. in Applied Physics, with her research focused on nanocomposites, polyaniline, in-situ growth, and energy storage. Her work explores the development and application of advanced materials in the field of energy storage, particularly emphasizing the synthesis and characterization of nanocomposites.

### Manufacture of Cellulose- and Lignin-Based Polymeric Biomaterials from Rice Straw for Use in the Footwear Industry

### H. Pérez-Aguilara\*, V.M. Serrano-Martíneza, M.P. Carbonell-Blascoa, E. Orgilés-Calpenaa and F. Arán-Aísa

<sup>a</sup>INESCOP, Footwear Technological Centre. Pol. Ind. Campo Alto, C/ Alemania, 102, 03600, Elda

#### Abstract:

Cellulose and lignin are the most abundant polymers in nature, however, they are not usually recovered and used in high value-added applications. In thisstudy, lignin and cellulose have been extracted from rice straw, which is a lignocellulosic waste very rich in both polymers. Despite its high lignin (37.39%) and cellulose (51.59%) content, the typical end-of-life scenario of rice straw waste is incineration. More than 650 million tonnes of rice straw are produced worldwide annually, which amounts to 950 million tonnes of CO2 eq. In this context, an economically and environmentally sustainable process has been developed for the recovery of cellulose fibres with suitable properties to be incorporated in the manufacture of polymeric materials (rubber, EVA or polyurethane), thus improving their physical-mechanical properties for application in the footwear sector. Polyols have also been extracted from the lignin recovered for use in the manufacture of polyurethane bioadhesives or polyurethane foams for use in the footwear sector. Furthermore, the antimicrobial capacity of polyols to functionalise the surface of insoles has been evaluated. Finally, the application of the different biomaterials manufactured as footwear components has been validated.

#### **Biography:**

Henoc Pérez obtained his Degree in Chemistry and PhD in Chemistry on New Strategies for the Synthesis of Organic Compounds from the Organic Chemistry Department at the University of Alicante in 2010. From 2014, he has been working at INESCOP in Elda, Alicante (Spain) in the Advanced Materials and Technology department, focusing his research on projects related to new and innovative methodologies for the extraction of bioactive products from animal and vegetable by-products for different industrial applications, such as sustainable biomaterials, materials functionalisation, biostimulants for plants, retanning agents for leather or the incorporation of the bioproducts obtained in new materials.

#### **Polymers Tribology in Food Packaging Equipment**

#### Silvia Rossi, Polymers Specialist \*

#### <sup>a</sup>Tetra Pak Packaging solutions Spa, Modena, Italy

#### Abstract:

In food packaging equipment plastic bushings and rollers can be exposed to demanding conditions in terms of loads, running speed, surrounding temperature and chemical environment. The choice of material coupling with lowest wear rate is critical to maintain the lifetime of the Filling Machine components. A distinctive requirement for material selection in food industries is the compliance to the regulation requested for food contact applications, thus excluding many polymeric grades that are containing fillers not approved. Reference material tribological coupling, PEEK bushing against AISI 316L shaft, suffers of premature wear with generation of black particles. The wear mechanism has been studied both with pin on disk tests and in a test rig, which replicates the coupling of the real components, in terms of geometries and operative conditions. The impact of friction coefficient on interfacial temperature was investigated through measurements and virtual simulations. Due to the high CoF and environmental conditions, an interface temperature exceeding polymer Tg is developed generating black particles. FT-IR characterization of wear debris showed the presence of thermally oxidated PEEK, confirming the root cause. The same methodology and experimental setup have been successfully applied to select alternative plastic grades.

#### **Biography:**

Silvia has a master's degree in Materials Engineering, and she has been working at Tetra Pak Packaging Solutions, R&D department, since 2017. Specialist in Polymers, from materials advanced selection to components failure analysis and characterization. Involved in several validation activities of new materials and polymers-based coatings, she managed plans with suppliers to quickly find solutions that guarantee quality and certifications compliance. Driver of root cause analysis of polymers degradation and wearing issues.

Research interests in polymers tribology, polymers wettability and polymers accelerated lifetime tests. Continuous scouting of new compounds and high-performance plastics to mitigate current global raw materials shortage.

# Targeting and maintaining stable chromatographic properties of polymethacrylate-based monoliths for separation of plasmid DNA

#### Ines Bergoč<sup>a</sup>\*, Boštjan Košir<sup>a</sup>, Leja Tominec<sup>a</sup>, Petra Lapajne<sup>a</sup>, Borut Mlakar<sup>a</sup>, Polona Skrt<sup>a</sup>, Urh Černigoj<sup>a</sup> and Aleš Štrancar<sup>a</sup>

<sup>a</sup>Sartorius BIA Separations d.o.o., Mirce 21, Ajdovščina, Slovenia

#### Abstract:

Rapid and efficient separation of macromolecules using polymer based monolithic chromatographic stationary phases is well established both in academia and industry. The preparation of a rigid macroporous polymeric material is typically done by thermally initiated

polymerization in a simple molding process. Although the polymerization process is well documented [1], the robust production of commercial chromatographic monoliths (effective volume ranging from 0.1 mL up to 40 L) is challenged by numerous parameters, for example the quality of raw materials; the effect of mold characteristics (different shapes, sizes, configurations etc.); the control over polymerization procedures and conditions... Therefore, several distinguished processing parameters need to be considered, monitored, and understood

throughout the formation of the monolith. Quality of raw materials typically results in significant deviations in the properties of the final product: a) mechanical ones like channel size, porosity, BET nitrogen adsorption surface area; b hydrodynamic properties such as column permeability; and c) chromatographic characteristics.

In the presented work we have focused on finding the correlations between the presence of specific additives in monomers on the formation and properties of a produced polymer. As an example, quantity of nitroxide radical present in the crosslinker, being monitored with electron paramagnetic resonance method, influences the process of nuclei formation during the polymerization, which affects the final polymer structure. This is reflected in changed (nonreproducible) chromatographic separation of plasmid DNA isoforms. Understanding the

phenomena enabled us to prepare a polymerization plan including selection of right combination of raw materials and process parameters ensuring the highest possible repeatability and reproducibility of analytical column production.

[1] Frantisek Svec, Tatiana B. Tennikova, Zdenek Deyl; Monolithic materials preparation, properties, and applications; JOURNAL OF CHROMATOGRAPHY LIBRARY- volume 67, 2003.

#### **Biography:**

Ines Bergoč is the Head of the Polymerization Department, a subdivision of the Research and Development (R&D) Department at Sartorius BIA Separations. Her research team focuses on understanding the mechanisms of polymerization, enhancing existing products, and developing novel materials, particularly for the purification of large molecules. Ines is actively involved in translating laboratory knowledge to large-scale production. Her team has achieved remarkable success with the development and production of SDVB chromatographic columns, spanning a range from analytical to 8 L columns. She holds a Ph.D. degree in Material Science, specializing in Polymer/Plastic Engineering, from the Faculty of Chemistry and Chemical Technology at the University of Ljubljana, Slovenia.

#### Self-sensing Structural Composites: A Piezoresistive Approach

#### J. Nunes-Pereira\*, J.M. Parente, P. Santos, V. Sadhu and A.P. Silva

C-MAST, Centre for Mechanical and Aerospace Science and Technology, Universidade of Beira Interior, Covilhã, Portugal

#### Abstract:

The environmental impact of plastics is a growing threat to public health and natural resources. In turn, the aerospace, automotive and energy production industries are increasingly relying on these materials to make structures more resilient and energy efficient due to the high mechanical strength and low density of polymer-based materials. It is, therefore, important to increase the reliability of this type of material to extend the useful life of structures, reduce maintenance time and costs, and thus reduce the consumption of raw materials. To address this need, Structural Health Monitoring (SHM) using piezoresistive self-sensing based on the intrinsic electrical properties of composites can be employed. Therefore, in this work, glass fibre and carbon nanotube (CNT) reinforced thermoset composites were fabricated to produce laminate panels and adhesive joints with self-sensing capabilities. The fabricated epoxy resin laminate panels with 8-layers of glass fibre and 0.5 wt% CNT exhibited a linear and synchronised piezoresistive response to cyclic bending with a maximum sensitivity (gauge factor, GF) of  $\approx 0.4$  and the ability to detect low-velocity impacts between 3 and 6 J. Bulk epoxy adhesives with 0.5 wt% CNT showed piezoresistive sensitivity with a maximum GF of  $\approx 0.8$  and the ability to detect the failure mode in lap shear testing of a bonded joint. In conclusion, the developed materials demonstrate promising piezoresistive self-sensing capabilities and can be used in SHM of structures for early detection of potential damage, thus contributing to increased reliability, reduced maintenance costs and reduced consumption of energy and repair materials.

#### **Biography:**

João Nunes-Pereira (Ph.D. in Sciences, 2013) is Assistant Researcher at the Centre for Mechanical and Aerospace Science and Technology (C-MAST) at the University of Beira Interior (UBI), Covilhã, Portugal. His research focuses on the development of multifunctional structural composites for the aerospace, automotive and energy generation industries, among others. Since 2022, he is Invited Assistant Professor at UBI in the field of Materials Science.

#### **Acknowledgements:**

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#### **RAFT Polymerisation of Fatty Acid Acrylamide Monomers Derived from Plant Oils**

#### Oliver Harris<sup>a\*</sup> and Dr Ryan Larder<sup>a</sup>, Dr Helen Willcock<sup>a</sup>, Dr Fiona Hatton<sup>a</sup>

<sup>a</sup>Loughborough University, Department of Materials, Loughborough, United Kingdom

#### Abstract:

Polymeric materials based on fatty acids have a combination of characteristics (functionality, hydrophobicity, tuneable T<sub>g</sub>) that give them great potential as partially renewable, high value added materials. Previous studies have demonstrated the synthesis and free radical polymerisation of a range of unsaturated pendant fatty acid acrylamide monomers via an industrially relevant transesterification reaction. However, despite it's similarity to the well understood biodiesel reaction there are key differences that currently limit the yield and purity of products. Additionally, no research has yet been conducted on the use of these monomers in controlled radical polymerisation systems (e.g. RAFT) which would enable the design of high performance materials. In this work we investigated the base catalysed transesterification of four different plant oils with N-hydroxyethyl acrylamide by conducting kinetics experiments, investigating potential side reactions and by greatly improving characterisation and isolation of the target product. Impure brine washed monomers were intentionally used in the kinetics studies of RAFT polymerisations in order to evaluate the suitability of the existing monomer synthesis method as a practical and sustainable solution.

Successful control of the reactions by RAFT was assessed by using <sup>1</sup>H NMR spectroscopy and GPC to obtain monomer conversion,  $M_n$  and D data. Further developments in this area will enable higher yield syntheses of monomers suitable for RAFT polymerisation, and the range of thermal properties (12<  $T_g$  <56 °C and -16<  $T_m$  <47) accessible dependent on the pendant fatty acid could open the doors for a wide range of unique, renewably sourced materials.

#### **Biography:**

Oliver graduated from Loughborough University with an MEng in Materials Science and Engineering in July 2021, where his research projects focussed on green technology. As a part of his studies he also spent a year in industry working at Zotefoams, a physically-blown crosslinked polymer foam manufacturer, which served as a source of inspiration to pursue a research project in sustainable polymers. Oliver started a PhD at Loughborough University in July 2021 in Dr Fiona Hatton's group, investigating sustainable polymers derived from plant oils. This work has encompassed monomer synthesis, RAFT polymerisation, NMR, GPC and thermal analysis.

#### Novel Green Pre-treatment for Improved Polyethylene Terephthalate (PET) Waste Degradability

#### F.Millucci<sup>a</sup>\*, R. Germani<sup>b</sup>, P. Sassi<sup>b</sup>, A. Donnadio<sup>c</sup>, M. Tiecco<sup>d</sup>, S. Corezzi<sup>a</sup>

<sup>a</sup>Department of Physics and Geology, University of Perugia, Via Alessandro Pascoli, 06123 Perugia, Italy <sup>b</sup>Department of Chemistry, Biology and Biotechnology, University of Perugia, Via Elce di Sotto 8, 06123 Perugia, Italy

<sup>c</sup>Department of Pharmaceutical Sciences, University of Perugia, Via del Liceo 1, 06123 Perugia, Italy <sup>d</sup>School of Pharmacy, University of Camerino, ChIP Research Center, via Madonna delle Carceri, 62032 Camerino, MC, Italy.

