



ABSTRACT BOOK

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Keynote presentation

General Entropy Approach Towards Ultratough Sustainable Plastics

Chaobin He

National University of Singapore, Singapore

Abstract: Not Available

Joining strength of Carbon Fiber Reinforce Polymer and Metals

Ninshu Ma¹, Weihao Li¹, Peihao Geng¹, Sendong Ren², Hongbao Xia³, Yunwu Ma⁴

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Abstract:

Using multi-materials to manufacture automotive structures is one of solutions to reduce the weight as well to meet the strength criteria for ensuring occupant safety during impact accidents. Polymer reinforced by carbon fibers (CFRP) keeps its light weight characteristics and exhibits much higher strength than the pure polymer. Therefore, it is paid a great attention for weight reduction of the vehicle structures. On the other hand, light weight metals such as aluminum or magnesium alloys and high strength steels are also widely employed for white bodies. Therefore, soundly and efficiently joining the CFRP and metals becomes very important. One of chemical joining processes is based on chemical reaction between CFRP and metals under certain thermal-pressure conditions. In this report, the thermal process was successfully realized using electrical resistance Joule heat, laser beam and friction heat, respectively. Furthermore, the influence of three joining conditions, temperature and pressure as well as the process time on the joining strength is presented. The obtained results can supply a guidance to join CFRP and metals soundly by applying suitable thermal-pressure conditions.

Biography:

Ninshu Ma has published 7 books and more than 200 papers in well-known journals and major international conferences. He chaired international symposium on Visualization of Joining and Welding (Visual-JW2019). He also chaired international conference on Welding Science and Engineering (WSE2019) and co-chaired WSE2011, WSE2013, WSE2017 and WSE2023. He also joined the development of commercial software JSTAMP and JWELD for metal forming and welding simulations, respectively. https://researchmap.jp/ma.ninshu

Nanocomposites of Conjugated Polymers with Cellulosic Nanomaterials, Graphenic Frameworks and Inorganic Nanotube Arrays: Challenges and Opportunities

Karthik Shankar*

University of Alberta, Canada

Abstract:

Conjugated polymers (CPs) are organic semiconductor platforms for low-cost solar cells, flexible displays, wearable consumer electronic gadgets, fluorescence imaging and chemiresistive sensors. In most of the aforementioned applications, achieving optimal performance using CPs requires the use of a heterojunction nanocomposite with another material such as an organic small molecule chromophore or an inorganic semiconductor. This is because of two reasons - the low charge carrier mobility (typically < 1 cm2/Vs) in CPs and the pronounced dependence of the optoelectronic properties of CPs on the stacking and organization of polymer chains i.e. on the morphology of CPcontaining films and membranes. Infiltrating CPs into ordered inorganic semiconductor nanorod/ nanotube arrays has been shown to result in high performance photodetectors, solar cells and chemical sensors. However, engineering challenges remain related to the imbibition of CPs into nanopores and the chain conformation inside the nanopores. We have found that optimally blending CPs with bare and functionalized cellulose nanocrystals (CNCs) allows the spontaneous formation of ordered nanocomposites wherein the chains of the CP wrap around the nanorod-like CNCs. An emerging class of nanocomposites consists of solution processed thin film blends of CPs with 2D materials such as graphene quantum dots (GQDs) and carbon nitride (CN) nanosheets. This Invited Keynote Lecture will discuss the different types of conjugated polymer based heterojunction nanocomposites, and highlight the corresponding challenges & opportunities.

Biography:

Karthik Shankar is Professor of Electrical and Computer Engineering at the University of Alberta, in Edmonton Canada. He completed M.S. (2002) and Ph.D. (2007) degrees in Electrical Engineering from Penn State University. From 2012-2017, he held a secondment to NRC-NINT. His research is focused on conjugated polymers, cellulose nanocrystals, graphenic frameworks, metal oxide nanomaterials and plasmonic substrates for optoelectronic device applications. He is an expert in quantum electronics and materials science. He is a recipient of the Petro-Canada Young Innovator Award. He has authored over 180 publications that have been cited >22,000 times. His h-index is 58 as of 2023.

Molecular Simulations of Polyelectrolyte Brushes and Associated Ions and Water

Siddhartha Das

Department of Mechanical Engineering, University of Maryland, College Park, MD

Abstract:

Functionalizing solid-liquid interfaces by grafting them with foreign materials (e.g., surfactants, polymer, polyelectrolytes, etc.) has been extensively employed for multiple applications ranging from drug delivery and oil recovery to sensing, water harvesting, and fabrication of nanofluidic diodes and transistors. In this talk, I shall present my group's research the all-atom Molecular Dynamics (MD) simulation-based exploration of the structure, ionics, and liquid transport at

interfaces grafted with such PE brushes. First, we provide hitherto unexplored details of PE-brushsupported counterions and water molecules resolved across atomistic scales for both cationic and anionic PEs. We find that the ultraconfinement effect introduced by the PE brushes causes a reduction in the mobility of these counterions and water molecules as well as a significant change in the energetics of the formation of water-water and water-PE-brush hydrogen bonds. We discuss the use of novel machine learning methods to unravel the properties of brush-supported water molecules. Second, we probe the PE brush structure and the properties of the brush-supported water molecules and counterions for the case where the brushes are grafted to the walls of a nanochannel. We discover the onset of overscreening (OS) within the PE brush layer caused by an interplay of nanoconfinement and counterion sizes. Finally, we establish this OS leads to (1) electroosmotic flows that are coion-driven and can be reversed (in direction) by increasing the strength of applied electric field and (2) ensures an electroslippage effect where electrokinetic energy generation and flow enhancement occur simultaneously in presence of background pressure-driven transport.

Biography:

Siddhartha Das, an Associate Professor in the University of Maryland (UMD), received his B.S. and Ph.D. from the Indian Institute of Technology Kharagpur. His research focuses on polymer systems, soft materials and interfacial transport. He has published 179 journal papers, received promotion to Associate Professorship with early tenure, got elected as Fellows to Royal Society of Chemistry U.K. and Institute of Physics U.K., won Junior Faculty Research Award from UMD engineering, Emerging Investigator awards from journals Soft Matter and Physical Chemistry Chemical Physics, and IIT Kharagpur Young Alumni Award, and got recognition as top 2% scientist by Stanford University.

Oral

Two-Dimensional Propagation of Thermal Waves Surrounding Dendrites Based on a Finite Difference Method

Séverine A.E. Boyer^{1*} and Alain Burr¹

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Abstract:

Based on the fundamental principles of heat phenomena [1], an original transient thermal modeling is proposed using finite difference calculation. The selected model-pattern is dendrite(s) distributed arbitrarily in the viscous-liquid fluid. The boundary conditions are simplified into 2D limits without changing the morphologies of the model-pattern.

The temperature distribution at the stage of the initial local disorder (first moment) and of the global stable organization (long durations) is assessed. The waves are propagating in the unstable fluid medium surrounding the dendrites. The waves are interpreted by both isoline and isocline pictures, referring respectively to the field of temperatures and its gradient. In the merging of the flow fields of the isoline of the temperature, fractal patterns are revealed within the interdendritic-liquid; they may lead to sites of extra-germination close by the main dendrites.

Oil and Char Derived from Waste Tires (Polymer Rubber) Pyrolysis as a New Potential Base for New Eco-Binder and Antioxidant Agent for Road Pavements

Paolino Caputo^{1*}, Abraham A. Abe¹, Michele Porto¹, Valeria Loise¹, Valentina Gargiulo², Giovanna Ruoppolo², Michela Alfè², Pietro Calandra ³, Francesco Cammarota² and Cesare Oliviero Rossi¹

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³CNR-ISMN, National Research Council, Institute of Nanostructured Materials, Via Salaria km 29.300, 00015, Monterotondo, Italy

Abstract:

As bitumen is derived from a non-renewable resource, efforts regarding its efficient and longlasting use as an asphalt binder have been brought to limelight. Two approaches that embody this objective are the research and development of alternative eco-binders as total or partial substitutes to bitumen in asphalt mixes and the discover of new potential anti-oxidant agents to be added in bituminous mixes to reduce susceptibility to oxidative aging thereby increasing the service life of asphalt pavements. In the present study, the testing of new-concept alternative binders and antioxidant agents obtained from the pyrolysis of waste tires (char and pyrolysis oil) is presented.

The bitumen modified with the char derived from waste tires pyrolysis, subjected to artificial aging unveiled that this pyrolysis product can exert a certain anti-aging effect, reducing the increase in rigidity typically obtained during aging. This was attributed to its higher carbon content (up to 80 wt.%) giving higher compatibility with the bitumen chemical nature and to its more uniform dispersion within the bituminous structure as found by AFM i.e., ultimately, to the establishment of more effective interactions.

On the other hand, the pyrolysis oil is very viscous at room temperature and it is similar to bitumen from the chemico-physical point of view. For this reason, this product can be used as base to new

eco-binder formulation in alternative of the bitumen. The new eco-binder has been improved by the use of additives in an attempt to improve its specific properties and, thus, to bridge the gap between this alternative binder and traditional bituminous binders.

These encouraging first attempts to use products from pyrolysis of wastes promote non-renewable resource conservation and they can make the use, recovery and recycling of resources more practical and effective, reducing production costs and facilitating a regenerative circular economy by complying the End of Waste (EoW) criteria in the framework of Waste Framework Directive of the EU (Directive 2008/98/EC).

KEYWORDS:

bitumen, additives, antioxidant agents, rapeseed oil, pyrolysis, tires, pyrolysis

Biography:

Caputo Paolino obtained his PhD in Life Science and Technology from the University of Calabria, Italy. He is currently a Temporary Research Associate (RTDa) in the department of Chemistry

and Chemical Technologies at the University of Calabria. He is also an afferent of the National Inter-University Consortium of Materials Science and Technology (INSTM) which is the largest consortium of its kind in Italy, drawing on the expertise of not less than 50 universities – and all those that are active in Italy in researching advanced materials and technologies. Paolino Caputo's research focuses on physical chemistry with a main focus on bitumen characterization and food based industrial materials and compounds. He has over 60 publications with over 900 citations. He is also one of the inventors of the Anti-smoke Patent (release date: October 31, 2018; number 102016000041219).

Valorization of Biomass from Insect Investigated for Commodities Plastic Degradation by a Circular Economy Approach

Patrizia Cinelli^{*,1}, Giovanna Strangis¹, Silvia Citernesi¹, Niccoletta Barbani¹, Norma Mallegni¹, Neetu Malik¹, Maria J. Lopez², Maurizia Seggiani¹

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²Unit of Microbiology, Department of Biology and Geology, CIAIMBITAL, ceiA3, University of Almeria, Almeria, 04120, Spain

Abstract:

One approach to solve plastic pollution, and compost contamination by plastic, is the use of enzymes, insect, and worms to degrade debris of commodities plastic, in compost and soil. Current study provides a preliminary overview of the main non-recyclable plastics in municipal waste streams, their characteristics, their possible sorting and lay the basis for a possible biological treatment using insects. For example, evidences of plastic assimilations were detected in Galleria mellonella. By the way order to make the approach more sustainable, and productive each by products has to be valorised as either fertilizer or as active molecules such as chitin extracted from the insect exoskeleton as conducted in the project RECOVER "Development of innovative biotic symbiosis for plastic biodegradation and synthesis to solve their end of life challenges in the agriculture and food industries". In the present study we report example of valorization of chitin and chitosan as functional polymers comparing those sourced from insect with traditional chitin and chitosan from crustaceous (as was developed in the project ECOFUNCO project (GA No 837863) "ECO sustainable multiFUNctional biobased COatings with enhanced performance and end of life options"). Particular reference will be made to extraction and applications of chitin/ chitosan in coatings and blends for food packaging and mulch films. Coatings with chitosan and chitin evidence valuable properties in barrier to oxygen and anti-microbial activity.

Biography:

Patrizia Cinelli is associate professor at Pisa University on Fundamentals of chemical technologies. PhD in Chemistry on "biodegradable and sustainable polymers for application in agriculture", partly performed at the United States Department of Agriculture (USDA), Peoria, IL, USA. Over 25 years of international experience in applied and green chemistry, polymer science and technologies. She has participated in over 20 European projects, acting as coordinator of the ECOFUNCO project GA 837863. She is co-author of over 120 papers in peer-reviewed journal, h-index 34, 14 book chapters, 9 patents on innovative materials. She works on sustainable polymers, and biomass valorization.

Molecular Dynamics Study of Polyamidoamine Oligomers Containing B-Cyclodextrins as Drug Carriers for Cancer Therapy

Giuseppina Raffaini^{1,2}

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Abstract:

Cyclodextrins (CDs) can solubilize hydrophobic drugs in water enhancing their bioavailability. The aza-Michael polyaddition of L-arginine and N,N'-methylene-bis-acrylamide gives the biocompatible and easily cell-internalized polyamidoamine ARGO7. By controlled synthesis, two ARGO7 oligomers, namely a trimer and a pentamer, bearing acrylamide terminal units, were experimentally obtained by prof. Paolo Ferruti and prof. Elisabetta Ranucci as precursors of the β -cyclodextrin-end-terminated oligomers P3 and P5, which have been shown to encapsulate curcumin, a promising anticancer drug, at both pH 7.4 and 4.5.

In this theoretical work Molecular Mechanics (MM) and Molecular Dynamics (MD) simulations of aggregation process between P3 and P5 carriers and curcumin were investigated. The drug molecules are found in the nanoaggregate formed during MD run due to favorable drug/carriers van der Waals interactions. H-bonds between β -CDs and π - π interactions among curcumin aromatic rings stabilized the formed nanoaggregates throughout the entire MD run, without degradation. The two carriers P3 and P5 are more energetically stable at pH 4.5 than at pH 7.4. The aggregation kinetics were faster at pH 4.5. In all cases, the curcumin molecules were partially exposed on the outer surface and partially incorporated into the aggregate core. In particular, the P3-curcumin aggregates showed some curcumin in host-guest inclusion complexes in the hydrophobic β -CD cavities, whereas in the P5-curcumin aggregates fewer drug molecules were encapsulated at both pH values. The different van der Waals interactions may be related to faster release observed at this acid pH, which is important for the internalization in cancer cells.

Biography:

Giuseppina Raffaini received Ms Sc. in Chemistry at Università degli Studi di Milano, the postgraduate diploma in "Advanced School in Polymer Science Giulio Natta", the Inter-university Master in Biomaterials, She done PhD in 2005 in Materials Engineering at Politecnico di Milano. In 2008 she became Assistant Professor, in 2014 Associate Professor at the Politecnico di Milano. Her research interests are molecular dynamics simulations of protein and drug adsorption on biomaterials, organic inhibitors in concrete, β -cyclodextrinsinclusion complexesfor drug delivery. She is co-author of 70 original peer-reviewed ISI papers. She is member of ACS, AlCIng, DCT-SCI Association.

Photoresins for the Suitable Development of Carbon Monoliths By 3D Printing

Jose Luis Diaz de Tuesta^{1*}, Hendryk Steldinger², Adriano Santos Silva^{3,4}, Adriano Henrique^{3,4}, Noelia Corrochano¹, Jan Gläsel², Helder T. Gomes^{3,4}, José Antonio C. Silva^{3,4}, Fernando Martínez¹ and Bastian J. M. Etzold²

¹Department of Chemical and Environmental Technology, ESCET, Rey Juan Carlos University, 28933, Móstoles, Madrid, Spain; ²Technical University of Darmstadt, Department of Chemistry, Ernst-Berl-Institut für Technische und Makromolekulare Chemie, 64287 Darmstadt, Germany; ³Centro de Investigação de Montanha (CIMO) and Laboratório Associado para a Sustentabilidade e Tecnologia em Regiões de Montanha (LA SusTEC), Instituto Politécnico de Bragança, Campus Santa Apolónia, 5300-253 Bragança, Portugal.

Abstract:

The properties of polymer-derived activated carbons can be finely controlled, since the composition of the polymer precursor is designed in manufacturing. In contrast to bioderived carbons, there are few deviations in the precursor materials and thus a more constant product properties. Also, polymer derived carbons can be designed in a way to retain the polymer structure. If the polymer precursor exhibits a high degree of crosslinking, direct pyrolysis can be conducted to produce the desired carbon material retaining their shape when transformed. Stereolithography (SLA) allow creating 3D printed structures of photopolymers that can be turned into carbon with tuned mechanical strength and electric or thermal conductivity using suitable resins. Recently, we prepared carbon monoliths from SLA 3D printed polymer based on a photoresin mixture of two monomers, 35% pentaerythritol tetraacrylate and 35% divinylbenzene. In addition, 30% bis(2-ethylhexyl) phthalate, phenylbis(2,4,6-trimethylbenzoyl)phosphine oxide and sudan1 were used as porogen, as photoinitiator and as dye, respectively. The 3D printed polymer monolith was stabilized by a thermal treatment in air (at 573 K for 6 h), pyrolyzed in nitrogen (at 1173 K for 0.3 h) and activated with CO2 (at 1133 K). The porous carbon monolith obtained show specific surface areas that reach values of 1300 m2 g-1, and have been assessed in three applications: wastewater treatment by Fenton, capture of post-combustion CO2 and separation of n/iso-Paraffins.

Biography:

Jose Luis Diaz de Tuesta concluded his doctoral thesis on doped carbon-based catalysts for catalytic wet peroxide oxidation with cum laude in 2016. Later, he joined the Polytechnic Institute of Bragança (Portugal) to continue working as researcher in different projects dealing with sustainable technologies for the preparation of carbon-based materials and nanomaterials with application as adsorbent and(or) catalysts in environmental applications, mainly wastewater treatment processes. In 2022, he joined to Universidad Rey Juan Carlos (Spain) and got two consecutive high-competitive grants to continue working in the same topics, including a project dealing the development of 3D printed carbons as electrocatalysts.

Production of Polyhydroxyalkanoates (PHBV) from whey and Preparation of Drug-Loaded Nanoparticles

Loreto Cabarcos, Nuria Otero, Christian Kennes, Silvia Diaz-Prado, María C. Veiga*.

Chemical Engineering Laboratory, Faculty of Sciences and Interdisciplinary Center for Chemistry and Biology (CICA), University of A Coruña, Spain

Abstract:

Polyhydroxyalkanoates (PHA) are biopolymers produced by some microorganisms. The production process can be based on the use of a mixed microbial cultures that use residues or industrial by-products as a substrate, such as whey. In this way, a high-quality material is obtained from highly

polluting waste at a low cost. This process is carried out in several steps. Briefly, volatile fatty acids are obtained from whey by anaerobic fermentation, which is followed by aerobic enrichment of microorganisms capable of accumulating PHA. The two processes are carried out with mixed microbial cultures.

At present, research has focused on obtaining these biopolymers for use in drug delivery. This is due to their exceptional characteristics: they are biodegradable, biocompatible materials and do not cause toxicity. Some proteins, such as human transforming growth factor (TGF-ß3), are essential in cell differentiation processes, but they have a short life, so they must be supplemented to the medium from time to time. Therefore, the nanoencapsulation of this protein is of great interest since its degradation is avoided.

This study presents results on PHA production and the subsequent preparation of nanoparticles. The production process was carried out using a mixed microbial culture and whey as substrate. Then, due to the presence of endotoxins, a purification of the material obtained prior to the formation of nanoparticles has been carried out. Finally, the formation of poly (3-hydroxybutyrate-co-3-hydroxyvalerate acid) (PHBV) nanoparticles with 12% HV content was carried out for use as a protein releaser, specifically the TGF-ß3 factor.

Biography:

Maria C. Veiga holds a Ph.D. in the field of environmental engineering (University of Santiago de Compostela, Spain). She is full professor of Chemical Engineering at the University of A Coruña (Spain). She worked as a post-doctoral scientist at Michigan State University (USA). Her fields of expertise are related to environmental biotechnology, with special focus on the development of sustainable bioprocesses for the removal of pollutants from wastewater streams and for the exploitation of industrial wastes for the production of biopolymers and bulk chemicals.

The Epoxy/Thiol-Ene Photopolymerization: A New Curing Method for Epoxy Resins

Ricardo Acosta Ortiz*

Center for Research in Applied Chemistry, Saltillo, Mexico

Abstract:

In this talk is discussed the research developed by our research group concerning a new method to photopolymerize epoxy resins in the presence of a thiol-ene system. This system include a compound with two or more tertiary amine groups functionalyzed with allyl groups, a multifunctional thiol such as the pentaerythritol tetrakis (3-mercaptopropionate) and the 2,2-dimethoxy 2-phenylacetophenone as radical photoinitiator. When the thiol-ene system is added to the epoxy resins at concentrations between 20-40 mol % an irradiated with UV light, the photocuring of the epoxy resins proceeds in 7 min obtaining a crosslinked co-network of the polyether-polythioether type. The epoxy/thiol-ene system display advantages over the conventional thermal curing of the epoxy resins, for instance, a considerable energy saving in comparison with conventional thermal curing that is usually carried out at temperatures between 120-180 °C and curing times between 6-12 h. The obtained polyether-polythioether co-network display enhanced toughness in comparison with the polyethers derived from the conventional thermal curing of epoxy resins, due to the presence of the flexible polythioethers. The combination of a hard phase such as the polyethers and a soft phase like the polythioethers in the co-network derived from the epoxy/

thiol-ene system, allowed us to obtain materials with shape memory materials. By replacing the multifunctional thiol used in the epoxy/thiol-ene system with a thiol-disulfide oligomer, resulted in the obtention of self-healing materials by means of a sulphide-thiol exchange reactions. Also, the versatility of our system allowed us to prepare epoxy nanocomposites using graphene oxide (GO) as filler. The basic species such as thiolates present in the system, attacked the epoxy groups in the GO to covalently bond this filler to the polymeric matrix, resulting in an increase of the mechanical properties. Recently, it has also been incorporated biobased epoxy resins derived from a terpenoid such nopol, in the epoxy/thiol-ene system. It was found that these biobased epoxy resin displayed high reactivity when they are photopolymerized using the epoxy/thiol-ene system.