#### Abstract:

Due to its widespread use and long environmental persistence, polyethylene terephthalate (PET) has surged as the iconic symbol of the current plastic crisis. Despite growing concerns about its negative impacts on ecosystems and human health, PET recycling rates remain alarmingly low due to degradation in material properties associated with traditional mechanical processes. To address this issue, chemical recycling (i.e. the selective breaking down of the polymer into high-quality monomers) has emerged as a promising alternative, enabling the remanufacturing of plastics with properties comparable to the pristine ones. However, high costs and substantial energy consumption still limit the widespread adoption of most chemical recycling methods. Here we demonstrate that a dissolution/precipitation treatment in propylene carbonate, a green solvent widely employed in cosmetic industries, significantly accelerates PET depolymerization. While conventional alkaline hydrolysis procedures typically require prolonged energy-intensive conditions (T>200°C, P~1.5 MPa), after pre-treatment PET can be fully depolymerized at 90°C in less than 5 minutes using minimal amounts of NaOH. Moreover, the proposed method retains high efficiency even when applied to recycle challenging materials, such as dyed fabrics and mixed waste. Green chemistry analysis indicates that the pre-treatment results in about 20-fold reduction of the environmental energy impact of alkaline hydrolysis, highlighting the elevated procedure's potential for industrial adoption.

[1] Millucci, F., Corezzi, S., Germani, R. PROCEDIMENTO PER LA DEGRADAZIONE DI PRODOTTI PLASTICI CONTENENTI POLIESTERI. Italian patent application no. 102024000008830, filed on 18/04/24.

[2] Millucci, F. et al. Novel green pre-treatment for enhanced PET hydrolysis (to be submitted to Nature Communications)

#### Biography:

Francesco Millucci is a third-year PhD student in physics at the University of Perugia, under the supervision of Prof. Silvia Corezzi. He earned his MSc in physics with highest honour from the University

of Perugia, with a thesis on the spectroscopic study of the volume phase transition in PNIPAM microgel. His current research is focused on the development of green strategies for polymeric materials recycling and upcycling. As part of his doctoral work, he spent six months at the FORTH/ICE-HT Institute in Patras, in the Nanotechnology and Advanced Materials Laboratory directed by prof. Costas Galiotis.

#### **Computer Simulations of Polymer/Graphene Oxide Composites**

### K.Karatasos<sup>a,\*</sup>, T. Rissanou<sup>b</sup>, K. Chrissopoulou<sup>c</sup>, G.S.Fanourgakis<sup>d</sup>, I Zuburtikudis<sup>e</sup> and H.A. Khalifeh<sup>e</sup>

<sup>a</sup> Aristotle University of Thessaloniki. Chemical Engineering Department, Thessaloniki, Greece

<sup>b</sup>Theoretical & Physical Chemistry Institute, National Hellenic Research Foundation, 48 Vassileos Constantinou Avenue, 11635 Athens, Greece

<sup>c</sup>Institute of Electronic Structure and Laser, Foundation for Research and Technology-Hellas, P.O. Box 1527, 711 10, Heraklion Crete, Greece

<sup>d</sup>Chemistry Department, Aristotle University of Thessaloniki, Thessaloniki , Greece <sup>e</sup>Abu Dhabi University, Department of Chemical Engineering, Abu Dhabi, U.A.E

#### Abstract:

Computer simulations have emerged as a unique tool to examine aspects of the physicochemical behavior of complex materials, in a level of detail usually not accessible in relevant experimental techniques. In the present work, a class of materials composed by graphene oxide (GO) and branched polymeric materials (either in free form or chemically attached to GO), are examined in order to assess the effects of the presence of the polymer molecules in the organization of the GO flakes in an aqueous environment, and in the ability of the formed composites to act as pollutant adsorbents and water purifying materials. To this end, equilibrium and non-equilibrium fully atomistic classical molecular dynamics simulations are employed to examine the driving forces for the self-assembly of the GO flakes in aqueous dispersions and to assess the mechanisms responsible for the enhancement of their capacity in water purification and desalination processes. The simulation results provide new insight on the relative importance of different factors (chemical composition of the GO, concentration, pH, size of the polymers etc) in the self-assembly process of the flakes, in the structural features of the resulting morphology, and in the interaction of the composites with pollutants and with ionic moieties which determine their ability to act as water purifying agents.

#### **Biography:**

Dr. Konstantinos Karatasos is a Professor in the Department of Chemical Engineering at A.U.T.H. His research interests include the study of the physicochemical behavior and the structure-property relationship of soft matter and composite materials. He has authored 70 articles in refereed journals and 3 chapters in books. He has participated in more than 120 conferences and served as a reviewer in more than 50 international journals and in research proposals in national and international bodies. He has participated in more the organization of meetings and schools, and he is a member of several scientific organizations.

#### Antibacterial Polymer Surfaces with Persistent Antimicrobial Activity

#### Maria Vamvakaki

<sup>a</sup>Institute of Electronic Structure and Laser, Foundation for Research and Technology - Hellas, 700 13 Heraklion, Crete, Greece and

<sup>b</sup>Department of Materials Science and Technology, University of Crete, 700 13 Heraklion, Crete, Greece

#### Abstract:

Antimicrobial surfaces have attracted great attention lately for use in medical devices, food processing and water purification systems. Among the different approaches employed, antimicrobial polymer surfaces that possess either antifouling or bactericidal properties have been shown to effectively inhibit the spreading of microbial infections [1]. Herein, functional polymer coatings exhibiting controllable antimicrobial properties were developed. Two types of polymeric materials were synthesised comprising (i) antifouling-bactericidal polymer brushes and (ii) self-polishing cross-linked polymer films. The solvent responsive behavior of the polymer brushes and their bactericidal activity for both Gram-positive and Gram-negative bacteria strains were evaluated. On the other hand, the ability of the cross-linked polymers to kill both bacteria strains and their self-polishing properties to renew the biocidal surface, were studied [2]. Overall, these dual-functional polymer surfaces exhibit unique antifouling-bactericidal and bactericidal-self-renewal properties, which render them promising for antimicrobial applications.

#### **References**:

- [1] Jain, A.; Duvvuri, L. S.; Farah, S.; Beyth, N.; Domb, A. J.; Khan, W. Adv. Healthcare. Mater. 2014, 3, 1969.
- [2] Koufakis, E.; Manouras, Th.; Anastasiadis, S. H.; Vamvakaki, M. *Langmuir* **2020**, *36*, 3482.
- [2] Manouras, Th.; Koufakis, E.; Vasilaki, E.; Peraki, I.; Vamvakaki, M. ACS Applied Materials and Interfaces **2021**, *13*, 17183.

#### **Biography:**

Maria Vamvakaki is a Professor at the Department of Materials Science and Technology, University of Crete and affiliated Faculty Member at IESL-FORTH. She holds a doctoral degree in Polymer Chemistry, University of Sussex, UK. Next, she became a research associate at the University of Sussex, a visiting Assistant Professor at the University of Cyprus and a visiting scientist at the University of Sussex. Prof. Vamvakaki is leading the Materials Synthesis Group, University of Crete. Her expertise focuses on the synthesis and characterization of polymeric, organic/inorganic materials, polyelectrolytes/polyampholytes and microgels/hydrogels. Current research interests include the synthesis of functional/stimuli-responsive polymers and their self-assembly in aqueous media in solution and at surfaces.

#### Water Effects in Amphiphilic Block Copolymers with Thermoresponsive Behavior

#### A. Kyritsis<sup>a</sup>\*, S. Kripotou<sup>a,b</sup>, A. Miasnikova<sup>c</sup>, A. Laschewsky<sup>c,d</sup>, C. M. Papadakis<sup>e</sup>

<sup>a</sup>National Technical University of Athens, Zografou Campus, 15780 Athens, Greece <sup>b</sup>University of West Attica, 12244, Athens, Greece <sup>c</sup>Universität Potsdam, Karl-Liebknecht-Straße 24-25, 14476 Potsdam-Golm, Germany <sup>d</sup>Fraunhofer Institut für Angewandte Polymerforschung, 14476 Potsdam-Golm, Germany <sup>e</sup>Technical University of Munich, James-Franck-Straße 1, 85748 Garching, Germany

#### Abstract:

Amphiphilic block copolymers can spontaneously form ordered structures either in solution or in films due to micelle formation or to bulk microphase separation. In the case where the hydrophilic block is a thermoresponsive homopolymer the self-organization of the copolymers may take various forms with the change of temperature. In this work we study the effects of water on the glass to liquid transition and the thermoresponsive transition in thermoresponsive diblock and triblock copolymers consisting of poly(methoxy diethylenglycol acrylate) (PMDEGA) and polystyrene (PS) blocks, in a broad range of polymer/water mixtures. We employ Differential Scanning Calorimetry (DSC) and Broadband Dielectric Spectroscopy (BDS) techniques for the investigation of the role of water to both transitions: glass to liquid and LCST-type coil to globule transition in the thermoresponsive polymers. In addition, our techniques

allow for the study of water freezing at subzero temperatures in the polymer/water mixtures studied. The results of this investigation are discussed in terms of hydrogen bonding, hydrophobic interactions, ordered (ice-like) and disordered state of interfacial water.

#### **Biography:**

The presenter is Professor at the School of Applied Mathematical and Physical Sciences, National Technical University of Athens - NTUA, Greece. He teaches elementary Physics and special topics of Physics of Dielectric Materials, Materials Science, Advanced Technological Materials and Nanotechnology at underand post-graduate level. His main research interests are focus on dielectric, thermal and hydration properties of inorganic and organic (polymers, biomaterials) materials, on structure-property relationships in polymer copolymers, blends and nanocomposites, on self-assembling polymeric materials, on colloids, ionic liquids, deep eutectic solvents and other glass-forming materials.

#### Breaking the classic boundary of shape memory polymers with dynamic network design

#### Tao Xie\*a

<sup>a</sup>College of Chemical and Biological Engineering, Zhejiang University, Hangzhou, Zhejiang Province, China

#### Abstract:

Shape memory polymers (SMP) are capable of undergoing programmable shape shifting in an on-demand fashion. Although such a behavior has been known for over half a century, rapid progress in the field of SMP has only been made in the last two decades. At the fundamental level, designing sophisticated shape memory behaviors beyond the simple shape-shifting between a permanent and a temporary shape has been the ever-lasting effort. In this talk, I will illustrate how designing dynamic polymer networks can expand the polymer shape memory behaviors beyond the radar screen. Specifically, I will first introduce a new class of SMP called thermadapt SMP for which the permanent shape can be mechanically programmed. Next, I will show how spontaneous phase transition in a hydrogel can be utilized to design SMP that can undergo autonomous yet on-demand shape-shifting.

#### **Biography:**

Tao Xie is Qiushi chair professor at the College of Chemical & Biological Engineering, Zhejiang University. He obtained Ph. D from University of Massachusetts at Amherst in 2001. He had since worked at the General Motors Global Research Lab and HRL Laboratories before returning to China in 2013. He is the inventor of over 80 patent and a recipient of Omnova Solution award (2001), R&D 100 award (2013), and Wang Baoren Award (2019, Chinese Chemical Society). He is a fellow of ACS PMSE division and an Associate Editor for ACS Applied Materials & Interfaces.

# Use of Analytical Techniques in the Study of an Industrial Metal-Polymer Surface Segregation Problem

#### Joshua Cunday<sup>a</sup>\*, Stephen J Bull<sup>a</sup>, Mark Geoghegan<sup>a</sup>

<sup>a</sup>School of Engineering, Newcastle University, Newcastle upon Tyne, United Kingdom

#### Abstract:

ABSTRACT BOOK

There are a number of surface segregation problems which affect industrial processes. In many processes there are deleterious consequences caused by the expulsion of materials from a thermoset during preparation, so mitigating these issues is of considerable value both in economic terms, but also environmentally.

Surface segregation of chemical species involved in reactions to metal surfaces has been studied in the

formation of a commercial rubber. In order to characterise this problem, a range of analytical techniques have been applied to both the metal and polymer surfaces. These include: elastic recoil detection, X-ray fluorescence, scanning electron microscopy/energy dispersive spectroscopy, energy dispersive spectroscopy mapping, X-ray photoelectron spectroscopy in both static and dynamic modes, particle-induced X-ray emission, optical microscopy, optical profilometry and scanning force microscopy.