Biography:

Ricardo Acosta Ortiz studied chemistry at the State University of Coahuila in Mexico and graduated as BSc in 1985. He then joined the chemistry research group at the Center for Research in Applied Chemistry (CIQA). He received a PhD degree at the Manchester Metropolitan University, UK in 1995. After one year of sabbatical staying at the laboratory of Prof James V. Crivello at Rensselaer Polytechnic Institute in Troy, NY in 2000, he obtained the position of senior researcher at CIQA. He has published more than 65 research articles

Amphiphilic Copolymers Containing Polystyrene and Polyglycidol Blocks with Various Architecture: Synthesis, Shape of Unimers, Aggregation Properties and Application for Enzymes and Enzyme Substrates Encapsulation

Stanislaw Slomkowski^{1*}, Mariusz Gadzinowski¹, Damian Mickiewicz¹, Bartosz Gostynski¹, Maciej Kasprów², Łukasz Otulakowski², Teresa Basinska¹, Barbara Trzebicka²

¹Centre of Molecular and Macromolecular Studies, Polish Academy of Sciences, Poland;

²Centre of Polymer and Carbon Materials, Polish Academy of Sciences, Poland

Abstract:

Amphiphilic copolymers found many applications, for example, in crude oil production, in production of protective coatings, for agriculture applications, in fabrication of household products, in food industry, in medicine and in many other fields. The vast majority of these copolymers contain poly(ethylene oxide) (PEO) as hydrophilic blocks. For decades PEO was considered health safe and approved for applications as food additive and important auxiliary drug component. However, many years of exposure on contact with PEO widely present in the environment resulted in development by many people of the adverse immune response. Thus, there is a search for hydrophilic polymer blocks, which could replace PEO. Interesting candidate for such application is polyglycidol (PGL) with main chain almost identical with that of PEO but equipped with one hydroxymethyl group in every monomeric unit. Therefore, studies of synthesis and properties of amphiphilic copolymers containing PGL are desired. The lecture will present design and synthesis of a library of copolymers consisting of the hydrophobic polystyrene (PS) and hydrophilic PGL blocks and having the following structures: PS-b-PGL, PGL-b-PS-b-PGL, PS-b-(PGL-g-PGL) and (PGL-g-PGL)-b-PS-b-(PGL-g-PGL). There will be presented information on conformation of unimers and dimers of these copolymers (based on DFT modelling) and information on their self-aggregation into nanoparticles and larger aggregates (by light scattering studies). Results of the studies of encapsulation of lipase and alkaline phosphatase into the aforementioned copolymer constructs and activity of encapsulated enzymes will also be discussed.

Acknowledgment: This work was financially supported by the National Science Centre (Poland) Grants UMO-2018/29/B/ST4/02178 and UMO-2018/29/B/ST8/01721

Biography:

Stanislaw Slomkowski received master degree (physic) from Lomonosov Moscow State University (SU), PhD and DSc degrees (chemistry) from Technical University in Lodz (Poland). He was the postdoctoral fellow at New York State University (Syracuse, USA), research associate at the University of Toronto, visiting Professor at the University Paris 7 and collaborating researcher at National Institute of Standards and Technologies (Gaithersburg, USA). Since 1972 he is permanently employed in Centre of Molecular and Macromolecular Studies, Polish Academy of Sciences (Lodz, Poland). His research interests are concentrated in polymers and polymer disperse systems for applications in pharmacy, medical diagnostics and medical treatment.

3D Printing Strategies to Control Biochemical Heterogeneity within 3D Scaffolds for Tissue Interface Engineering

Murat Guvendiren*

New Jersey Institute of Technology, Otto H. York Department of Chemical and Materials Engineering, University Heights, Newark, NJ

Abstract:

3D printing has become a common manufacturing technique to create tissue engineering scaffolds and live tissues. In this presentation, novel strategies developed in our research laboratory will be discussed to fabricate complex 3D hydrogels as well as 3D polymeric scaffolds with user-defined and tunable spatial control of biochemical and mechanical properties for musculoskeletal tissue engineering. First, we will present a novel approach to bioprinting dense cellular structures within continuous or heterogenous support and/or functional hydrogels. We will demonstrate our results to control stem cell osteogenesis within built-in vasculature using these devices. We will then focus on controlling stem cell heterogeneity within 3D printed solid polymeric scaffolds with airbrushed functional hydrogel membranes for interface tissue engineering.

Biography:

Murat Guvendiren is an Assistant Professor and the Director of the Materials Engineering program in the Chemical and Materials Engineering Department at NJIT. His research focuses on 3D printing of tissues and organs, and advanced functional materials. Dr. Guvendiren is the recipient of NJIT Excellence in Research award (2022), NCE Rising Star in Research award (2022), NSF CAREER award (2021), NJIT Excellence in Innovative Teaching award (2021), NJIT Innovation in Engineering Education Award (2020), and MTF Biologics Junior Investigator award (2019). He is an elected Senior Member of the National Academy of Inventors (NAI) since 2022.

Polymeric Hydrogels for Wearable Biosensors

Wen Zhong*, Helen Hsu and Yitian Wang

Department of Biosystems Engineering, University of Manitoba, Canada

Abstract:

Hydrogels are highly hydrated, porous and soft materials with a touch similar to that of the human skin, therefore, have attracted extensive interests in the development of wearable biosensors. Both natural (e.g., polysaccharides, proteins) and synthetic polymers have been utilized in the development of multifunctional hydrogels with high mechanical strength, high stretchability, 3D printability and self-healing capacity. Incorporated with such conductive agents as carbon materials and/or conductive polymers, these hydrogels show great potentials in the development of a variety of biosensors, including E-skin for health monitoring and management, E-nose that detects hazardous gases (like ammonia gas), growth sensors that monitor plant growth, and humidity responsive actuators. These hydrogels can also be developed into triboelectric generators, which convert environmental mechanical energy into electricity to allow sustainable operation of self-powered biosensors.

Biography:

Wen Zhong obtained her PhD degree in Textile Engineering in Donghua University (China) in 2002 and had her postdoc training at the Department of Biosystems Engineering in the University of California, Davis. She joined the Department of Textile Sciences at the University of Manitoba in 2005 and the Department of Biosystems Engineering in 2015. She has also been affiliated with the Department of Medical Microbiology. Her research expertise is in the areas of biomaterials, nanotechnology and biosensors. She published in high impact journals like Science Advances, ACS Nano, Advanced Materials, and Advanced Functional Materials.

The Effect of Wood Fiber Length and Fiber Content on the Dielectric Properties of Maple Fiber-Polypropylene Composites

Farshid Basiji^{1*}, Fouad Erchiqui¹, Ahmed Koubaa¹, Abdessamad Baatti¹

University of Québec in Abitibi-Temiscamingue (UQAT), Canada

Abstract:

The interest in bio-based polymers and composites with dielectric constants suitable for cuttingedge applications (electrical, electronics, transport, etc.) is in high demand at both academic and industrial levels. To this end, several laboratories and research centers are working on the development of new dielectric materials. However, the effect of plant fiber morphology on the dielectric behavior of bio-composites does not seem to be sufficiently elucidated in the literature. It is within this framework that this work is oriented and aims to investigate the impact of fiber size on the dielectric properties of a family of bio-composites, based on a thermoplastic resin (polypropylene, PP) and cellulosic reinforcements (extracted from Canadian sugar maple). The dielectric parameters of interest are the dielectric constant (ϵ ') and dissipation factor (ϵ '') as a function of frequency, temperature, and reinforcement length. For this purpose, three lengths are considered (short (50 µm), medium (75 µm), and long (100 µm) fibers) for frequency 2.4 GHz and ambient temperature (24 °C). For the study, we developed four sample families of bio-composites (PP-Wood) as a function of fiber length and mass concentration (5, 10, 15, and 20 vol.%). Thermocompression molding was used for this purpose. The samples were then characterized for their dielectric properties.

Biography:

Farshid Basiji, a dedicated Wood and Paper Science and Technology researcher, holds both a bachelor's and a master's Degree from a prestigious university in Iran, notable for his substantial contributions to the field. During his master's program, he conducted pioneering research on wood-plastic composites, specifically investigating the impact of fiber length on mechanical properties. This work resulted in the publication of two research papers, including one focusing on the effects of Filler Content and compatibilizing agents on Particle-Reinforced Composites. Currently pursuing a Ph.D. in Engineering in Canada under the supervision of Dr. Fouad Erchiqui at the University of Quebec, Farshid is driving research in Wood Bio-Plastic Composites, showcasing his unwavering commitment to sustainable materials and technological advancement.

Machine Learning and Guided Nanostructures of Organic Electronics and Ionics

Jihua Chen*

Center for Nanophased Materials Sciences, Oak Ridge National Laboratory, USA

Abstract:

Guided assembly of polymers and organic molecules can provide a way towards intriguing nanostructures and enhanced functionality of organic electronis, polymer ionics, and medicine. (1-2) The weak intermolecular interactions during the slow crystallization process are modifying the nucleation and assembling kinetics via surface energy, and thus playing a key role in defining these organic, polymeric or ionic complexes in their ability to store energy of transport charge.

We demonstrated herein that using AI and low-dose TEM, one can study the relationships of these intermolecular forces and resultant nanointerfaces after the guided assembly process. Energy filtered TEM at reduced accelerating voltage and illumination conditions provides nanoscale elemental mapping. We use a polymer - small molecule organic semiconductor complex as an example for organic thin film transistor, and a polymer guided salt complexe for solid electrolyte. The revealed nanostructures are connected with impedance spectroscopy or transistor performance.

Biography:

Jihua Chen has been a R&D staff member at the Center for Nanophase Materials Sciences (CNMS), Oak Ridge National Laboratory (ORNL) since 2011. He obtained a PhD in Macromolecular Science and Engineering from the University of Michigan-Ann Arbor in 2006. Working at the conjunction of soft electronics, battery, medicine, and data science, he is applying AI to tackle problems in manufacturing and healthcare. Dr. Chen authored and coauthored 160+ scientific publications, with a H index of 55 and over 10k citations on Google Scholar.

Insights Into Hydrogen Bonding of Polydisperse Polyethylene Glycol from Molecular Dynamics Simulations

Markus M. Hoffmann

SUNY Brockport, Department of Chemistry and Biochemistry, USA

Abstract:

Interest in using polyethylene glycol (PEG) as a green chemical solvent is growing because of its low toxicity, biodegradability and interesting solvent characteristics that allowed its successful use in one-pot, multi-component synthesis reactions. Thus, there is an increased need for a physicochemical understanding of PEG as a solvent to further its use in chemical synthesis. Due to its chemical structure, inter- and intramolecular hydrogen bonding can be expected to play a major role for the molecular level interactions and dynamics. Molecular dynamics (MD) simulations were undertaken to study the intermolecular interactions in PEG 200, a polydisperse mixture of ethylene glycol oligomers with an average molar weight of 200 g/mol. Several force-fields were tested how well they produced measured physical properties. Agreement with literature values improved upon adjustments of the partial charges on the hydroxyl groups and the potential function for the -O-CH2-CH2-OH dihedral. The extent of these adjustments varied from oligomer to oligomer. These force-field adjustments resulted in a lowering of hydrogen bonding interactions overall and a shift towards intra-molecular hydrogen bonding. Intramolecular hydrogen bonding was found to be particularly favored for tetraethylene glycol. To the best of our knowledge these simulations are the first ones reported for a polydisperse mixture of ethylene glycol oligomers.

Biography:

Hoffmann studied chemistry as an undergraduate at the Technical University Darmstadt in Germany. In 1992, he moved to the US to pursue a graduate degree in physical chemistry and completed his Ph.D. at Washington University in St. Louis, MO, in 1997. After a post-doc with the Pacific Northwest National laboratory, he has since 2000 been a Professor in Physical Chemistry at State University of New York, College at Brockport.

Thermoplastic Elastomers with Inherent Antimicrobial Properties for Reduction in the Spread of Harmful Microbes

Kacie M. Wells¹

¹North Carolina State University, Raleigh, NC / Fiber & Polymer Science Program

Abstract:

The global Covid-19 pandemic shed new light on the true dangers of viruses and how reducing the spread of microbes is crucial for our health. While great strides have been made to mitigate the virus and prevent future outbreaks, there are still major threats such as antimicrobial resistant pathogens that are a growing concern. Preventative measures are a critical area in reducing the impact of surface-spreading microbes. Our approach is the use of inherently self-disinfecting anionic block copolymers which have been shown to kill over 99.9999% of multiple microbes in minutes. The mid-block sulfonated block copolymer produces a water-activated pH-drop near its surface, inactivating gram-positive, gram-negative, and spore-forming bacteria (such as C. difficile), as well as viruses (including SARS-CoV-2). We employed various casting solvents to prepare the polymer films and form different microstructures leading to changes in antimicrobial performance. We also implemented treatment of the films, solvent-vapor annealing and hydrothermal annealing, to further change the microstructure, altering the tortuosity of the pathways for proton diffusion, giving the potential to improve the antimicrobial performance of the polymer films. With these films treatments we have been able to elucidate time-dependent morphological responses of the block copolymer to Gram-positive (Staphylococcus aureus) and Gram-negative (Escherichia coli)

bacteria. The film treatments resulted in changes to the bacterial inactivation kinetics, which we compared and analyzed using a model assuming a two-stage inactivation process. These polymers present a new method for preventing the spread of infectious microbes and helping to slow the rise of antimicrobial resistant pathogens.

Biography:

Kacie Wells completed her B.S. degree at the University of Connecticut in Materials Science & Engineering before working as an R&D engineer, then going on to obtain an M.S. degree in Textile Engineering at North Carolina State University. After working a few years in industry, she decided to return to N.C. State to pursue her Ph.D. in Fiber & Polymer Science. She joined Dr. Richard Spontak's research group where she learned about block copolymers and how to cast, treat, characterize, and perform antimicrobial testing of those polymers, leading her to be named first author on 2 submitted publications.

Utilization of Corn Stover-Derived Nanocellulose as Oil-In-Water Emulsion Stabilizer

Lingling Liu*

Iowa State University, USA

Abstract:

Agricultural byproducts such as corn stover are widely available low-cost materials for preparation of nanocellulose, which is an emerging green chemical with versatile applications. Corn stoverderived nanocellulose can be prepared by bleaching, alkaline, 2,2,6,6-tetramethylpiperidin-1-oxyl (TEMPO) oxidation, and ultrasonication treatments. TEMPO-oxidized cellulose nanofibril (TEMPO-CNF) with a width of 4 nm, length of 353 nm, and surface charge of 1.48 mmol/g COO- can be prepared from corn stover. The as-prepared TEMPO-CNF had a crystallinity index of 69.50%. Via thermogravimetric analysis, the residual weight of TEMPO-CNF is larger than that of corn stover samples. TEMPO-CNF can be used to stabilize lemongrass essential oil loaded oil-in-water emulsion. In addition, TEMPO-CNF improved the freeze-thaw and centrifugal stability of oil-inwater emulsions stabilized by small molecular weight surfactants (e.g., Tween 80). The prepared nanoemulsion was stable against centrifugation, freeze-thaw and room temperature storage (tested up to 30 days). This study highlights the value-added use of agricultural byproducts to enhance the stability of emulsions stabilized by synthetic surfactants. The developed emulsions comply with the growing interest in using natural substances to prepare stable emulsion products.

Biography:

Lingling Liu is an adjunct assistant professor at the Department of Agricultural and Biosystems Engineering at Iowa State University. She oversees the agricultural nanotechnology and nutritional engineering lab. She received her Ph.D. degree in Food Science from the University of Georgia in 2018. Her research focuses on agricultural byproduct utilization, nanocellulose, nanoemulsion, biobased materials, coatings/films, food nutrition, and food shelf life enhancement.

Immobilization of Laccase Enzyme on Poly(maleic anhydride-alpha-styrene) Films

Nicolas González¹, Jenny Blamey², Valeria Villalobos¹, Marcela Urzúa^{1*}

¹Departamento de Química. Facultad de Ciencias. Universidad de Chile

²Facultad de Química y Biología Universidad de Santiago de Chile, Santiago, Chile

Abstract:

In the environmental and toxicological field, there is a growing interest in phenolic contaminants. These can have negative effects on human and animal health. Enzymatic oxidation has been explored as a remediation method, one example being the use of the enzyme Laccase. However, the use of free enzymes in wastewater treatment faces challenges due to their instability and limited re-usability under environmental conditions. In contrast, enzymes immobilized in a matrix show higher thermal stability, longer lifetime and versatility in terms of pH and working temperature. In addition, they allow an easy recovery of enzymes for reuse, and offer the possibility to design a variety of bioreactors. However, enzyme immobilization faces limitations, such as diffusion restrictions and short immobilization period. Thus, covalent immobilization of enzymes on solid surfaces emerges as an alternative. In this context, poly(maleic anhydride-alt-styrene) films, PAMSt, and their derivatives, stand out as potential polymeric matrices for enzyme immobilization. This study proposes to obtain PAMSt films and PAMSt functionalized with L-glutamic acid, Glu, to covalently immobilize Lacase enzyme without losing its enzymatic activity. The functionalization of PAMSt functionalized with L-glutamic acid was followed by FTIR, 13C and 1H NMR. The PAMSt and PAMSt-Glu films were characterized by ellipsometry, contact angle, AFM and XPS. The enzyme activity was determined by UV-vis spectroscopy in a solution with 0.16 M Syringaldazine model substrate. The results showed that the enzyme Laccase is covalently immobilized on the PAMSt and PAMSt-Glu films via the maleic anhydride group contained in the main chain of the copolymer. The enzymatic activity results, indicate that this stability is dependent on the chemical nature of the side chain. In conclusion, copolymers derived from maleic anhydride containing amino acids allow the covalent immobilization of the enzyme Lacasa, being dependent on the presence of the maleic anhydride group. Acknowledgments: FONDECYT Regular project 1231631

Biography:

Marcela Urzúa is Doctor of Sciences with a mention in Chemistry in the Pontificia Universidad Católica de Chile, Chile. She has a Postdoctorate in Polymer-Surface at the Faculty of Sciences of the University of Chile. Currently, She is an Associate Professor of Department Chemistry at the Facultad de Ciencias, Universidad de Chile. She has been the Principal Investigator and co-Investigator in different projects of investigation. Her areas of interest are polymer chemistry and surface physicochemistry in polymer.

Structural Investigation of Human Hair

Cristiano L. P. Oliveira^{1*}, Cibele R. R. C. Lima¹, Augusto C. C. Bandeira¹, Cassio Alves²

¹Physics Institute, University of São Paulo, São Paulo - Brazil, ²Course of Exact Sciences, Federal University of Paraná, Pontal do Paraná, Paraná – Brazil

Abstract:

Human hair is a biopolymer that has two major morphological regions well distinct: the cuticle and cortex. Between the cells of the cuticle and cortex, cell membrane complexes (CMCs) are present, consisted of proteins and lipid bilayers. The main function of the cuticle, the outer structure, is to provide mechanical protection for the cortex, which contains a helical fraction comprising a crystalline phase (intermediate filaments - IFs) embedded in amorphous matrix that is sensible to water, largely influenced by the relative humidity. Hair treatments with chemical products and the use of thermal devices, can promote important structural changes like protein denaturation, water removal and surface damages on the cuticle. We combined a number of techniques, Small-Angle X-ray Scattering (SAXS) in situ measurements (varying the temperature), thermogravimetry coupled to mass spectrometry (TG/MS), optical microscopy (OP), X-Ray computer tomography (XRCT) and differential scanning calorimetry (DSC) to obtain structural details on the human hair and structural changes upon chemical and thermal treatments[2]. Caucasian virgin hair, Caucasian bleached hair, Caucasian straightened hair and Caucasian bleached and straightened hair were investigated. As will be shown, several results could be obtained providing important structural details as changes on porosity of the inner structure of hair, changes on the CMC structure and hair surface characterization. These results are very important for the basic knowledge on hair structure but also for the cosmetic companies and professionals on hair styling to understand the implications of their products and treatments.

Nanosize Azodye Layers for Liquid Crystal Photoaligning and Photopatterning

Vladimir G. Chigrinov

Hong Kong University of Science and Technology, Clear Water Bay, Kowloon, Hong Kong

Department of Theoretical Physics, Moscow Region State University, Mytishi, Russia

Nanjing Jingcui Optical Technology Co., LTD, Nanjing, China

Abstract:

Photoalignment and photopatterning has been proposed and studied for a long time [1]. Light is responsible for the delivery of energy as well as phase and polarization information to materials systems. It was shown that photoalignment liquid crystals by azodye nanolayers could provide high quality alignment of molecules in a liquid crystal (LC) cell. Over the past years, a lot of improvements and variations of the photoalignment and photopatterning technology has been made for photonics applications. In particular, the application of this technology to active optical elements in optical signal processing and communications is currently a hot topic in photonics research [2]. Sensors of external electric field, pressure and water and air velocity based on liquid crystal photonics devices can be very helpful for the indicators of the climate change.

We will demonstrate a physical model of photoalignment and photopatterning based on rotational diffusion in solid azodye nanolayers. We will also highlight the new applications of photoalignment and photopatterning in display and photonics such as: (i) fast high resolution LC display devices, such as field sequential color ferroelectric LCD; (ii) LC sensors; (iii) LC lenses; (iv) LC E-paper devices, including electrically and optically rewritable LC E-paper; (v) photo induced semiconductor quantum rods alignment for new LC display applications; (vi)100% polarizers based on photoalignment; (vii) LC smart windows based on photopatterned diffraction structures; (vii) LC antenna elements with a voltage controllable frequency.