It will be shown in this presentation that the use of these different techniques in combination yield valuable information about the chemical processes that take place during curing. Different techniques are required not simply to obtain extra information but to account for occasions when individual techniques have limited capacity. An example of an effective analytical combination is that of elastic recoil detection (ERD) and X-ray photoelectron spectroscopy (XPS). ERD provides excellent quantitative information of elemental concentration as a function of depth, yet quantitative bonding information would be limited to inference if it weren't for dynamic XPS analysis. Alling the two allows for the polymer segregation to be studied in its entirety.

#### **Biography:**

In 2017, [Your Name] relocated to Newcastle upon Tyne to pursue a degree in Chemical Engineering. In 2021, they graduated with an MEng (First Class Hons) in Chemical Engineering with a focus on Sustainable Engineering from Newcastle University. As part of their master's program, they conducted a year-long research project on "Enhanced Carbon Capture using Nickel Nanoparticles and Amine Degradation in the Presence of Nickel Nanoparticles." Following this, [Your Name] began a 4-year industrially sponsored PhD at Newcastle University, focusing on understanding the mould fouling phenomenon during tyre moulding. Throughout their PhD, they have presented their research at various domestic and international conferences, contributing to discussions in both academic and industrial communities.

### Effect of h-BN and m-BN nanosheets on Gas barrier and Weather resistance properties of Thermoplastic Polyurethane

#### Rishabh Tiwari<sup>a\*</sup>, B.S. Butola<sup>b</sup> and Mangala Joshi<sup>c</sup>

<sup>a\*, b, c</sup>Department of Textile and Fiber Engineering, Indian Institute of Technology Delhi, New Delhi, India-110016

#### **Abstract:**

The incorporation of boron nitride nanosheets (h-BN) into thermoplastic polyurethane (TPU) films has attended significant attention for enhancing gas barrier properties. This study investigates the effect of varying concentrations of h-BN and Ethoxy grafted h-BN (m-BN) on the gas barrier performance of TPU films. m-BN were synthesized through sonication-assisted alcoholysis reaction technique and subsequently incorporated into TPU matrix via solution mixing to prepare masterbatch followed by melt mixing and subsequently prepared films via compression molding, with different concentrations (1 to 10wt%) of h-BN/ TPU and m-BN/TPU. The permeability of the nanocomposite films to gases such as oxygen (O2), nitrogen (N2) and helium (He) was evaluated using a gas permeability tester. Results demonstrated a substantial enhancement in the gas permeability with the m-BN as compared to h-BN. Specifically, TPU films with 3 wt.% m-BN exhibited up to a 28% reduction in helium, 43% reduction in oxygen and a 66% reduction in nitrogen permeability compared to neat TPU film. This enhancement is attributed to the high aspect ratio, better exfoliation and dispersion, which creates more tortuous path for gas molecules, thereby impeding their diffusion through the polymer matrix. These films are exposed in natural weathering conditions for upto 5 months and artificial weathering condition upto 300h. Moreover, mechanical testing revealed that the inclusion of mBN improved the tensile strength and Young's modulus of the TPU films. These findings suggest that m-BN is a promising nanofiller for the development of advanced TPU-based barrier materials for applications in the food packaging, protective coatings, Lighter Than Air systems (aerostat and airships) and in the flexible electronics. References: 1. Adak, Bapan, Mangala Joshi, and B. S. Butola. "Polyurethane/functionalized-graphene nanocomposite films with enhanced weather resistance and gas barrier properties." Composites Part B: Engineering 176 (2019): 107303. 2. Kim, Dukeun, et al.

"Sonication-assisted alcoholysis of boron nitride nanotubes for their sidewalls chemical peeling." Chemical Communications 51.33 (2015): 7104-7107. 109377. 3. Laosamathikul, Witita, Toshiki Sawada, and Takeshi Serizawa. "Alcoholysis-Assisted Exfoliation of Boron Nitride Nanosheets from Hexagonal Boron Nitride." Transactions of the Materials Research Society of Japan 42.5 (2017): 135-138. 4. Mandlekar, Neeraj, et al. "Degradation Study of Aromatic and Aliphatic TPU Films in Accelerated Weathering: Impact on the Gas Barrier and Mechanical Properties." Lighter Than Air Systems: Proceedings of the International Conference on Design and Engineering of Lighter-Than-Air Systems 2022 (DELTAs-2022). Singapore: Springer Nature Singapore, 2022.

#### **Biography:**

Rishabh Tiwari is a Ph.D. research scholar in the Department of Textile and Fiber Engineering at IIT Delhi, India. He holds both a master's and a bachelor's degree in Polymer Science and Engineering. With strong hands-on experience in polymer processing, coatings, characterization techniques, and the development of composites and nanocomposites, his research focuses on advancing materials science through innovative applications and sustainable solutions in polymer-related industries. Passionate about his field, Rishabh is dedicated to contributing to the development of high-performance, environmentally friendly materials and pushing the boundaries of polymer and fiber engineering.

#### Effect of Epoxy-Based Chain Extender on The Mechanical Properties of R-Pet For Food Contact

### Gustavo Kampa<sup>a</sup>\*, Norton Komora<sup>b</sup>, Cátia Zoraida<sup>a</sup>, Mariana Marques<sup>a</sup>, Marisa Brancoa, Sibele Cestari<sup>a</sup> and Renato Reis<sup>a</sup>

<sup>a</sup>Extrusion, Composition and Advanced Materials, Centre for Innovation in Polymer Engineering (PIEP), Universidade do Minho, Campus de Azurém (Edifício 15), Guimarães, Braga, Portugal

<sup>b</sup>Casa Mendes Gonçalves LDA, Golegã, Santarém, Portugal

#### Abstract:

Plastic food packaging is an essential part of products, whether it is to provide the food with protection against external agents or to maintain its organoleptic properties during its shelf-life [1]. However, plastic packaging, as well as plastics in general, were produced for many years based on a linear economy model, which focused on the efficiency, quality and design of products with little or no concern for their end-of-life, with significant waste generation in the environment associated with materials that are highturnover consumer goods, for example [2]. To overcome this problem, incorporating recycled polymers into food packaging could be a strategy to use in order to reduce the virgin polymer content and promote a circular economy [3]. The main objective of this research is to replace virgin polyethylene terephthalate (PET) in bottles in the food sector (sauces and seasonings) with 100% thermomechanically recycled PET (R-PET). Since R-PET does not have the same tensile and impact resistance as its virgin counterpart, the incorporation of an epoxy-based chain extender additive was studied. The compositions were made in a co-rotating twin screw extruder Coperion ZSK 26 (L/D ratio 40), with different concentrations of chain extender (0.10 to 1.00%, and some of which have an antioxidant additive) to evaluate the effect of the additive on the mechanical properties of RPET, with rupture tensile and falling dart impact tests being carried out. By better of presenter Size: 200\*200 understanding the mechanical properties of extruded compositions, it will be a significant indication for their application in food packaging. References [1] A. S. Bauer, M. Tacker, I. Uysal-Unalan, R. M. S. Cruz, T. Varzakas, and V. Krauter, "Recyclability and redesign challenges in multilayer flexible food packaging—a review," Foods, vol. 10, no. 11. MDPI, Nov. 01, 2021. doi: 10.3390/foods10112702. [2] M. Shamsuyeva and H. J. Endres, "Plastics in the context of the circular economy and sustainable plastics recycling: Comprehensive review on research development, standardization and market," Composites Part C: Open Access, vol. 6. Elsevier B.V., Oct. 01, 2021. doi: 10.1016/j.jcomc.2021.100168. [3] U. R. Gracida-Alvarez, H. Xu, P. T. Benavides, M. Wang, and T. R. Hawkins, "Circular Economy Sustainability Analysis Framework for Plastics: Application for Poly(ethylene Terephthalate) (PET)," ACS Sustain Chem Eng, vol. 11, no. 2, pp. 514-524, Jan. 2023, doi: 10.1021/acssuschemeng.2c04626. Keywords: PET; Chain extender; Extrusion; Mechanical properties.

#### Acknowledgements:

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#### **Biography:**

Gustavo Kampa's main focus has been in the industrial sector, particularly thermoplastics and related products. He graduated in Industrial Chemistry from the University of Beira Interior in 2020 (Covilhã, Portugal), is a master's student in Polymer Engineering at the University of Minho (Guimarães, Portugal), and is currently dedicated to Innovation & Development (R&D) in the area of Extrusion, Composition and Advanced Materials at PIEP.

#### **Polymeric eBike - Replacement of Conventional Materials**

#### Ana Barroso<sup>a\*</sup>, Filipa Carneiro<sup>a</sup>, Joel Antunes<sup>a</sup>, Catarina Rebelo<sup>a</sup>, Joana Silva<sup>a</sup> and Susana Costa<sup>a</sup>

<sup>a</sup>PIEP – Innovation in Polymer Engineering, Guimarães, Portugal

#### Abstract:

The Polymeric eBike project is dedicated to developing a modular and configurable electric bike that reconciles production standardization with customization for varied applications. Designed with a single frame adaptable to different modules and business models, the eBike caters to specific needs such as cargo transport, anti-vandalism for bike-sharing, and customizable features for corporate or community use. Constructed from PA6 reinforced with 30-35% glass fiber, the frame is both lightweight and robust. For the protection of critical electronic components, especially the battery, polycarbonate (PC) reinforced with 30-35% carbon fiber is employed to enhance impact resistance and safety. These polymeric composites enable intricate designs, better performance, and corrosion resistance. Numerical simulations will replicate real-world scenarios to predict the structural behavior of the bike frame. These simulations demonstrate the validation of the performance of these materials on normal operation, protection against environmental factors, weight reduction, and enhanced safety. This ongoing project underscores the potential of polymeric materials to innovate electric bike-sharing systems by offering adaptable, efficient, sustainable and safe solutions for diverse market needs.

#### **Biography:**

Ana Barroso is a Portuguese industrial designer in the product design & development team at "PIEP -Innovation in Polymer Engineering", with a degree in Product Design and currently pursuing a Master's in Product Engineering at the University of Minho. Experience includes polymer-based product development, innovation and ecodesign, with a focus on integrating sustainable practices in new solutions and material innovation.

### **Virtual Presentations**

# Versatile Hindered Amine-Supporting Polymer for Capturing Acidic Pollutants to Form Unique Polymer Composites

#### Eri Yoshida\*

Toyohashi University of Technology, Toyohashi, Aichi, Japan

#### Abstract:

The global environment faces pressing issues such as increasing CO2 emissions leading to global warming, ocean acidification, depletion of fossil fuels, plastic waste pollution, and the deterioration of water quality due to perfluorinated acids and their salts. These issues are often interrelated, necessitating a simultaneous and versatile approach for comprehensive environmental improvement. This study demonstrates a versatile polymer material that addresses some of these issues through simple acid-base reactions.

A hindered amine, 2,2,6,6-tetramethylpiperidine (TP), possesses high basicity and lacks nucleophilic attack ability, allowing it to capture even weak acids. A TP-supporting polymer effectively captured carbonic acid (CA) in water by introducing gaseous CO2, converting TP into its ammonium bicarbonate form. The CA-loaded polymer formed complexes with poly(sodium 4-styrenesulfonate) (PSS) through ion exchange, storing the CA within the complex aggregates, which exhibited ribbon-like or sheet-like morphologies. Additionally, the TP-supporting polymer incorporated perfluorinated carbonic acid into its microspheres through dispersion polymerization in an aqueous medium.

These findings indicate that the hindered amine-supporting polymer produces unique composite materials by capturing pollutant acids, which promises to improve the marine environment and water quality.

#### **Biography:**

Eri Yoshida earned her Ph.D. in Polymer Engineering from the Tokyo Institute of Technology in Japan. She joined the Kyoto Institute of Technology as an Assistant Professor. In 1999, she conducted research on supercritical CO2 at the University of North Carolina at Chapel Hill as a visiting scientist. In 2004, she moved to Toyohashi University of Technology, where she is currently an Associate Professor. Her research interests include CO2 capture technologies, chemical recycling of waste plastics, and artificial biomembrane models using synthetic polymer vesicles.

#### Calculation Of Number-Average Functionality And Gel-Point For Stepwise Polymerization

#### Hui Deng<sup>a</sup>\*, Yan Han<sup>b</sup>

<sup>a</sup>Wanhua Chemical(Beijing) Co.,Ltd./ RuiYan Tech Co.,Ltd.; Beijing, China <sup>b</sup>Wanhua Chemical(Beijing) Co.,Ltd. ; Beijing, China

#### Abstract:

The number-average functionality is proposed a simplified equation which can be used to predict the reaction progress of the stepwise polymerization expediently. According to the equation, once the average functionality of one reactant ([Equation], for example) is fixed, there will be a critical functionality of [Equation]. The reaction system has no risk to gel with the increase of component A if [Equation] is below the critical functionality, while gelation will occur with the increase of component A if [Equation] is higher than the critical functionality, and the gel point is the degree of reaction when [Equation] diverges to indefinitely large. The deduced equation is suitable for polymerization between R-A<sub>n</sub> and R'-B<sub>n</sub>, in which one of the components could be consumed completely, such as polyurethane, polyester, or other stepwise polymerization reactions. The equation can calculate the number-average functionality of polymer mixtures, especially for grafting or branched polymerization.

#### **Biography:**

Hui Deng graduated from Shanghai Jiao Tong University with a bachelor's degree in 2010. Currently, working as an engineer at Wanhua Chemical (Beijing) Co., Ltd., Hui focuses on the development of polyurethane products.

Yan Han graduated from Dalian University of Technology with a master's degree in 2008. As an engineer at Wanhua Chemical (Beijing) Co., Ltd., Yan is primarily involved in the development of polyurethane products.

#### Spiropyran-Merocyanine-Based Photoswitchable Polymer Systems

# Vadim V. Annenkov<sup>\*</sup>, Viktor A. Pal'shin, Stanislav N. Zelinskiy, Maxim S. Sudakov, Mariya S. Strelova, Elena N. Danilovtseva

Limnological Institute Siberian Branch of Russian Academy of Sciences, Irkutsk, Russia

#### Abstract:



The merocyanine moiety is interesting for the design of smart polymer systems. Its cyclization into spiropyran under light (460 nm) or at neutral pH values is accompanied by pH decrease. We synthesized merocyanine/ spiropyran-containing copolymers with hydrophilic (acrylic acid, 1-vinylimidazole, acrylamide derivatives of short polyamines) and hydrophobic (hydrocarbon derivatives of acrylamide) monomers. The behavior of polymers in aqueous medium was studied by light scattering, UV-Vis spectrometry, potentiometry and viscometry. We studied and discuss the following properties and application areas of the new polymers:

- interaction with oligonucleotides, capture of the complexes by living cells, and release of oligonucleotides under the influence of illumination and/or pH;

- triple (pH, light and temperature) sensitive polymers;
- coatings with light controllable surface (adhesion, contact angle);

- light triggers pH-sensitive processes such as interpolymer complexation and polyampholyte chain collapse.

This research was funded by the Russian Science Foundation, grant number 22-15-00268, https://rscf.ru/en/project/22-15-00268/.

#### Biography:

Vadim Annenkov was graduated from Irkutsk State University, Russia, in 1984. He received Ph.D. in Macromolecular Science from Irkutsk Institute of Chemistry in 1989 and D.Sc. degree from Irkutsk State University in 2001, Professor from 2009. He is a Deputy Director of the Limnological Institute SB RAS, Irkutsk, Russia. He has near 170 scientific articles and 18 patents. Research interests include synthesis and properties of hydrophilic polymers; physical chemistry of polymer solutions; mathematical simulation of macromolecular systems; study of the molecular mechanisms of biomineralization; biomimetic methods for nanoparticles synthesis; design systems for immune and genetic diagnosis.

#### Development of an Eco-Friendly Rubber Shoe Sole using Fly Ash as a Filler

#### K.C.C.K. De Silva<sup>a\*</sup>, S. M. Egodage<sup>b</sup> and W.A. Cyril<sup>a</sup>

<sup>a</sup>The Plas;cs and Rubber Ins;tute of Sri Lanka (PRISL), Rajagiriya, Sri Lanka. <sup>b</sup>Department of Chemical and Process Engineering, University of Moratuwa, Sri Lanka.

#### Abstract:

Dry rubber-based incorporated with several other components are used in the preparation of rubber shoe soles. These additives have both favorable and unfavorable environmental impacts.

Hence, product manufacturers tend to use additives with low negative impacts on the environment if they prove to be financially beneficial. Within this research, a rubber formula was redesigned by replacing an existing filler, "ball clay (BC)" with "fly ash (FA)". FA is a by-product and waste of coal combustion in power generation plants which is less expensive and harmless to environment. A series of rubber compounds were prepared by varying the BC loading from 50 to 0 phr at intervals of 10 phr loading, while keeping the total BC/FA loading at 50 phr and the other additives at constant quantities. Rubber vulcanizates were prepared at 150 °C under 25 MPa pressure for 13 minutes. Cure characteristics of rubber compounds and physico-mechanical properties, such as tensile properties, tear strength, compression set, abrasion resistance and hardness, of rubber vulcanizates were investigated according to international standards. The results obtained exhibited that both Delta cure and cure rate index increased with the increase of FA loading suggesting a positive impact of FA on the curing process. Abrasion resistance and resistance to flex cracking increased, while compression set was decreased with the increase of FA loading. Moreover, tensile strength, 300% Modulus and tear strength exhibited synergistic effects. These results suggested that eco-friendly rubber shoe soles could be produced with FA, preferably by replacing BC up to 30 phr.

#### **Biography:**

Karunamuni Chamal Chirantha Karunarathna De Silva (K.C.C.K. De Silva), a Sri Lankan researcher. I conducted this research as part of the Diploma in Polymer Technology at the Plastics and Rubber Institute of Sri Lanka (PRISL). I hold a bachelor's degree in Polymer Chemistry from the University of Sri Jayewardenepura, Sri Lanka. My research was supervised by Prof. Shantha Egodage and Mr. W.A. Cyril from the Department of Chemical Engineering at the University of Moratuwa, Sri Lanka.

# Revealing the Role of Chain Conformations on the Origin of the Mechanical Reinforcement in Glassy Polymer Nanocomposites

#### Hilal Reda<sup>\*a</sup> and Vangelis Harmandaris<sup>a,b,c</sup>

<sup>a</sup>Computation-based Science and Technology Research Center, The Cyprus Institute, Aglantzia 2121, Nicosia, Cyprus,

<sup>b</sup>Department of Applied Mathematics, University of Crete, Heraklion GR-71409, Crete, Greece

#### Abstract:

Understanding the mechanism of mechanical reinforcement in glassy polymer nanocomposites is of paramount importance for their tailored design. Here, we present a detailed investigation, via atomistic simulation, of the coupling between density, structure, and conformations of polymer chains with respect to their role in mechanical reinforcement. Probing the properties at the molecular level reveals that the effective mass density as well as the rigidity of the matrix region changes with filler volume fraction, while that of the interphase remains constant. The origin of the mechanical reinforcement is attributed to the heterogeneous chain conformations in the vicinity of the nanoparticles, involving a 2-fold mechanism. In the low-loading regime, the reinforcement comes mainly from a thin, single-molecule, 2D-like layer of adsorbed polymer segments on the nanoparticle, whereas in the high-loading regime, the reinforcement is dominated by the coupling between train and bridge conformations; the latter involves segments

#### connecting neighboring nanoparticles.

#### **Biography:**

Hilal Reda is currently an associate researcher at the Cyprus Institute according to fellowship from a Marie Skłodowska Curie Individual Fellowship. He works on the development of polymer nanocomposites (PNCs) for novel applications, which have attracted considerable interest in recent years due to the enhanced properties of PNCs, including mechanical rigidity, stiffness and toughness, electrical and thermal conductivity, etc. This project proposes a multiscale computational methodology to predict the mechanical properties of PNCs, which involves microscopic simulations, homogenization approaches and continuum models. He now continues his work as an associate research scientist in the SimEA project.

#### Furan-based polymers designed ad hoc for sustainable monomaterial food packaging

#### Valentina Siracusa<sup>a\*</sup>, Nadia Lotti<sup>b</sup>

<sup>a</sup>Department of Chemical Science (DSC), University of Catania, Italy <sup>b</sup>Department of Civil, Chemical, Environmental and Materials Engineering, University of Bologna, Italy

#### Abstract:

Although plastic packaging is often considered one of the main responsible of plastics environmental impact, in case of food packaging some valuable effects must be considered. Indeed, packages protect food, extending its shelf life and reducing food waste, which is one of the main plagues of the modern era. Another current concern is the accumulation of wastes in the environment, which is pushing governments and society towards an efficient management of plastic and to the transition towards the circular economy. However, recycling is not always a cost-effective or a feasible alternative, due to the lack of proper recycling policies (in developing countries) and, in case of food packaging, to organic matter contamination and multilayer structure. Thus, biodegradable plastics represent the only alternative to landfill. In this scenario, 2,5-furandicarboxylic acid (FDCA) can be considered an interesting chemical building block to realize sustainable mono-material packaging, with excellent mechanical and gas barrier properties. Of particular interest, the eco-design of novel furan-based polyesters for the realization of flexible films. It has been indeed demonstrated that flexible packaging is more sustainable than rigid one and very effective in protecting food with the minimum amount of material and waste, helping to reduce food waste by offering optimum protection (Flexible Packaging Europe, 2021). This contribution aims to present an overview of the most important results obtained by the research group coordinated by me which have allowed the extrapolation of important property-structure correlations with particular attention to functional properties, i.e. mechanical properties and gas barrier properties.

#### **Biography:**

Siracusa Valentina received her degree in Industrial Chemistry and completed her PhD and post-PhD study. From 2006 she is Associate Professor in Chemistry for Engineering Courses and for Life Cycle Assessment Study (LCA) courses. She collaborates to several research projects, she is author of more than 120 papers in high impact factor scientific journals, she is author of several book chapters for Wiley, Springer, Elsevier and she is Editorial Board Member and Lead Guest Editor of International Journals. Her research interest includes: synthesis and full characterization of biodegradable and bio-based polymers; gas barrier behavior and in moisture condition, at different temperature; Life Cycle Assessment (LCA) study of polymers.

# Identifying Relationships Between Hybrid Carrageenan Chemical Structures and The Viscoelastic Properties of The Formed Hydrogels

#### Loic Hilliou \*\*, Alice Monteiro \*, João M. Alves \*, Bruno Faria \*

<sup>a</sup>Institute for Polymers and Composites, University of Minho, Guimarães, Portugal

#### Abstract:

Hybrid carrageenans (HC) are a family of sulfated polysaccharides, mainly used in the food industry for their gelling, stabilizing and thickening properties. However, the gelling mechanism of carageenans remains unclear to this point [1]. In this presentation, different types of HC extracted from commercial carrageenophytes and treated with alkali to remove biological precursors, are delivered with simplified chemical structures when compared with earlier studies [2]. The gels formed in the presence of a single cation will be studied with linear and nonlinear rheology. The study aims to 1) question the linear dependence of the gel elasticity with the content in kappa carrageenan disaccharides on the hybrid carrageenan polymer chain 2) document the gel mechanical behavior under large deformation which so far received little attention in spite of its industrial relevance [1,2].

[1] Hilliou, L. Structure–Elastic Properties Relationships in Gelling Carrageenans. Polymers 2021, 13, 4120.

[2] Souza, H.K.S.; Kraiem, W.; Ben Yahia, A.; Aschi, A.; Hilliou, L. From Seaweeds to Hydrogels: Recent Progress in Kappa-2 Carrageenans. Materials 2023, 16, 5387.

#### Acknowledgements:

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#### **Biography:**

Loïc Hilliou (ORCID 0000-0002-9936-8088) is associate researcher at the Institute for Polymers and Composites, University of Minho, Portugal, and in charge of the rheology lab of this institute. His research is about the relationships between the materials properties, their process-induced structure and rheology and the final properties of the resulting products. Recent studies focused on the extrusion of polymer based systems, on hybrid carrageenan hydrogels, on formulation of pastes for 3D printed lithium batteries, on polyhydroxyalkanoates, and the rheological understanding of extrusion-based additive manufacturing. He published over 40 papers on these topics during the last five years.