Depolymerization Photochemistry by Molecular Dynamics

Dmitri S. Kilin*

Department of Chemistry & Biochemistry, North Dakota State University, Fargo, ND

Abstract:

Several aspects of electromagnetic field to matter interaction are addressed by computational modeling of transitions between ground and excited state potential energy surfaces, driving molecular system away from the equilibrium. Photoinduced bond breaking events are enhanced for molecular systems placed in the center of resonant microcavity via formation of a bound matterto-field polaritonic state. A description of matter-to-electromagnetic radiation interaction is is integrated with on-the-fly ab initio molecular dynamics and electronic structure methods. Validity and predictive power of several algorithms applicable for the IR and UV-vis range excitations are discussed. A vibrational polariton algorithm is tested by exploring an ensemble of hydrogen fluoride molecules in the IR cavity. A time-dependent excited state dynamics (TDESMD) algorithm is applied to a several UV-photoactivated reactions ranging from formation of luminescent defects at surface of carbon nanotubes [1] to photodegradation of polymers and plastics [2] to photopolymerization of molecular precursors for fabrication of silicon nanostructures. [3] Introduced TDESMD algorithm seems most useful in the limit of multiple reaction pathways and multiple products. Validation of TDESMD predictions is based on comparison of computed and measured distribution of products and mass spectra. Optical properties, such as lifetimes, and photoluminescence quantum yield of the molecular structures are computationally evaluated through implementation of nonequilibrium dynamics of excited electronic states.

Biography:

Kilin completed his B.S. and M.S. degrees in physics at Belarus State University, (Minsk, Belarus) and received his doctoral degree from Chemnitz University of Technology, (Chemnitz, Germany) in Michael Schreiber's group in 2000. After subsequent postdoctoral internships with Jeff Cina at the University of Oregon, Oleg Prezhdo at the University of Washington, and David Micha at the University of Florida, he joined the University of South Dakota as a research faculty. In 2015 he became an assistant professor, and in 2021 an associate professor in the Department of Chemistry and Biochemistry at North Dakota State University.

Development of Potential Nanocomposite Copolymer Desiccant Films for Moisture Adsorption-Desorption Process

Norazilawati Muhamad Sarih^{1*} and Farah Aqilah Md Zulkiflie¹

¹Department of Chemistry, Faculty of Science, Universiti Malaya, Kuala Lumpur, Malaysia.

Abstract:

Dehumidifying air via refrigerant cooling method consume tremendous amounts of energy. Independent humidity control systems using desiccants have been introduced to improve energy efficiency. This research is aimed to find the alternative of commonly use solid desiccant, silica gel due to its weak physical adsorption properties, as well as to overcome the limitation of liquid desiccants that may affect indoor air quality and cause corrosion. This study reports on the synthesis of poly(vinyl alcohol-co-acrylic acid), P(VA-AA) via solution polymerisation from the

hydrolysis of poly(vinyl acetate-co-acrylic acid), P(Vac-AA). This viable copolymer was incorporated with graphene oxide (GO) at different concentration (0%, 0.5%, 2%, 3% and 5%) to enhance the adsorption-desorption process. The samples were tested for their ability to adsorb moisture at different relative humidity (RH) and their capability to maintain optimum sorption capacity for every 10 repeated cycles. The nanocomposite film with 2% GO, P(VA-AA)/GO2 exhibited the highest moisture sorption capacity at 0.2449 g/g for 60% – 90% RH at 25oC, as compared to its pristine copolymer which could only adsorb 0.0150 g/g moisture. The nanocomposite desiccant has shown stable cycling stability and superior desorption in the temperature range of 45oC - 65oC with up to 88% moisture desorption.

Biography:

Norazilawati Muhamad Sarih obtained her PhD. degree in Polymer Chemistry from Durham University, UK in 2010. Later she was appointed as a Senior Lecturer at the Department of Chemistry, Faculty of Science, Universiti Malaya in the same year. She has taught a variety of courses from BSc. until PhD level. She supervised 12 postgraduates (PhD. and MSc. degrees) and monitored more than 35 final year project students. She holds several administrative positions at the Departmental and the Faculty levels. She was appointed as Associate Professor in 2021. Currently, she is the Vice-President of the Malaysia Carbon Management Society since 2019.

Access to Poly(organophosphazenes) by Macromolecular Substitution

Harry R. Allcock

Atherton Professor, Departments of Chemistry, Chemical and Biochemical Engineering, The Pennsylvania State University, University Park, Pennsylvania USA

Abstract:

Several hundred potentially useful high polymers are accessible by the conversion of poly(dichlorophosphazene) (NPCl2)n to organic derivatives [NP(OR)2]n or [NP(NHR)2]n by the process of macromolecular substitution. This allows the attributes of the inorganic skeleton (thermo-oxidative stability, optical transparency, torsional mobility, elasticity, and biocompatibility) to be combined with the diverse properties of the organic side groups. The talk will cover both the synthetic and structure-property correlations accessible through this system and will review some existing and developing applications.

Biography:

Harry R. Allcock has devoted his career to the development of inorganic-organic rings and polymers. He was born in 1932 in England and obtained his Ph.D. degree in organosilicon chemistry from the University of London. He then held postdoctoral appointments at Purdue University and the Canadian National Research Council in Ottawa, before spending five years at the American Cyanamid Research Laboratories in Connecticut. In 1966 he moved to the Pennsylvania State University where he and his coworkers have explored the broad scope of polyphosphazenes and have published more than 650 papers and several books on these polymers and materials.

Improved Flocculation Efficiency of Cationic Polymers Via Self-Assembling

Laura Romero-Zerón^{1*} and Siddhartha Vuttla²

^{1,2}University of New Brunswick/Chemical Engineering Department, New Brunswick, Canada

Abstract:

Cationic polymers are used in wastewater treatment to aid the formation of macro-flocs. In this exploratory study, we hypothesized that the flocculation efficiency of cationic polymers could be enhanced via self-assembling. Three polymers with cationic charges of 40%, 60%, and 80% were evaluated. The cationic surfactant dodecyl trimethylammonium chloride (DTAC) and b-cyclodextrin (b-CD) were used to produce supramolecular flocculants via self-assembling with the polymers. The wastewater used was produced water from bitumen recovery operations (Pelican Lake Reservoir, Alberta, Canada). The self-assembled supramolecular systems (SPS) were produced by adding to the respective polymer solution concentration, the pre-established concentration of DTAC and b-CD (2:1 molar ratio). For instance, if a 30-ppm SPS was produced, the concentrations of each of the chemicals added were 30-ppm polymer, 30-ppm DTAC, and 30-ppm b-CD. Then, the SPSs were added to the wastewater. The efficiency of the SPSs at different concentrations was evaluated via UV-Visible Transmittance and visual observation of the macro-flocs generated. The experimental results demonstrate enhancement of the flocculation efficiency from 0.5% to a maximum of 7.1%. More significantly, the concentration of cationic polymer required could be reduced up to 6 times (from 30 ppm to 5 ppm), without affecting the flocculation efficiency of the SPS. Therefore, selfassembling indeed improves the flocculation efficiency of the cationic polymers and reduced the required polymer concentration. This implies that formulation of flocculant systems through selfassembling enhances the functionality of cationic polymers, however more research is justified to better understand the mechanisms and enhanced performance of these SPSs.

Biography:

Laura Romero-Zerón, Ph.D., P. Eng. is a Chemical Engineer and professor in the Dept. of Chemical Engineering at the University of New Brunswick. Fredericton, Canada, since 2004. Her research interests include remediation of hydrocarbon contaminated soils, selective adsorption of pharmaceutical drugs and toxins using natural fibers, recycling and upcycling of plastic waste, recovery, and identification of biosurfactants, polymer-surfactant self-assembling systems, evaluation of synthetic and biopolymers functionality, rheological evaluation of polymer-surfactant systems, and pyrolysis of biomass waste to produce value-added bio-additives. Romero-Zerón has published more than 67 scientific papers including two book chapters and has edited two technical books.

Polyurethane Elastomers Toughened by Amphiphilic ABA Tri-Block Copolymers as the Soft Segments

Yanbin Fan^{1*}, Jun Ma², Daoyong Chen², Shaoguang Feng¹, Adam L. Grzesiak¹

¹The Dow Chemical Company; ²Fudan University, China

Abstract:

Increasing the strength while not sacrificing the ductility of polymeric elastomers helps in expanding the application range and this meanwhile improves the durability of the materials.

However, compromise on the strength or ductility usually occurs because the regulation rules for the two attributes are mutually exclusive. In this work, leverageable strategies for toughening polyurethane elastomers applying ABA tri-block copolymers as the soft segments have been successfully developed, where A represents a polyester end block showing miscibility with the urethanes, while B is a middle polymer block showing great immiscibility with the urethanes. It is confirmed that this deliberately adjusted amphiphilicity of the soft segments triggers the formation of small and uniform hard domains that demonstrate an intriguing mechano-responsive orientability under uniaxial deformation. In this way, the polymer chains can be highly stretched and aligned to form nanofibril-like structures, and meanwhile the oriented polymer chains in the same direction can cooperatively resist the external loading stress, making the polyurethanes extraordinarily ductile and strong. Specifically, when poly(ε -caprolactone)-block-poly(ethylene glycol)-block-poly(ε -caprolactone) was used as the soft segment, a polyurethane with a recordhigh tensile strength and a remarkably increased ductility at the same time was obtained. When the strategy was extended to modify poly (dimethyl siloxane) based polyurethanes, a significant increase in both tensile strength and ductility was simultaneously achieved.

Biography:

Yanbin Fan is currently a Research Scientist and the Adhesive Platform Leader in Asia Pacific Corporate R&D at Dow. His research areas include polymer structure-property relationships, sustainable polymers and smart adhesion systems. Yanbin received his Ph.D. in Polymer Sciences from Fudan University in 2014 and started his industrial career at BASF SE at the same year. He has authored 37 patent applications and 9 research papers. Yanbin is also the recipients of various industrial awards including the 2021 BIG Sustainability Award and 2020 R&D100 Award (Finalist).

Enhanced Expression of the Gene Cluster for Plant-Derived Aromatic Compound Detoxification by Lignin Degradation Products

Eri Kumagawa^{1,2*}, Yukari Ohta²

¹Graduate School of Science and Technology, Gunma University, Gunma, Japan

²Gunma University Center for Food Science and Wellness, Gunma, Japan

Abstract:

Lignin is a natural polymer with many potential applications, useful chemicals, materials, and clean biofuels. Recently, the enzymes with excellent selective conversion ability and biological funneling functions, have shown good possibility in improving utilization. To design a lignin conversion system based on microbial metabolism, it is important to identify genes involved in lignin metabolism and to understand their functions. According to transcriptome analysis using the lignin model dimer (GGGE) of Novosphingobium sp. MBES04, we reported that the gene cluster was specifically upregulated. Even though strain MBES04 does not utilize GGGE as an energy source, the biological advantage of having its metabolic pathway (β -etherase system) was unclear. The goal of this study was to clarify the role of the gene cluster and to understand the significance of the strain MBES04 having the gene for the β -etherase system. This gene cluster is strongly induced by products of the β -etherase system, suggesting that it contributes to the detoxification of compounds containing aromatic and heteroaromatic rings from plant sources. In addition, the growth of the strain MBES04 was enhanced by cluster induction in crude extracts from the Eucalyptus. Therefore, we conclude that the β -etherase system of the strain MBES04

works as a switch for the induction of gene clusters in lignin partial degradation products, and the strain MBES04 adapts and maintains survival in environments with organic compounds of plant derivatives by upregulating clusters.