#### Application of geopolymer material on open pit Mine Road: A Review

#### Abdoul Wahab<sup>a</sup>\*, Wei Zhou<sup>b</sup>, Xiang Lu<sup>a</sup>, Tian Ya<sup>a</sup>, Ernest Nii Laryea Amartey<sup>c</sup>, Zhongchen Ao<sup>a</sup>, Zhongao Yang<sup>a</sup>, Linyou Jiang<sup>a</sup>, Yuqing Yang<sup>a</sup>

<sup>a</sup>School of Mines, China University of Mining and Technology, Xuzhou, China

<sup>b</sup>State Key Laboratory of Coal Resources and Safe Mining, China University of Mining and Technology, Xuzhou 221116, China

<sup>c</sup>School of Safety Engineering, China University of Mining and Technology, Xuzhou, 221116, China

#### Abstract:

This review assesses the use of geopolymer as an environmentally friendly alternative for constructing and repairing roads in open pit mines, offering a sustainable solution to mitigate concerns related to waste dumps. Most industrial solid and mine waste are piled up at waste dumps, negatively impacting the environment. The review highlights the adverse environmental effects of accumulating industrial and mine waste, advocating for the recycling of these materials as aggregates in geopolymer road construction. Further examining the entire spectrum of geopolymer road materials, this work discusses their preparation, properties, and applications within open-pit mines road. The focus extends to the mechanical properties of geopolymer road material, emphasizing its notable compressive strength at ambient temperature. Among other things, the review underscores the positive impact of geopolymer on road quality, smoothness, strength, and service life of mining transport roads, suggesting its potential to enhance operational efficiency in mine environments.

#### **Biography:**

Abdoul Wahab Ali Moussa is Ph.D. student, studying Mining Engineering third year at China University of Mining and Technology, specializing in Engineered Solutions for Open pit mine road reparation, Dust Suppression, Erosion Control, and Soil Stabilisation. A pioneering, Abdoul Wahab Ali Moussa is passionate about health and safety and providing innovative solutions that are cost-effective to the mining industry, governments, and infrastructure sectors.

#### Impact Resistance of Layered Aramid Fabric: A Numerical Study on Projectile-Induced Damage

#### Larisa Titire<sup>a\*</sup> and Cristian Munteniță<sup>a</sup>

#### <sup>a</sup>"Dunarea de Jos" University, Galați, Romania

#### Abstract:

The aim of this work is to comparatively analyze, by numerical simulation, the impact behavior of aramid fabric. The layered panel will be impacted by two projectiles specific to the NIJ protection level HG1. The protection level in this study is according to NIJ Standard 0123.00. This standard is used to establish protection levels. The two projectiles specific to the NIJ HG1 protection level are 9mm Luger and .357 Mag. Law enforcement personnel use body armor designed to protect the torso. Different types of armor protect officers from various hazards. Body armor protects against penetrating bullets and physical injuries from projectile impact. These vests have a soft armor that protects against handgun projectiles and a stiffer tactical armor made of both soft and hard materials that protects against rifle ammunition. Law enforcement agencies should assess the types of hazards that their personnel may encounter when purchasing body armor and select body armor with appropriate features to protect against these risks. With the help of numerical simulation, the mechanisms of destruction of the aramid fabric on impact are identified. The protection performance is analyzed as a function of the influence of the number of layers and the projectile velocity variation. The strand is modeled at the individual level, each strand consisting of hundreds or even thousands of fibers, which makes the simulation very difficult. The material properties for the yarn, as well as for the projectiles, are selected from the literature.

#### **Biography:**

Dr. Larisa Titire studied at the "Dunarea de Jos" University, Romania and graduated as MS in 2020. She then joined the research group of Prof. Cristian Muntenita at the INTERDISCIPLINARY RESEARCH CENTER IN THE FIELD OF MECHANICAL ENGINEERING - CCIDIM. She received her PhD degree in 2023 at the same institution. She obtained the position of an Assistant at the 'Dunarea de Jos" University.

#### **Optimization of Clutch Friction Disc Material Using Neural Networks**

#### Balasoiu George<sup>a</sup>\*, Muntenita Cristian<sup>a</sup>, Amortila Valentin<sup>a</sup> and Titire Larisa<sup>a</sup>

<sup>a</sup>Dunarea de Jos University of Galati, Romania

#### Abstract:

This paper presents a comparative analysis of four sets of clutch discs from different automotive gearbox manufacturers, using SEM and EDX techniques to determine the chemical composition of the materials. For each disc, three measurements of the friction coefficient between the disc and steel were performed

to highlight the differences among the analyzed discs. The results were used to build a neural network, using Easy NN software, with the goal of optimizing the friction material. The percentages of constituent elements were used as input data, while the maximum, minimum, and average values of the friction coefficient and the temperature generated during friction were employed as output data. To evaluate the neural network, the correspondence between the importance of input data and their sensitivity to output data changes was analyzed. It was found that the model with three hidden layers shows a significant correlation between the six most essential elements and their sensitivity. Based on this neural model, the chemical composition of the friction disc materials was optimized using the "Query" mode, minimizing the differences in friction coefficients and the developed temperature. -

#### **Biography:**

PhD student George Balasoiu studied at the "Dunărea de Jos" University of Galați, Romania. He graduated with his first bachelor's degree in 2014 and completed both his master's degree and his second bachelor's degree in 2020. Since 2020, he has been a PhD student and an Assistant in the Mechanical Engineering Department of the Faculty of Engineering. In 2024, he joined the research group of Assoc. Prof. Cristian Muntenita at the Interdisciplinary Research Center in the Field of Mechanical Engineering (CCIDIM).

#### Influence of Curcumin in Overall Migration of Polyurethane Films for Fruits and Vegetables Packaging

#### David Ruiz\*a, Yomaira Uscáteguia, Luis-Eduardo Diazb, Manuel F. Valeroa

<sup>a</sup>Universidad de La Sabana, GEMA research group, Chía, Cundinamarca, Colombia <sup>b</sup>Universidad de La Sabana, Bioprospecting research group, Chía, Cundinamarca, Colombia

#### Abstract:

Overall migration is one of the most important safety criteria for materials in contact with food. In this research, it was shaped polyurethane films with curcumin as additive for fruits and vegetables packaging. It was compared the overall migration of three formulations. First, polyurethane without curcumin. Second, polyurethane with 0,25% w/w curcumin. Third, polyurethane with 0,5% w/w curcumin. It was carried out tests of overall migration, Fouriertransform infrared spectroscopy (FTIR) and thermogravimetric and differential thermal analysis (TGA and DGA). The obtained results showed that the highest overall migration formulation was curcumin at 0,25% w/w, and the lowest migration rate was the formulation at 0,5% of curcumin w/w. On the contrary of the general assumption, where while higher is the additive concentration higher is the overall migration, in this research it demonstrated that the

intermolecular interactions between polymer and additive molecules is a relevant factor to keep in mind, due to these interactions could reduce the migration of materials despite mass increasing of additives. This hypothesis is sustained through FTIR, TGA and DGA results. This research could be useful to a better understanding of overall migration phenomena.

#### **Biography:**

ABSTRACT BOOK

David Ruiz was born in Bogotá, Colombia, and holds a bachelor's degree in Environmental Engineering. He is currently pursuing a Ph.D. in Biosciences at Universidad de La Sabana, focusing his research on food packaging. Since January 2021, David has also been a lecturer at the same university, where he continues to share his expertise with students.

#### The Effects of Hydrogel Type on The Kinetics of Dehydration Process

#### Jelena D. Jovanovic<sup>a\*</sup>, Vesna V. Panic<sup>b</sup>, Nebojsa N. Begovic and Borivoj K. Adnadjevic<sup>d</sup>

<sup>a</sup>Institute for General and Physical Chemistry, Studentski Trg 12-16/V 11158 Belgrade, Serbia <sup>b</sup>University of Belgrade, Innovation Center of Faculty of Technology and Metallurgy, 4 Karnegijeva Street,

### 11000 Belgrade, Serbia °Faculty of Physical Chemistry, University of Belgrade, Studentski Trg 12-16, 11158 Belgrade, Serbia

#### Abstract:

Hydrogels are prominent materials with smart response to external stimuli, swelling ability, biocompatibility, etc. Dehydration of hydrogels, as a complex reversible and endothermic physicochemical process of removing water from material, which takes place under conditions of simulated energy exchange and mass transfer, is of remarkable practical and theoretical importance, because hydrogels could be assumed as model systems suitable for modeling the kinetics of dehydration of living tissues and foods.

Our investigation is aimed to get insight into the effect of hydrogel type on the applicability of novel kinetic models that can describe hydrogel dehydration precisely and with a higher degree of reliability: Vyzovkin's isoconversion method, Webull's distribution of reaction times, distribution apparent energy activation model, logistic function, etc.

We used hydrogels based on poly(acrylic acid), poly(methacrylic acid), alginate and gelatin. All hydrogels were synthesized in our laboratory, equilibrium swollen in distilled water and their non-isothermal (heating rates 5-30 Kmin<sup>-1</sup>) and iso-thermal dehydration (293K-360K) were recorded by thermogravimetric measurement, under N<sub>2</sub> atmosphere.

Kinetics parameters: rate constants (k), activation energy (Ea), preexponential factor (InA), and dependences of Ea and InA on the degree of dehydration ( $\alpha$ ) were determined. The kinetic's complexity of dehydration processes was discussed based on the dependences of Ea and InA on  $\alpha$ . The correlations among the values of k, Ea and InA with the xerogels' structural properties were determined. The complex nature of hydrogels' dehydration kinetics was revealed and explained as the consequence of phase state of the absorbed water, fluctuating structure and thermal activation of the hydrogel.

#### **Biography:**

Dr Jelena Jovanovic, research professor, is R&D Director at Institute of General and Physical Chemistry, Belgrade, Serbia. Dr J. Jovanovic has extensive career which covers numerous areas: advanced and smart materials, polymers, composites, hydrogels, poly(siloxanes), synthesis and polymerizations, and physicochemical processes (adsorption, extraction, swelling, dehydration, drug-release) both under conventional and non-conventional conditions (microwaves, ultrasonic, cavitation). Hydrogels are within the topic of her interest along with the effects of external fields on the reaction kinetics. She worked on the development of novel methods of kinetics analyzes. Dr J. Jovanovic has extensive international and leadership experience.

### **Poster Presentations**

### Technical, environmental, and safety aspects of producing colloidal lignin particles on the pilot scale

#### Elham Khalati<sup>a\*</sup>, Pekka Oinas<sup>a</sup>

<sup>a</sup>Aalto University School of Chemical Engineering, Espoo, Finland

#### Abstract:

ABSTRACT BOOK

Lignin is a renewable biopolymer with different functional groups that make it a promising substitute for petroleum-derived resources. Approximately 50-70 million tons of lignin is produced annually as the by-product of pulp and paper industry. However, roughly 98% of lignin is burned to generate heat. The inherent heterogeneity of this material limits its application; thus, researchers have employed different techniques to enhance its dispersibility in water and polymers. Lignin transformation into colloidal particles via a three-solvent polarity exchange has shown promising results on the lab-scale. The main steps of the process are dissolving lignin, diluting the solution, forming colloidal lignin particles (CLPs), recovering used solvents, and drying concentrated CLPs. Upscaling of this new production method directly from the lab to

the full-scale operation is not viable. For this purpose, the pilot plant acts as a bridge between lab-scale technology and its commercialized adoption and application. This research focuses on various aspects of designing the related pilot plant with a daily production capacity of 20 kg of dry CLPs. In this work, the process is simulated in Aspen Plus<sup>®</sup>. Based on the simulation results, technical diagrams are prepared, and environmental, safety, and economic aspects of the process are investigated. For enhancing safety, the pilot plant was planned to be in an ATEX-certified container, thereby shielding the environment from leakages or explosions. The operation of the process is also improved by optimizing tuning parameters of process controllers. The designed pilot plant provides a promising basis for commercialization of the CLPs production process.

#### **Biography:**

I am Elham Khalati, and I have a master's degree in the field of process engineering. Currently, I am a doctoral student in the Plant Design group under the supervision of Professor Pekka Oinas, at Aalto University School of Chemical Engineering. My research area is related to conducting techno-economic assessments and process modeling to produce bio-based materials including lignin-derived materials on pilot and commercial scales.

#### **Colorless and Soluble High-Performance PFAS-free Polyimides from Aliphatic Anhydrides**

#### Sara Greco\*ª, Marta Falconeª

<sup>a</sup>Valsynthese SA, CH-3900 Brig, Switzerland

#### Abstract:

Fully aromatic polyimide materials, as Kapton<sup>®</sup>, are widely used for flexible electronic substrates or as insulators, thanks to their wide range of thermal stability as well as excellent dielectric and mechanical properties. However, there are limitations in their processability and employment at large scale in new technologies due to their low solubility and deep amber staining, resulting from charge transfer interactions, established between polymer rigid chains. Currently, researchers are focusing on designing resins with excellent thermal and chemical stability, transparent and colorless with a high processability, in terms of viscosity and solubility. Balancing among all those properties for this class of materials it is easily achievable when aromatic diamines are combined with perfluorinated aromatic dianhydrides. An alternative solution to per-and polyfluoroalkyl substrate (PFAS) is the utilization of complete aliphatic dianhydrides in combination with aromatic diamines. In this work, aliphatic substrates as bicyclo [2.2.2] oct-7-ene-2,3:5,6-tetracarboxylic dianhydride (BTA) and bicyclo [2.2.2] octane-2,3,5,6-tetracarboxylic 2,3:5,6-dianhydride (HBTA) have been tested as PFAS-free moiety for highly performant polyimides. Those dianhydrides combined with the right diamines gave promising results in terms of discoloration and solubility, making those substrates suitable for a large-scale polyimides development as pre-polymer and polymer varnishes solutions, for high thermal resistant materials adapt for optoelectronic applications and enameling purpose respectively.

#### **Biography:**

Sara Greco obtained the Batchelor degree in Chemistry at the University La Sapienza (Rome) in 2019 with mark 110/110 cum laude, after which she started her master's degree in Material Chemistry at the University of Padua. At the same time, she applied for a position at Valsynthese SA (Switzerland) where she is currently working at, dealing with organic synthesis for various projects. At present, she is finalizing her master thesis at Valsynthese company, in collaboration with the University of Padua, for the research of new polyimide materials.

# Comparative Analysis of 3D Printing and Injection Molding for Biocomposites: Quantifying Limitations in 3D Printing

#### Sunil Kumar Ramamoorthy<sup>a</sup>\*, Paul Forbid Mukoroh<sup>b</sup>, Fathi Gouda<sup>c</sup>, and Mikael Skrifvars<sup>a</sup>

<sup>a</sup>Swedish Centre for Resource Recovery, University of Boras, Boras, Sweden <sup>b</sup>Arcada University of Applied Science, Helsinki, Finland <sup>c</sup>Department of Engineering, University of Boras, Boras, Sweden

#### Abstract:

The production methods could affect the properties of the components produced. This study investigates the impact of a production method, 3D printer, on water absorption, mechanical and thermal properties of the biocomposites produced from poly(lactic) acid and wood particles. The results were analyzed comparatively with injection molding. A minor change (0.1 mm) in the layer thickness in 3D printing affected the biocomposites' properties significantly. The water absorption in 3D printed biocomposites caused swelling leading to permanent dimensional changes and initiated many failure nodes across layers. The water absorption of the injection molded biocomposites was primarily due to the material properties while the water absorption of the 3D printed biocomposites was due to the combination of intrinsic porosity of the 3D printing and the material properties. Water absorption in injected molded biocomposites was due to the gradual absorption of water from surface to the core. Increasing the biocomposites' surface contact with water in 3D printing increased the water absorption. Additionally, increasing the layer thickness in 3D printing increased the water absorption further. 3D printed biocomposites mechanically performed better on decreasing the layer thickness. Lower porosity on decreasing the layer thickness was the predominant factor. A structure's overall strength increased when there were more contact sites and greater interlayer bonding due to smaller layer thickness. Injection molded biocomposites had higher density and better mechanical properties than 3D printed biocomposites due to solid specimens resulting in reduced failure sites. The results from this comparative study highlights the limitations of 3D printing.

#### **Biography:**

Sunil Kumar Ramamoorthy is employed as a researcher at the Swedish Center for Resource Recovery, specializing in polymer technology. Prior to this role, Sunil held positions as a scientist at a research institution in Sweden and as a visiting professor at a university in India. He is actively involved in teaching and examining students at the bachelor's, master's, and PhD levels in a range of disciplines including mechanical engineering, chemical engineering, textile engineering, and resource recovery. Sunil serves as a guest editor for academic journals. His research focus lies in the development of bio-based polymer materials.

#### Efficient and Recyclable Solid-Supported Pd(II) Catalyst for Microwave-Assisted Suzuki Cross-Coupling in Aqueous Medium

#### Abdulrahman M. Alazemi,\*\* Kamal M. Dawood, b\* Hamad M. Al-Matar\*, and Wael M. Tohamy\*

<sup>a</sup>Chemistry Department, Faculty of Science, University of Kuwait, Safat 13060, Kuwait <sup>b</sup>Department of Chemistry, Faculty of Science, Cairo University, Giza 12613, Egypt

#### Abstract:

Solid-supported catalysts play efficient and crucial roles in organic synthesis. A solid-supported palladium(II) complex based on **chitosan** was synthesized and fully characterized using all possible tools (Fourier transform infrared spectroscopy, thermogravimetry analysis, differential scanning calorimetry, X-ray photoelectron spectroscopy, energy-dispersive X-ray spectroscopy, inductively coupled plasma atomic emission spectrometry, scanning electron microscopy, transmission electron microscopy, and Brunauer–Emmett–Teller analysis). The catalytic activity of the solid-phase catalyst in Suzuki cross-coupling reactions was evaluated in aqueous solvents under both conventional heating and microwave irradiation conditions. The recyclability and thermal stability of the prepared catalyst were also examined,

and the catalyst was found to be active till five consecutive runs without a notable loss of activity under the microwave condition, with the turnover number and turnover frequency values reaching 19,019 and 114,114 h-1, respectively.

#### **Biography:**

My research interests are in the convergence of synthetic organic chemistry, catalysis, and materials science. The main focus of my research is on: Designing new molecules, using organic synthesis protocols, that have different functional groups for applications such as electronics, photonics, and energy conversion systems. My second line of research focuses mainly on exploring physical properties of solid catalysts as a new avenue in green chemistry for molecular transformations. Planning to further extend my knowledge in polymers upconversion such as Triplet-triplet Annihilation Upconversion (TTA-UC). This is a great opportunity for me.

# *Dillenia indica* mucoadhesive hydrogel infused with amphiphilic polyphenol: Emerging adsorbent and antioxidant

#### Debolina Ghosh<sup>a</sup>\*, Sagnik De<sup>b</sup>, Deepmoni Deka<sup>a</sup>, Gopal Das<sup>a,b</sup>

<sup>a</sup>Centre for the Environment, Indian Institute of Technology, Guwahati, Assam,India <sup>b</sup>Department of Chemistry, Indian Institute of Technology, Guwahati, Assam,India

#### Abstract:

The work demonstrates the use of mucoadhesive materials that were taken from the fruits and seeds of Dillenia indica (DI), a plant that is widely distributed in India, to create a hydrogel. To improve the hydrogelation property, an artificially generated amphiphilic polyphenol (L) has been added to the hydrogel networks. Additionally, the potential for radical scavenging and the overall phenolic content of the DI-L hydrogel were examined. At an initial concentration of 10 mg/L of Fe (III) solution, the DI-L hydrogel demonstrated good sensitivity and effective adsorptive removal of Fe (III) from the aqueous medium with an adsorption capacity of 6.157 mg/g. Consequently, our results emphasize the most creative use of converting fruit mucoadhesive into environmentally friendly solutions.

#### **Biography:**

Debolina Ghosh works as a PhD student at the Indian Institute of Technology (IIT) Guwahati, India, in the Center for Environment. Her passion is translational research with a focus on environmental issues and the focused remediation aspects of such knowledge. Her main objective is to broaden and deepen her current knowledge to tackle global environmental concerns and make a meaningful and practical contribution to society. The esteemed Prime Minister's Research Fellowship (PMRF) has been awarded to Debolina. She is now developing plant-based natural hydrogels for use in environmental applications.

#### Single-Step Synthesis 19F MRI Tracers with Enhanced Sensitivity via Gradient Copolymerization-Induced Self-Assembly

#### Vyshakh M. Panakkal\* and Ondrej Sedlacek.

Department of Physical and Macromolecular Chemistry, Faculty of Science, Charles University, Prague, Czech Republic.

#### Abstract:

We synthesize functional polymer nanoparticles using the polymerization-induced self-assembly (PISA) method. In a typical PISA process, a solvophilic block is a chain-extended using an initially soluble monomer that later, upon polymerization, becomes the insoluble core of the polymer micelles. Here,

we demonstrated the one-step synthesis of polymer micelles by gradient copolymerization-induced self-assembly, which can be done using monomers with different reactivity in aqueous conditions. The resulting polymer nanoparticles, with a fluorine core due to one of the monomers, hold potential as a magnetic resonance imaging (MRI) tracers. Unlike the traditional method of chain extension of a pre-made macro-chain transfer agent, the different reactivities of poly(ethylene glycol) methacrylate (PEGMA) and N,N-(2,2,2-trifluoroethyl)acrylamide (TFEAM) monomers in aqueous dispersion lead to a gradient composition in the final polymer. This compositional gradient results in self-assembly while enhancing the fluorine signal from the resulting polymer nanoparticle. We conduct studies on the reactivity parameters of the copolymerization in aqueous and non-aqueous polymerization conditions, validating our theory for the gradient structure of the resulting polymer. After optimizing the fluorinated polymer nanoparticles' structure and composition, we have confirmed the potential applications in phantoms using 19F MRI in vitro. The authors acknowledge the financial support from the Ministry of Health of the Czech Republic (project no. NU22-08-00286)

#### **Biography:**

Vyshakh Manayath Panakkal is a final-year doctoral student at the Faculty of Physical and Macromolecular Chemistry at Charles University, Prague. He focuses on developing novel polymer nanoparticles using polymerization-induced self-assembly for biomedical applications. He has presented his work at national and international conferences and published in leading Journals.

Leucine-based Pseudo-proteins as Promising Biomaterials for Biomedical Applications: In Vitro Evaluation Of Immunomodulatory Effects On J774 Monocyte-macrophage Cell Line

Ksovreli Mariam<sup>1\*</sup>, Zibzibadze Nino<sup>1</sup>, Kachlishvili Tinatin<sup>1</sup>, Nadaraia Lili<sup>2</sup>, Gverdtsiteli Marekhi<sup>3</sup>, Kantaria Temur<sup>3</sup>, Piot Olivier<sup>4</sup>, Courageot Marie-Pierre<sup>4</sup>, Terryn Christine<sup>5</sup>, Tchelidze Pavel<sup>6</sup>, Katsarava Ramaz<sup>3</sup>, Kulikova Nina<sup>1</sup>

<sup>1</sup>Institute of Cellular and Molecular Biology, Agricultural University of Georgia, 0159 Tbilisi, Georgia <sup>2</sup>Carl Zeiss Scientific and Education Center, New Vision University, 0159 Tbilisi, Georgia <sup>3</sup>Institute of Chemistry and Molecular Engineering, Agricultural University of Georgia, 0159 Tbilisi, Georgia <sup>4</sup>BioSpecT Unit, University of Reims Champagne-Ardenne, 51100 Reims, France <sup>5</sup>DICT, University of Baims, Champagne, Ardenne, 51100 Reims, France

<sup>5</sup>PICT, University of Reims Champagne-Ardenne, 51100 Reims, France 6 Faculty of Healthcare, East European University, 0159 Tbilisi, Georgia

#### Abstract:

This study aimed to investigate the immunomodulatory effects of leucine-based pseudoprotein (LPP) films on J774 monocyte-macrophage cells. Specifically, the research focused on how these films influence key physiological parameters, including surface phenotype, cytokine/chemokine secretion profile, metabolic activity and cells motility. The study utilized four distinct types of LPP films: 1L6 (composed of carbonic acid, L-leucine, and 1,6-hexanediol), 8L6 (composed of sebacic acid, L-leucine, and 1,6-hexanediol), and a copolymer (CoP) constituted of 70 mol% 1L6 and 30 mol% 8L6 and a mixture (Mix) also comprising 70% of 1L6 and 30% of 8L6. Immunophenotyping revealed that cells grown on CoP LPPs exhibited decreased CD86 expression, a marker of pro-inflammatory M1 macrophages, indicating a shift towards a less inflammatory phenotype. Conversely, CD206 expression, characteristic of M2 macrophages, was significantly increased in cells grown on Mix LPPs, with similar trends observed in cells grown on 1L6 and CoP LPPs. Elevated IL-10 and CCL22 levels across all LPP-treated cells further supported the shift towards M2 polarization, while IL-1β production remained unchanged, suggesting no pro-inflammatory response. Additionally, cells grown on CoP LPPs showed enhanced migration ability, a trait associated with M2 macrophages, indicating that these LPP films may promote an anti-inflammatory macrophage phenotype. The ability of LPPs, particularly CoP LPPs, to induce M2 polarization underscores their potential for biomedical applications, such as wound healing. These findings suggest that the effects of LPP films on macrophage behavior may be influenced by differences in surface topography, warranting further investigation into the specific adhesion complexes and signaling pathways involved.