Biography:

Eri Kumagawa is a PhD student at Gunma University, Japan. Her research focused on the utilization of lignin as an alternative to petroleum derived products. She have previously worked on the search and characterization of the novel enzyme which cleaves the β -ether bond of lignin. She found the thermotolerant and alkaliphilic enzyme, from Altererythrobacter sp. B11. Currently, She is interested in valuable material production using the metabolic capacity of microorganisms and enzymes.

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Oral

Multiple Light Scattering as a Preliminary Tool for Bio-Film Formulation

Catia Giovanna Lopresto^{1*}, Maria Gabriela De Paola¹, Rosy Paletta¹, Vincenza Calabrò¹

¹University of Calabria, Italy

Abstract:

Bioplastics receive constantly increasing attention as interesting alternatives to fossil-derived plastics, due to their renewability and degradability. Among them, edible coatings and films have been focused by a growing amount of research. Starch-based films are a promising alternative to synthetic films in food packaging. Even if their chemical, physical, and mechanical properties were widely studied in the literature, the characteristics of the film-forming dispersions were poorly addressed. Film-forming dispersions influence the formation and quality of films produced. In this work, we propose a method based on multiple light scattering analysis to characterize film-forming dispersions stability by Turbiscan®. The investigation of stability and destabilization phenomena in dispersions can predict good or scarce film formation and quality, and detect possible phase separation before their visibility to the unaided eye. We prepared different starch-based dispersions with the addition of carboxymethyl cellulose or pectins. Then, we analyzed how the addition of additives in such dispersions and the preparation method (with or without sonication) influenced the film formation and quality, in terms of optical and mechanical properties. Therefore, the Turbiscan® can be considered a very useful tool in the choice of the optimal dispersion formulation, even before performing tests on film formation.

Biography:

Catia Giovanna Lopresto completed her Master's Degree in Chemical Engineering at University of Calabria (Italy) in 2011, grade 110/110 and honors, Catia Giovanna Lopresto obtained her first PhD in Mechanical Engineering in 2014, and a second PhD in Life Science and Technology in 2023, both at University of Calabria. During her research activity about bioconversion, extraction and green processes, she worked as a visiting researcher at DTU (Denmark), University of Genova (Italy) and KU Leuven (Belgium). Moreover, she participated to several national and international conferences, she held some academic courses, she co-supervised some degree thesis in Chemical Engineering, she wrote about twenty book chapters and papers in international journals, and she revised several manuscripts in scientific journals.

Crystallographic Texture Evolution in Ultra High Molecular Weight Polyethylene During Uniaxial Tension

Sahitya Movva¹, Reeshemah K. Burrell², Parisa Pooyan^{1,3}, Hamid Garmestani 1,2,4, Karl I. Jacob^{1,3,4}

¹ School of Materials Science and Engineering, Georgia Institute of Technology, Atlanta, G²

Department of Mechanical Engineering, Center for Materials Research & Tech, FAMU-FSU College of Engineering, Tallahassee, FL

³ The George W. Woodruff School of Mechanical Engineering, Georgia Institute of Technology, Atlanta, GA

⁴ Renewable Bioproducts Institute, Georgia Institute of Technology, Atlanta, GA

Abstract:

The crystallographic texture evolution of ultra high molecular weight polyethylene (UHMWPE) subjected to different strains (up to engineering strains of 3.00) under uniaxial tension is presented in this work. A somewhat linear polyethylene with 60% crystalline region and 40% amorphous region has been used in this study. Wide angle X-ray diffraction has been utilized to study the crystallographic texture of the undeformed and deformed UHMWPE samples with the help of pole figures. The texture components of the undeformed and deformed UHMWPE samples have been presented using the orientation distribution functions (ODFs). The texture evolved with the increase in the strain deformation of the samples. Texture components have been observed to change with elongation as well as with ODFs plotted at different rotations. (001)[010] texture component is present in the ODFs of all the samples indicating that this component certainly contributes to the mechanical properties of the samples.

Increasing Polymer Concentration in the Precursor Solutions Systematically Improves the Phase Purity of the Crystalline Oxide Particles in Electrosprayed Films.

Amit Ranjan* and Yogendra Yadawa

Department of Chemical and Biochemical Engineering, Rajiv Gandhi Institute of Petroleum Technology, Jais, Amethi, UP, India

Abstract:

Polymer assisted sol-electrospraying improves the phase-purity of the oxide particles after calcining the deposited films, which was otherwise not possible by electrospinning. Unlike electrospinning, the purity of the rhombohedral zinc titanate particles systematically improved upon adding PVP in the precursor solution and a one-hundred percent pure batch was obtained by sol-electrospraying route at the PVP weight fraction of 31.25%. With an increase in PVP fraction, the crystallite size also decreases. After careful characterization by multiple analytical and spectrospcopic techniques, the explanation offered for this observed trend is that the sol clusters having different atomic arrangements differ in their electrostatic multipole moments. As a result their interaction with the applied electrostatic field are different causing them to undergo spatial separation under the applied field. The clusters with different arrangements in the as-deposited films nucleate into different structures and yield different crystalline phases upon calcination. However in electrospraying mode, PVP polymer chains form cages inside the droplets suppressing separation of the clusters and yielding a homogeneous distribution of sol clusters in the deposited films, and thereby giving a single rhombohedral phase upon calcination. Application of these particles is explored by evaluating their performance as a visible light sensitized photocatalyst, and it is found that they adsorb, reduce, and degrade 4-nitrophenol, and important environmental pollutant, with reaction rates enhanced in presence of light.

Biography:

Amit Ranjan obtained his PhD from the Department of Chemical Engineering and Materials Science at the University of Minnesota, where he worked on the theoretical formulation of self-assembly in diblock copolymer. After working as a post doc at the UNC Chapel Hill and Harvard University, he joined the faculty of Chemical Engineering at the Rajiv Gandhi Institute of Petroleum Technology. His group explores subjects pertaining to the interface of polymer-inorganic materials and one of the current research pursuits in his group is to investigate how polymers can be utilized in improving the photocatalytic behavior of oxide materials.

Bacterial Membrane-Disrupting Mechanism due to Antimicrobial LL-37 Peptide Action

Małgorzata Jurak^{1*}, Agnieszka Ewa Wiącek¹, Katarzyna Pastuszak¹, Bożena Kowalczyk², Jacek Tarasiuk², Marta Palusińska-Szysz²

¹Institute of Chemical Sciences, Maria Curie-Skłodowska University in Lublin, Poland

²Institute of Biological Sciences, Maria Curie-Skłodowska University in Lublin, Poland

Abstract:

The human cathelicidin LL-37 is a cell-permeable antimicrobial host defense peptide. The peptide acts directly on bacteria by disrupting the bacterial membrane integrity via interacting with lipids. Thus, the initial contact of the peptide with the outer leaflet of the membrane is needed. In this study, to mimic the external leaflet of the cell membrane the Langmuir monolayer was used with the addition of LL-37 to the subphase of the Langmuir trough to represent the extracellular fluid. The properties of the model bacterial membranes (Langmuir monolayers) formed by phospholipids isolated from the Legionella bacteria (L. micdadei, L. dumoffii, and L. gormanii) cultured on the medium with or without the addition of choline were determined, along with the effect of antimicrobial LL-37 peptide on the intermolecular interactions, packing, and ordering under the monolayer compression. Our experimental observations indicate that the cationic side chains of the peptide bind to anionic bacterial membranes preferentially. Upon binding, LL-37 can penetrate into the hydrophobic tails of phospholipids, destabilizing the membrane integrity. The above process can entail membrane disruption and ultimately cell death. The LL-37 action depends on the changes in the lipid membrane composition caused by the utilization of exogenous choline by the Legionella species. This finding is relevant for the formation of pharmaceutical therapeutics against antibiotic-resistant bacterial diseases.

Biography:

Małgorzata Jurak is currently an Assistant Professor at the Department of Interfacial Phenomena, Institute of Chemical Sciences, Faculty of Chemistry, Maria Curie-Skłodowska University (MCSU) in Lublin, Poland. She studied the basic and applied chemistry at MCSU and graduated (MSc) in 2004. Then she obtained the DSc degree in 2009 and the habilitated doctor degree in 2019. Her scientific interests include: physicochemical phenomena at interfaces, intermolecular interactions, wetting, surface free energy, surface structure analysis, biomimetic systems, model eukaryotic and prokaryotic membranes, effects of biologically active molecules (polysaccharides, peptides, drugs, antioxidants), polymer-based biomaterials and their biomedical applications.

Multi-Scale Investigation of Morphological, Physical and Tensile Properties of Flax Single Fiber, Yarn and Unidirectional Fabric

Souher Aldroubi^{1,2*}, Bohumil Kasal^{1,2}, Libo Yan^{1,2}, Erik Bachtiar²

¹Technical University of Braunschweig, Germany;

²Fraunhofer Institute for Wood Research Wilhelm-Klauditz-Institut WKI, Germany

Abstract:

In this study, the morphological, physical, and tensile properties of flax were experimentally investigated at three different scales (single fiber, yarn and unidirectional fabric). The cross-sectional area was determined directly using microscopic image and indirectly via linear density with gravimetric and vibroscopic methods. All specimens were tested in tension until failure. The results showed that measured properties and their variability were scale-dependent. The tensile strength and modulus of elasticity were gradually decreasing with the scale and the variabilities were decreasing when going from fibers to yarns and fabric. This difference in the properties should be considered for any multi-scale analysis of the flax reinforcement. The average failure strains of single fiber, yarn and fabric were 2% (±30%), 1.7% (±12%) and 1.7% (±2.8%), respectively. Due to the consistency of failure strain at different material scales, it can be recommended as design criterion. The tensile behavior and the failure mechanisms of single fiber manifest the composite polymeric structure of flax cell wall. The results of this study can be used for better design and preparation of plant-based natural fiber reinforced polymer composites.

Biography:

Souher Aldroubi is a renowned engineer and researcher specializing in natural fiber reinforced polymer composites. As a doctoral candidate nearing dissertation submission, has dedicated five fruitful years to researching the applications of natural fibers in the automotive and construction sectors. The research project focuses on the hydrothermal aging solely and coupled with mechanical stresses of flax-epoxy composites. Flax fiber itself is a growing hierarchical complex polymeric composite. The investigation of flax fibers' durability contributes to their reliable usage in constructions. Aldroubi has actively contributed to conferences, and industry events. Expertise and enthusiasm make Aldroubi eager to participate and share valuable insights at the upcoming Polymers-2023 conference.