#### **Biography:**

Mariam Ksovreli is a PhD student and junior researcher at the Agricultural University of Georgia. She is skilled in working with both primary and immortalized cell cultures and has experience in animal work and preparing samples for microscopy (TEM, SEM, LCM). Her research focuses on the biomedical applications of biodegradable pseudo-proteins, particularly their role in macrophage and fibroblast interactions in wound healing. She has authored several publications, including recent studies on leucine-based pseudo-proteins in Polymers and the International Journal of Molecular Sciences. Mariam aims to improve wound care through innovative biomaterials.

# Green Reinforcement of Plastic Packaging by Starch Addition: A Coupled Computational and Experimental Study

#### P. Calandra<sup>a\*</sup>, A. Pecchia<sup>a</sup>, B. Tirri<sup>a</sup>, F. Mercuri<sup>a</sup>, F. Lo Celso<sup>b</sup>, C. Oliviero Rossi<sup>c</sup>, V. Loise<sup>c</sup>, P. Caputo<sup>c</sup>

<sup>a</sup>CNR-ISMN National Council of Research – Montelibretti (RM), Italy & INSTM <sup>b</sup>Università degli Studi di Palermo, Dipartimento di Fisica e Chimica, Palermo, Italy <sup>c</sup>University of Calabria, Rende (CS), Italy & UdR INSTM della Calabria

#### Abstract:

Poly Lactic Acid (PLA)/ Poly Butylene Adipate-co-Terephthalate (PBAT) blends are used as packaging green materials since they constitute hydrophilic and biodegradable plastic. With the aim of improving the mechanical characteristics of PLA/PBAT blends as biodegradable packaging materials for food products the addition of starch has been considered. In silico study performed by classical molecular dynamics (MD) highlighted that the addition of starch can reinforce the polymeric structure via starch-polymer interactions, suggesting that starch can be a suitable material to be added to the PLA/PBAT blend to obtain more resistant packaging materials. Experimental analysis of the mechanical properties of PLA/PBAT blends containing different amounts of starch confirmed what foreseen by MD, highlighting increases in Young modulus and glass transition as a function of added starch. Starch amount of 10 wt% turned out to be the optimum to maximize the elongation bearable under tensile stress before rupture. The coupled theoretical/experimental approach constitutes added value of the present work, furnishing important data on the reinforcement of the packaging material performances and a molecule-based interpretation and comprehension of the observed phenomenon.

#### **Biography:**

ABSTRACT BOOK

Pietro Calandra is a chemist, physicist, writer and science popularizer working at the National Research Council of Italy as senior researcher. He has a long experience in the study of complex chemical systems, with particular attention to strongly interacting molecular systems (fluids) and on the behavior of smart materials under external (electric, magnetic, mechanical) stimuli. He is involved in material science with more than 120 scientific papers. He manages several research projects on the designing of novel materials by re-using waste materials in the ambit of circular economy.

#### Chemical Recycling and Physical Tuning of Necklace-shaped Polydimethylsiloxanes Bearing Anthracene Dimer Units

#### Atsuro Moria\*, Harutake Hayashia, Agamoni Pathaka and Masashi Kunitakeb

<sup>a</sup>Grad. Sch. of Sci. and Tech., Kumamoto Univ., Kumamoto City, Kumamoto Pref., Japan

<sup>b</sup>Inst. of Industrial Nanomaterials., Kumamoto Univ., Kumamoto City, Kumamoto Pref., Japan

#### Abstract:

Currently, polymer recycling technologies that do not compromise energy costs or material properties are eagerly desired to solve the plastic waste problem in the world. There might be two development directions for polymer recycling; degradation technologies of ordinary plastics and new degradable plastic materials. Herein, we introduce the latter, new degradable siloxane polymer materials based on anthracene dimer units. We have focused on anthracene units, which undergo reversible dimerization and de-dimerization under UV light and heat, and dimethylsiloxane, attracting attention for their decarbonization. The necklaceshaped siloxane polymers bearing anthracene dimer units were photo-polymerized by UV irradiation (365 nm) from anthracene-terminated dimethylsiloxane as a monomer. Monodisperse monomers were synthesized by hydrosilylation, and polydisperse monomers were synthesized by ring-opening equilibrium polymerization. Various polymers were produced from monodisperse or polydisperse monomers with different lengths of siloxane chains, and the structure-physical properties correlation was evaluated as polymer films. Fragile and opaque films were obtained from monodisperse monomers, indicating crystalline polymers. Besides, transparent and flexible films were obtained from polydisperse monomers, indicating amorphous polymers. All polymers were decomposed almost 100% to the original monomers by heating at 160 °C. Furthermore, the re-photopolymerization was achieved using recycled monomers, thus realizing monomerpolymer conversion based on photopolymerization and thermal depolymerization. The physical properties, such as glass transition temperatures and flexibilities of polymers were controllable in terms of the average siloxane length between anthracene dimers, indicating their potential for use in rubbers and elastomers.

#### **Biography:**

Atsuro Mori is a master student at Kumamoto University, Japan. He was born in Kumamoto Pref. in 2000 and grew up there. He will start working as a corporate researcher next year.

# Architectural Influence of Polymer Brush-Modified Tri-compartmental Anisotropic Particles in Stabilizing Pickering Emulsion

### Subhashree Subhasmita Pradhan<sup>1</sup>\*, Ashank Upadhyay<sup>1</sup>, Samiksha Shrivastava<sup>2</sup>, Awaneesh Singh<sup>2</sup>, Sampa Saha<sup>1</sup>

<sup>1</sup>Department of Material Science and Engineering, Indian Institute of Technology Delhi, New Delhi-110016, India

<sup>2</sup>Department of Physics, Indian Institute of Technology (BHU), Varanasi-221005, Uttar Pradesh, India.

#### Abstract:

We aimed to create tri-compartmental polymeric particles (TPs), with selective areas conjugated with hydrophilic patches, to produce an array of amphiphilic particles with various architectures. Briefly, the electrohydrodynamic co-jetting technique was employed to create four sets of TPs comprising PLA (polylactide) in one/two compartments and a blend of PLA and a macro-initiator at a ratio of 90/10 in other compartments (s). Upon grafting a hydrophilic

polymer brush (poly(2-dimethyl aminoethyl methacrylate) (polyDMAEMA)) onto the surface of macroinitiator (10 wt%) containing compartment using Surface Initiated Atom Transfer Radical Polymerization (SIATRP), particles were expected to become amphiphilic. By locating the macroinitiator in various compartments (TBP 1-4), an array of amphiphilic particles with various architectures was created and characterized. This study allowed us to produce a repertoire of anisotropic particles with varying amphiphilicity to investigate their role as Pickering emulsion stabilizers beyond Janus geometry. The relative performance of the brush-modified TPs (TBPs) in stabilizing octanol/water-based emulsion was explained with the aid of their HLB balance, interfacial tension, location of the macroinitiator, and the macroinitiator content/grafting density. Hydrophilic rich lobe polyDMAEMA TBPs, were shown to stabilize emulsion for up to 8 days, making them

the most efficient. In addition to polyDMAEMA, TPs were grafted with hydrophilic poly(ethylene glycol methyl ether methacrylate) brushes to improve their hydrophilicity, resulting in a stable emulsion lasting up to 11 days. We used dissipative particle dynamics simulations to analyze oil-in-water emulsion with TBPs to confirm our experimental results. Except at high grafting density, experimental and numerical modeling correlated well.

#### **Biography:**

My name is Subhashree Subhasmita Pradhan, and I am a fourth-year PhD student at India's Indian Institute of Technology Delhi (IIT Delhi) in Materials Science and Engineering. My research focuses on advanced polymeric anisotropic particles and their diverse range of applications, which includes those in the fields of environment and biomedicine. The University of Calcutta granted me a Master of Technology degree in polymer science and technology prior to this. Two research articles, a review paper, and a book chapter of mine have appeared worldwide by esteemed publishers such as Springer Nature and Elsevier.

### DTI Analysis of The Implantation of Biomaterials Derived From Polyaniline For Tissue Regeneration in The Spinal Cord

### Puebla-Garcia Melissa<sup>a,\*</sup>, Ortega-Cruz Thania<sup>a</sup>, Christopher-René Torres-San-Miguel<sup>b</sup>, and Morales-Guadarrama Axayacatl<sup>a</sup>

<sup>a</sup>Centro Nacional de Investigación en Imagenología e Instrumentación Médica, Departamento de Ingeniería Eléctrica, Universidad Autónoma Metropolitana Iztapalapa, CDMX, Mexico.

<sup>b</sup>Instituto Politécnico Nacional, Sección de estudios de posgrado de la Escuela Superior de Ingeniería Mecánica y Eléctrica Unidad Zacatenco, CDMX, Mexico.

#### Abstract:

Diffusion Tensor Imaging (DTI) analysis is a magnetic resonance imaging technique used to study the microstructure of brain tissue, particularly white matter, providing information on the integrity of neural pathways and neuronal connectivity. In this work, DTI is used with the objective of evaluating the effectiveness of polylactic acid – polyaniline (PLA-PANI) implants as scaffolds, in promoting functional recovery and anisotropy in the epicentre of spinal cord injuries in rats.

To carry out this analysis, the implantation of PLA-PANI scaffolds in rats with spinal cord injuries was carried out. Subsequently, the DTI technique was used to quantify the structure and connectivity of the spinal cord in the implanted rats compared to control rats. Some of the parameters that were evaluated using DTI include the anisotropic fraction, axial and radial diffusivity, as well as axonal projections calculated from the diffusion direction of water molecules in the tissue.

In addition to the DTI analysis, it is important to complement this evaluation with the functional and behavioural characterization of the rats through motor function and autonomy tests, to evaluate functional recovery after treatment with PLA-PANI implants. Taken together, this comprehensive approach allows evaluation of both structural changes in the spinal cord and functional improvement in the implanted rats, which would contribute to the development of therapeutic strategies to improve recovery after spinal cord injuries

#### **Biography:**

Final year student of Biomedical Engineering, the latest studies and works have focused on biomaterials. In recent times she has studied the performance of materials in animal models, with the intention of disseminating scientific information and continuing this development. She is interested in participating in laboratories and working with researchers who are studying similar topics. She is currently a research assistant at the National Research Center for Imaging and Medical Instrumentation.

# Analysis of the Implantation of Biomaterials Derived from Polyaniline for Tissue Regeneration in the Spinal Cord using Magnetic Resonance Spectroscopy

### Ortega-Cruz Thania<sup>a,\*</sup>, Puebla-Garcia Melissa<sup>a</sup>, Christopher-René Torres-San-Miguel<sup>b</sup>, and Morales-Guadarrama Axayacatl<sup>a</sup>

<sup>a</sup>Centro Nacional de Investigación en Imagenología e Instrumentación Médica, Departamento de Ingeniería Eléctrica, Universidad Autónoma Metropolitana Iztapalapa, CDMX, Mexico.

<sup>b</sup>Instituto Politécnico Nacional, Sección de estudios de posgrado de la Escuela Superior de Ingeniería Mecánica y Eléctrica Unidad Zacatenco, CDMX, Mexico.

#### Abstract:

Magnetic resonance spectroscopy (MRS) is a technique that allows analysing the chemical and molecular properties of a sample by measuring the absorption, emission or scattering of electromagnetic radiation in vivo. In the context of this work, MRS has been used to evaluate the feasibility of polylactic acid - polyaniline (PLA-PANI) scaffold implants, in promoting cell regeneration, neuroprotection, and functional recovery in spinal cord injuries in rats.