Interplay of Matrix Stiffness and Stress Relaxation in Directing Mesenchymal Stem Cells Osteogenic Differentiation

Emilie Prouvé^{1,2,3}, Murielle Rémy¹, Cécile Feuillie¹, Michael Molinari¹, Pascale Chevallier^{2,3}, Bernard Drouin^{2,3}, Gaétan Laroche^{2,3}, and Marie-Christine Durrieu^{1*}

¹Univ. Bordeaux, CNRS, Bordeaux INP, CBMN, UMR, Pessac, France ; ²Laboratoire d'Ingénierie de Surface, Centre de Recherche sur les Matériaux Avancés, Département de Génie des Mines, de la Métallurgie et des Matériaux, Université Laval, Québec G1V 0A6, Canada ; ³Centre de Recherche du Centre Hospitalier Universitaire de Québec, Hôpital St-François d'Assise, Québec G1L 3L5, Canada

Abstract:

The aim of this study is to investigate the impact of poly(acrylamide-co-acrylic acid) hydrogels stiffness and stress relaxation on the osteogenic differentiation of human mesenchymal stem cells (hMSCs). Varying the amount of crosslinker and the ratio between the monomers enabled to obtain hydrogels with controlled mechanical properties, as characterized using unconfined compression and Atomic Force Microscopy (AFM). Subsequently, the surface of the hydrogels has been functionalized with a mimetic peptide of the BMP-2 protein, in order to favor hMSCs osteogenic differentiation. Finally, hMSCs were cultured on the hydrogels with different stiffness and stress relaxation: 15 kPa-15%, 60 kPa-15%, 140 kPa-15%, 100 kPa-30%, and 140 kPa-70%. The cells on hydrogels with stiffnesses from 60 kPa to 140 kPa presented a star-like shape, typical of osteocytes, which has only been reported by our group for two dimensional substrates. Then, the extent of hMSCs differentiation has been evaluated by using immunofluorescence and by quantifying both the expression of osteoblast markers (Runx-2, osteopontin) and osteocyte markers (E11, DMP1, sclerostin). It has been found that a stiffness of 60 kPa led to a higher expression of osteocyte markers as compared to stiffnesses of 15 and 140 kPa. Finally, the strongest expression of osteoblast and osteocyte differentiation markers has been observed for the hydrogel with a high relaxation of 70% and a stiffness of 140 kPa.

Alumina Based Reinforcements for Acrylate Matrix Composite for Dentistry

Radmila Jančić Heinemann^{1*} and Marija M. Vuksanović²

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Abstract:

Dental composite materials need to have specific properties concerning their mechanical properties but also the aesthetic demands. Acrylates have been used for decades in dental applications as they have good biocompatibility and are inert for the patient. Dentures are prepared using the PMMA and the improvement of their properties can be achieved in two ways: by addition of itaconate the conversion of the monomer is improved but mechanical properties are lowered, by addition of ceramic particles the mechanical properties changed. Alumina particles were chosen as they have several modifications that enable the tuning of composite properties.

Alumina particles were prepared using the sol-gel technique and further heat treatment to obtain a chosen crystal structure. Addition of ferrous oxide and choice of calcination temperatures enabled to prepare different crystal structures. It was shown that those structures influence hardness, modulus but also the toughness of the prepared materials and those properties could be optimized. Adhesion properties could also be influenced using those particles.

Adhesion was tested using three different methods – wetting angle measurement, hardness testing and cavitation. All methods were in accordance and gave the insight about the improvement of mechanical properties and adhesion of the composite compared to the matrix.

Medical Textiles in 2023: Key Players to Guarantee Blood Supply Throughout the Body

Robert Guidoin

Department of Surgery, Université Laval and Centre de Recherche du CHU de Québec, Québec, Canada

Abstract:

Medical textiles are fiber-based materials for medical application. They must have a number of properties that make them acceptable: non-toxic, non-carcinogenic, non-allergenic, resistant to bacterial colonization and biocompatible. Medical textiles have a critical role in preserving human life: recent the COVID pandemic highlighted their irreplaceable necessity as the N95 masks protected healthy people from illness by limiting the spread of respiratory droplets. They can be classified as:

1 Implantable: they are designed to be used within the human body for a wide range of restorative uses: blood conduits to restore the blood flow throughout the body, suture wounds, cardiac valves, hernia prostheses, artificial tendons, and artificial ligaments.

2 Textiles for protection in the operating room: they are used for surgical and various medical gowns. A balancing comfort and function in textiles worn by the personnel is recommended. The protection of the patient is the key issue.

3 Extracorporeal devices: artificial kidneys to remove the waste products of the blood, artificial liver to supply fresh plasma, and hollow fiber membrane oxygenators for oxygen supply and carbon dioxide elimination.

4 Scaffolds: support for tissue engineering and regeneration medicine by selecting core-shell hydrogel microfibers or various nanofibers produced by electrospinning.

Medical textiles are located at the interfaces between technical disciplines and life sciences. Depending upon the applications, the manufacturers select fibers types based upon their characteristics. The importance of medical textiles is immense: development of new medical devices in implantology, guarantee of a healthy life in the operating room and outside.

Biography:

Robert Guidoin is professor of surgery (biomaterials) at Laval University, Canada. He is fellow of the International College of Fellows of Biomaterials Science and Engineering, and the American Institute for Medical and Biological Engineering. He has made important contributions in the field of vascular and endovascular grafts, heart valves, mechanical hearts, membrane oxygenators, auditor ossicles, breast implants and intra-uterine devices. He has published more than 300 scientific papers, 24 book chapters, 2 books as co-editor, and has presented his research at numerous meetings worldwide. Robert Guidoin is an internationally leading expert in cardiovascular devices, especially those used for percutaneous techniques.

Biodegradable films: An Alternative for Synthetic Pollution

Claudia Romero*, Gonzalo Velazquez, Silvia Bautista

Instituto Politécnico Nacional, Centro de Desarrollo de Productos Bióticos, Departamento de Desarrollo Tecnológico, Yautepec, Morelos, México

Abstract:

Pollution by synthetic plastics is a serious and growing environmental concern that has motivated the development of biodegradable materials with similar properties while preventing waste disposal problems. Among the renewable biopolymers used as a raw material to obtain biodegradable films, there are polysaccharides, proteins, and lipids, all of them derived from plant or animal sources. Starch is the commonly used agricultural raw material, since it is a renewable source, inexpensive, widely available, and relatively easy to handle. Some non-conventional sources for obtaining starch with better physicochemical and functional characteristics are okenia, banana and mango starches. Also, films can be made from fruit kernel or crustacean exoskeleton. In general, films are water sensitive and present inferior mechanical and barrier properties than synthetic polymers. This weakness could be improved by the preparation of composites with inorganic natural reinforcing materials. Among these fillers, is sodium montmorillonite (MMT). The introduction of fillers to a polymeric matrix increases its strength and stiffness and as a result, water vapor permeability and mechanical properties of films are improved. In my research I have found that the order of aggregation of MMT and glycerol in biopolymers films modify the final film properties because there is a competition for the active sites in the montmorillonite. Another way to decrease the sensitivity of films is by using the hydrophobic nature of essential oils and they also have antimicrobial activity. Research has been conducted testing with bacteria and fungi.

Biography:

Claudia Romero has a food engineering degree, master's degree in food science and a PhD in food technology. She has been director of several projects from my research center and from CYTED. She has written some articles and chapter books. She has supervised bachelor's, master's, and doctorate students. Her research area is in characterization and development of biodegradable films and their application to preserve fruits and vegetables.

The use of Silane Coupling Agents to Anchor Imidazoles to Titanium Dioxide and their Effects on Several Polymer Matrices when used as a Filler.

Javier Vallejo Montesinos^a, Luis Román Rosas Orta^a, Paulina Palafox González^b, Maximiliano Toledo Hernández^a, Veronica Ariadna Pérez Martínez^b, Bernardo Franco^c, Jorge Alejandro Alegría Torres^b, and David Contreras López^d

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Abstract:

In this work, the effect of the side group of a series of silane coupling agents, as well as the subsequent anchoring of an imidazole derivative, for titanium dioxide particles, within several

polymer matrices: polypropylene polylactic acid, and chitosan-starch, with emphasis on their mechanical properties and their crystallization kinetics, and their rate of degradation. For polypropylene differences, the 3-Glicydoxypropyltrimethoxysilane was the best in photostability overall. On the other hand, 3-Chloropropyltrimethoxysilane promoted the degradation. All the other silane coupling agents avoided the anatase's photocatalytic activity, inhibiting the polymer matrix's degradation. Differences were the following: the chlorine group was the best regarding low variability in Young's modulus, good resistance to degradation, and lower values for both activation energy and crystallization enthalpy. The amine, glycidoxy, and Imidazole groups were similar concerning the thermal and viscoelastic behavior.

On the other hand, this work implemented a novel synthetic workflow to generate functionalized particulate and film composites. Chitosan-starch films were analyzed for their water retention capacity, film moisture, mechanical properties, and antimicrobial capacity against Escherichia coli and Bacillus subtilis. It was found that the rutile particles functionalized with 3-aminopropyltrimethoxysilane or imidazole showed antimicrobial activity against both bacteria, both alone and on chitosan-starch films. Also, the rutile-amine particulate composite showed general cell damage in direct contact with a reporter E. coli strain, suggesting the release of ions that produce cell stress.

Biography:

Vallejo has a Ph.D. in Polymer chemistry and is currently a Researcher at Universidad de Guanajuato, specializing in organosilicon polymers, surface modification, physical chemistry, and polymer chemistry with skills and expertise in polysiloxanes, alumina, material characterization, physical chemistry, materials, sulfates, polymers, nanomaterials, GPC, polymer composites, functionalization, polymerization, nanocomposites, composites, polymer nanoscience, nanoparticles, surface properties, nanomaterials synthesis, polyethylene and polypropylene.

Elasto-mechanical Characterization of Liquid Reinforced Soft Solid Composites

Vinu Unnikrishnan^{1*} and Karthik Kundapur²

College of Engineering, West Texas A & M University, Canyon, TX

Abstract:

Soft solid composites with liquid inclusions belong to a group of flexible materials in which a soft solid matrix is reinforced with liquid inclusions. The incorporation of liquid phase, into the soft matrix provides unique characteristics that can differ from those of the individual constituent materials. By controlling the type and volume fraction of the liquid inclusions, the properties of liquid reinforced soft composites can be tailored to the specific needs. In this work, the elastomechanical properties of liquid reinforced soft composites are determined experimentally for various volume fractions of the inclusion phase. In the second part of this work, the experimental data are compared with various micromechanical based theoretical formulations. Such liquid reinforced soft composite materials are advantageous in various applications in soft robotics, flexible electronics, targeted drug delivery systems and biomechanical applications.