Specifically, MRS can be considered as a non-invasive technique used to analyse the chemical composition of biological samples. With MRS, the aim is to quantify changes in metabolites, such as the levels of neurotransmitters, amino acids, lipids and other compounds in the spinal cord of rats treated with PLA-PANI implants. Furthermore, it is considered important to complement the MRS with the functional and behavioural characterization of the rats to evaluate recovery after treatment with PLA-PANI implants. This allowed the molecular and chemical changes to be correlated with the functional improvement observed in the treated rats.

In summary, MRS could be a valuable tool to evaluate the effects of PLA-PANI implants on the spinal cord at a molecular and chemical level, contributing to the development of therapeutic strategies to improve recovery after spinal cord injuries, through the provision of data that contributes to improving the understanding of some of the mechanisms involved in cellular and functional regeneration.

#### **Short Biography:**

Biomedical Engineering student, the latest studies and works have focused on biomaterials. She is currently a research assistant at the National Center for Research in Medical Imaging and Instrumentation. Her field of interest is research in biomaterials, specifically to promote cell regeneration, functional recovery in spinal cord injuries, as well as analysis with medical imaging techniques.

#### Mechano-responsive and Photochromic Dithienylethene-polycaprolactone Conjugates

#### Medeina Steponavičiūtė<sup>a\*</sup>, Debashis Majee<sup>a</sup> and Stanislav Presolski<sup>a</sup>

<sup>a</sup>Division of Science, Yale-NUS College, Singapore 138527, Singapore

#### Abstract:

Despite the constantly growing number of studies devoted to mechanochemical polymers and various mechanophores characterized by fluorescence, only a few of them study DTEs and their applications in polymer mechanochemistry. Within this study, we introduce the two DTE mechanophores with different possible attachment points (-2,2' and -5,5') for polymers. Polymer poly( $\varepsilon$ -caprolactone)s (PCL) was used for this study because of its wide application and strategic convenience. Polymers with DTE in the middle of the mechanophore were synthesized by controlled ring-opening polymerizations using DTE as bifunctional initiators. Six different molecular mass DTE polymer compounds were analyzed using ultrasonication experiments, spectroscopic analyses, and theoretical calculations. Results showed that using an external force makes it possible to cleave the closed form of the DTE molecules and thus change their optical properties. This strategy can be repeated several times but is superior to other known systems. DTE

compounds with -5,5' attachment points are also characterized by greater resistance compared to DTE -2,2'. The presented concept of mechanical cleavage of bonds and photo deactivation of DTE compounds provides further advances in polymer mechanochemistry and the application of these molecules in stress-sensing materials.

Keywords: polymer mechanochemistry, DTE, ultrasonication,

#### **Biography:**

Medeina Steponavičiūtė, the author of this study, is a researcher and lecturer at Vilnius University (Lithuania) and a post-doc researcher at Yale-NUS College in Singapore. Where her research is primarily focused on the synthesis and modification of hydrogels for CuAAC 'click' chemistrybased 3D printing. She also has a keen interest in living Radical Polymerization, the synthesis and properties of charge-carrying molecular brushes, the synthesis and properties of stimuliresponsive polymers, bioinspired and biomimetic polymers, and conservation and restoration chemistry. Medeina's PhD, which she obtained at Vilnius University, was centered on the synthesis and properties of catechol groups containing brush copolymers.

#### Nanofibrillation of Technora and Production of Nanofiber Nonwoven Fabric

#### Gayeon Jeong<sup>1\*</sup>, Hyeri Kim<sup>2</sup>, Dohyeong Kim<sup>1</sup>, Garam Park<sup>2</sup>, Jaseung Koo1<sup>2</sup>

<sup>1</sup>Department of Organic Applied Materials Engineering, Chungnam National University, Daejeon, Korea <sup>2</sup>Department of Bio-Applied Chemistry Research, Chungnam National University, Daejeon, Korea

#### Abstract:

Technora is a type of copolymer aramid fiber known for its higher strength and elongation compared to Kevlar. When Technora, which exists in the form of filaments, is nanofiberized, its diameter is reduced to the nano scale, the aspect ratio increases, and its physical properties are enhanced. However, literature on nanofiberization often indicates that the process can be time-consuming or require additives. Therefore, research was conducted to achieve nanofiberization in a shorter period and to obtain nanofibers with maintained particle shape through supercritical drying. Nanofibers that underwent an appropriate drying process retained a soft feel and a non-agglomerated state. A nonwoven sheet manufacturing process using this nanofiber solution was also studied. The resulting nonwoven fabric combines the thermal stability of aramid fibers with a thin thickness. Establishing a nanofiberization process for copolymer aramid fibers can positively impact the domestic aramid fiber industry.

### **E-Poster Presentations**

Photo- and pH-Sensitive Systems Based on Polyacids and Polyamines with o-Nitrobenzyl Ether Groups

Elena N. Danilovtseva<sup>\*</sup>, Viktor A. Pal'shin, Stanislav N. Zelinskiy, Maxim S. Sudakov, Mariya S. Strelova, Vadim V. Annenkov

Limnological Institute Siberian Branch of Russian Academy of Sciences, Irkutsk, Russia

### Abstract:

The o-nitrobenzyl ether group (ONEG) is a photosensitive fragment that irreversibly decays when illuminated at a wavelength of 350 nm. The introduction of ONEG into the polyamine chain allows us to

obtain oligomers capable of transforming into short polyamines (3-5 nitrogen atoms) under the action of light. These compounds are promising as DNA (RNA) carriers in gene therapy and genetic engineering because the controlled degradation of polyamine allows the release of nucleic acid from the complex with polyamine at the desired place and time. We found the ability of ONEG to be hydrolyzed by tertiary nitrogen atoms from the polyamine chain as a catalyst. This reaction is inhibited by protonation of amine groups at low pH values or in complexes with polyacids, including oligonucleotides. The interactions of polyamines and ONEG-containing polyamines with carboxyl-containing polyacids, polyampholytes and oligo-DNA were studied by potentiometry, turbidimetry, light scattering and gel electrophoresis.

The light-induced decay of ONEG has been used in the development of photosensitive coatings for cell immobilization. The hydrolytic self-destruction of ONEGs in the polyamine chain allows the creation of nucleic acid complexes with finely tuned behavior in living organisms: excess complex will self-destruct, minimizing side effects.

This research was funded by the Russian Science Foundation, grant number 22-15-00268, https://rscf.ru/en/project/22-15-00268/.

#### **Biography:**

Elena Danilovtseva was graduated from the Department of Chemistry, Irkutsk State University, Russia in 1984. She received her Ph.D. in Macromolecular Science from the Institute of Chemical Sciences, Almaty, Kazakstan in 1991. She is a Senior researcher in Limnological Institute SB RAS, Irkutsk, Russia. She is author of near 115 scientific papers and 12 patents. Her scientific interests include synthesis and properties of water-soluble polymers; complexes of polymers with metal ions; molecular mechanisms of biosilicification; biomimetic methods for the preparation of nanoparticles and hybrid materials; design of functionalized coatings; application of fluorescent compounds in study of living organisms.

### Progress in Self-repairing Water-Blocking Materials for Engineering Uses in Water-Associated Settings

#### Wentong Lu\*, Yiyao Zhu, Hao Tian, Peilong Zhou, Jincheng Wang

Department of Polymer Materials and Engineering, College of Chemistry and Chemical Engineering, Shanghai University of Engineering Science, Shanghai 201620, People's Republic of China.

#### Abstract:

In various engineering manufacturing sectors, particularly in river and marine engineering, groundwater projects, and deep-sea operations, the presence of water poses significant challenges due to its pervasive nature and the inability to be controlled like soil, rocks, or vegetation. Water, composed of countless tiny molecules, exhibits the characteristic behavior of gravitationally driven flow towards lower points, permeating even the smallest crevices. Prolonged water infiltration can lead to extensive leakage, posing challenges for machinery and metal components requiring dry working environments. In large-scale construction projects, machinery primarily consists of metal and its alloys, often coated with corrosion-resistant layers. However, these coatings have limited lifespans due to corrosion and abrasion during operation. Therefore, sealing materials play a crucial role in isolating water interference. Conventional sealing materials, when subjected to prolonged water exposure, often exhibit inadequate durability. Thus, adopting a "treating water with water" approach, employing elastic materials capable of water absorption and expansion, becomes imperative. Introducing water-absorbing fillers into elastic materials enhances their performance. Common fillers like superabsorbent polymers (SAP) or crosslinked sodium polyacrylate (PAANa) exhibit excellent water absorption properties, expanding their volume hundreds to thousands of times.

The main theme of this work is the utilization of perfluoropolyether diol (PFPE), possessing dipole-dipole interaction capabilities through C-F bonds. Leveraging dipole-dipole interactions and metal coordination, self-repair is promoted. While water affects metal coordination efficiency, dipole-dipole interactions

remain largely unaffected, even in harsh water conditions, facilitating self-healing. This comprehensive approach offers promising avenues for enhancing the durability and performance of materials in water-related engineering applications, addressing critical challenges in construction and maintenance in such environments.

#### Ballistic Impact Study of an Aramid Fabric by Changing the Projectile Trajectory

#### Larisa Titireª\* and Cristian Munteniță

<sup>a</sup>"Dunarea de Jos" University, Galați, Romania

#### Abstract:

Textile fabrics made of aramid fibers are widely used, in soft or rigid form, for personal protective systems against various types of ballistic threats. Ballistic impact refers to a high-velocity impact caused by a thrusting source, often involving a low-mass object. To use these materials effectively in structural applications, it is crucial to have a good understanding of their ballistic behavior when subjected to high-velocity impact. Upon contacting the ballistic material, it undergoes intricate ballistic penetration processes that require comprehensive and quantitative examination for enhanced comprehension. The aim of this study is to analyze the mechanism of damage of the aramid fabric by changing the projectile impact trajectory based on numerical simulations. By performing numerical simulations and examining the penetration process in detail, a thorough understanding of the behavior of the aramid fabric is aimed to be obtained. The obtained results are analyzed based on the von Mises stress distribution (panel and projectile, projectile only, main wires), projectile deformation, projectile velocity during ballistic impact and based on photographs obtained during impact.

#### **Biography:**

Dr. Larisa Titire studied at the "Dunarea de Jos" University, Romania and graduated as MS in 2020. She then joined the research group of Prof. Cristian Muntenita at the INTERDISCIPLINARY RESEARCH CENTER IN THE FIELD OF MECHANICAL ENGINEERING - CCIDIM. She received her PhD degree in 2023 at the same institution. She obtained the position of an Assistant at the 'Dunarea de Jos" University.

#### Wind Turbine Blades Materials Behavior in Abrasive Wear Conditions

#### Cristian Muntenita<sup>a</sup>\*, Larisa Titire<sup>a</sup>\*, Geanina Podaru<sup>a</sup>, Romeo Marin<sup>a</sup>, Amortila Valentin<sup>a</sup>

<sup>a</sup>"Dunarea de Jos" University, Galati, Romania

#### Abstract:

Taking into account that one of the most available renewable energies is the wind energy, the wind turbines get more and more used in order to harvest this one. The wind turbine propeller blades are exposed to several environment aggressive factors, one of these being the abrasive wear generated by the impact of hard particles, like sand or dust, with the blade. Due to high rotational speed of the blades, the resulting wear leads to material degradation. As the most used materials are layered composites, several researches' goals are the improvement of the resistance to abrasive wear. In this work, samples of a commercial wind turbine blade, made by composite materials, are subjected to abrasive wear tests, in order to identify the weaknesses leading to premature degradation of the blade material. With this goal an air streamed wearing particles test rig was used. The obtained results shown that the most important factor against the abrasion is the surface layer. Once this one is compromised, the damage evolution of the blade material is rising exponentially. Also, a protection method was investigated, consisting into the application of an abrasive resistant auto adhesive polymeric film on the surface of the blade. The results of the tests shown an improvement of the material resistance against abrasive wear.

#### Organising Partner GED Biomedical Innovations AB

Per Albin Hanssons vag 41 Malmo- 20512, Sweden Phone: +46 40 666 53 35 Administrative Office Yuktan Technologies Pvt Ltd 20 Cecil Street, #05-03 Plus, Singapore 049705 contact@yuktan.com

**Email:** committee@polymersconference.com **Web:** https://polymersconference.yuktan.com/