Biography:

Vinu Unnikrishnan is an Assistant Professor in Civil Engineering in the College of Engineering, at West Texas A&M University. He earned a Ph.D. in Civil Engineering in 2007 from Texas A&M

University, College Station, and currently holds 4 U.S. patents on biofidelic soft materials, has authored over 45 journal papers, 92 conference publications and 4 book chapters on various topics in mechanics of nano- and bio-materials. He has a strong expertise in applied mechanics, and is a leading expert on development, simulation, and validation of novel concepts in advanced materials systems in Mechanical, Aerospace and Civil Engineering applications.

Do Functionally Graded Cores of Polymeric Layers Improve Impact Resistance?

Romesh C. Batra* and Berkan Alanbay

Presenter* and Co-author names {For Ex: (David Mansom^{1*}, John Smith², Fred Cox³)}

Department of Biomedical Engineering and Mechanics, Virginia Polytechnic Institute and State University, Blacksburg, VA

Abstract:

A functionally graded material (FGM) has material properties continuously varying in one or more spatial directions that eliminates interfaces between different materials and hence likely stress singularities. A structure comprised of an FGM is expected to provide improved performance, e.g. higher failure load, than an identically shaped structure of either a homogeneous or lavered material. Here we study the response of a sandwich structure comprised of thin fiber-reinforced polymeric face sheets and the core composed of eight layers of polymeric foam. Three arrangements of core layers, namely, the mass density of the core layers increasing from the lowest to the highest, the highest to the lowest and the an optimized one. The optimization algorithm finds the thicknesses of the two face sheets and the eight core layers as well as the lay-up of the eight layers. It minimizes the total mass of the structure and either the back face deflection or the total reaction force transmitted by the sandwich structure to the rigid substrate perfectly bonded to it. In each case the sandwich structure has the same initial, boundary and loading conditions. It is found that the optimum lay-up of the core layers depends upon the quantity to be minimized, and does not correspond to the mass density varying from the lowest to the highest. Whereas large thick layers of low density foams minimize the total reaction force, high density thick foam layers provide the least back face deflection.

Biography:

Romesh Batra is University Distinguished Professor and Clifton C. Garvin Professor at Virginia Polytechnic Institute and State University. His team's work, published in > 470 refereed journal articles, has been widely recognized by his peers through > 17,600 citations on Scopus with H = 68, and the following honors: USACM 2019 Belytschko Medal, 2016 ASME Robert Henry Thurston Lecture Award, 2015 ASME Honorary Membership, 2009 Engineering Science Medal, an Honorary D.Sc. from Thapar University in 2006, and Alexander von Humboldt Award for senior scientists (1992). He is a Fellow of the USACM, AAM, SES, ASME, and the ASEE.

Donor-Acceptor Polymer Nanoparticles for Mitigating Bacterial Infections

Nicole Levi,^{1*} Santu Sarkar,1 Erica Vargas,¹ Bradley Burden^{,1} and Shaina Yates¹

¹Department of Plastic and Reconstructive Surgery, Wake Forest University School of Medicine, North Carolina

Abstract:

Application of localized heat for mitigating bacterial biofilms offers a new avenue to eliminate challenging medical infections, especially those that are resistant to antibiotics. This report describes polymer nanoparticles comprised of Poly[4,4-bis(2-ethylhexyl)-cyclopenta[2,1-b;3,4-b'] dithiophene-2,6-diyl-alt-2,1,3-benzoselenadiazole-4,7-diyl] (PCPDTBSe) for photothermal ablation (PTA) of Staphylococcus aureus (SA). Nanoparticles had a size of 65-130nm. The minimum inhibitory concentration (MIC) of the nanoparticles determined the appropriate working concentration to be 50µg/mL. PTA was performed, using a 5W, 800nm infrared laser for 60s to generate temperatures in excess of 70oC. The log reduction of S. aureus was quantified using fluorescence assays and colony forming unit (CFUs), demonstrating greater than 3 log reduction of viable bacteria, which is the crucial threshold for for clinical relevance. Following successful eradication of SA using PCPDTBSe nanoparticles, the particles were blended into silicone elastomer to create a photothermal nanocomposite capable of eliminating SA biofilms, both in vitro and in vivo. Stimulation of silicone alone with 612 J/cm2 of 800nm light had no effect on planktonic or biofilm SA, whereas ablative temperatures resulted in a 95-100% reduction in viable bacteria. Sub-ablative temperatures resulted in a 75% reduction in planktonic bacteria treated with gentamicin and a 90% reduction in biofilm-residing SA, compared to controls treated with gentamicin alone and no infrared stimulation. Depending upon the laser parameters used (1.2-3W/ cm2 for 10-45s) there was a reduction of 33-94% CFUs following treatment with the heat-generating nanocomposite plus antibiotics. Our results demonstrate the potential for heatgenerating biocompatible nanocomposites to augment antibiotics used to treat S. aureus biofilms.

Biography:

Nicole Levi, Ph.D., is an Associate Professor and Director of Materials Research Innovation and Development in the Department of Plastic and Reconstructive Surgery at Wake Forest University School of Medicine. She has training in Physics and Biomedical Engineering, with specific expertise in the field of nanotechnology. One facet of her research involves the synthesis of nanoparticles composed of donor-acceptor conjugated polymers that can both fluoresce, and be optically-stimulated to generate heat. Dr. Levi has demonstrated that these novel nanoparticles have high photothermal conversion efficiency and are useful for treatment of both cancer and bacterial infections.

A 3D Hydrogel Droplet Array for Quantifying Proteins from Minimal Amount of Cells

Huiyan Li*

University of Guelph, Canada

Abstract:

Protein quantification in intact cells can provide important information on cellular activities. Immunocytochemistry has been widely used for protein detection from intact cells, but the assay is semi-quantitative, and requires a relatively large amount of cells which is not always available. Flow cytometry is another common method for cellular protein detection. The assay is quantitative, but signal acquisition requires a flow cytometer that suffers from potential clogging and compromised data quality due to cell debris and clumps. Also, a flow cytometric assay typically needs hundreds of thousands to millions of cells and cannot be used for imaging of cellular proteins. In this work, we have developed a highly sensitive and simple-to-implement platform for simultaneous protein imaging and quantification from a small number of intact cells. We characterized the 3D structure of the cell-containing alginate hydrogel droplets immobilized on a glass slide using a confocal microscope. The images showed that the average height of the droplets were approximately 300 microns, with a diameter of approximately 1500 microns. Further, we compared the size and concentration of the gold nanoparticles for optimal metal enhanced fluorescence, and found that smaller sizes of gold nanoparticles provided higher fluorescent signals. Using EpCAM protein, we determined the minimum number of cells required. With as low as 625 cells per spot, we were able to detect the protein with significant difference from the IgG control. This required cell number was 8-fold lower than that needed for conventional immunocytochemistry.

Biography:

Huiyan Li obtained her B.Eng from Harbin Institute of Technology, China. She then moved to Canada and completed her M.A.Sc at the University of Victoria. She received her PhD in Biomedical Engineering at McGill University. After a postdoc training in UVic-Genome BC Proteomics Center, Dr. Li joined the Biomedical Engineering group as a research fellow at Harvard Medical School – Massachusetts General Hospital. In 2020, Dr. Li joined the University of Guelph and started her research lab. Her research focuses on developing micro- and nano technologies for the study of health and diseases. Her work has been published in top peer-reviewed journals and has been highlighted in major scientific magazines.

Characteristics of Hybrid Bioactive Coatings on the Plasma Activated Polye there there are a constrained on the plasma and t

Agnieszka Ewa Wiącek^{1*}, Kacper Przykaza², Małgorzata Jurak¹

¹Faculty of Chemistry, Maria Curie-Skłodowska University, Lublin, Poland; 2 Biomedical Faculty, Medical University of Lublin, Poland

Abstract:

PEEK (polyetheretherketone) is a biocompatible, physicochemically stable polymer with a modulus of elasticity similar to that of human bone. Thanks to that it is an attractive material for orthopedic implants. However, PEEK is also biologically inert, so sufficient bonding to the surrounding bone tissue during implantation may not be possible. The two main strategies are helpful to get around this problem and improve the PEEK bioactivity, e.g. surface modification and composite preparation. Air plasma-activated PEEK surfaces with deposited layers of bioglass, chitosan and mixed were investigated. The surfaces resulted by immersion/hybrid method for wettability/surface free energy changes were tested. In addition, FTIR (Fourier transform infrared spectrometry), SIMS (Secondary ion mass spectrometry) and SEM (Scanning electron microscopy) methods were used to determine, control and visualized the composition of the coatings. Additionally, the tested systems were incubated in SBF (Simulated body fluid) to verification of the impact of modifications on the bioactivity/biocompatibility of the PEEK surface. During surface preparation by impregnation with bioactive materials, the main challenge is to maintain the excellent mechanical properties of PEEK, hence all modifications concerned only its top layer. Developing a PEEK surface coated with bioactive layers could provide an effective way to achieve both mechanical and biological benefits.

Biography:

Agnieszka Ewa Wiącek studied chemistry at Maria Curie-Skłodowska University and was employed in the Department of Physical Chemistry. She received D. Sc. degree in chemistry in 2000 and Dr. habilitation degree in physical chemistry in 2013 writing dissertation titled "Effect of the selected biologically-active substances, mainly phospholipids and (phospho)lipases on the interfacial properties of dispersed systems". She has published about 90 research articles which were cited according to Google Scholar more than 1600 times. Additionally she is author/co-author of 100 conference' articles. She is promoter of master of science and licentiate thesis (more than 50) and 2 doctoral thesis. She participated in 6 scientific projects. In 2018 she obtained the position of an Associate Professor at MCSU.

Non-Covalent Protein Polymers are Involved in Inheritance, Disease and Memory

Yury O. Chernoff*

Georgia Institute of Technology, USA

Abstract:

Transmissible protein isoforms (prions) cause human and animal diseases, and control heritable traits in yeast and other fungi. Most prions non-covalent fibrous polymers (amyloids), composed of identical protein molecules that are linked via intermolecular cross-beta structures. Pre-existing prion directs formation and location of beta-structures in the newly immobilized molecule, thus manifesting itself as a structural template. Therefore, prions transmit structural protein changes that are not encoded in DNA sequence. This molecular mechanism is also involved in human pathologies such as Alzheimer's disease, making yeast prions a useful model for studying molecular foundations of amyloid diseases. Some prion proteins also form biomolecular condensates via liquid-liquid phase separation. These condensates are reminiscent of hypothesized early forms of life, and can sometimes convert into solid fibrous amyloids. The process of prion formation and propagation is regulated by chaperone proteins, that control protein folding and are involved in defense again proteotoxic stresses. Chaperone-mediated fragmentation of prion polymers generates oligomers, that immobilize new protein molecules and convert them into a prion form. Thus, prions employ the cellular stress defense machinery for their own replication. Environmental and physiological conditions modulate prion formation via influencing the chaperone machinery. Metastable prions manifest themselves as carriers of the molecular memory of stress. Deciphering of the enzymatic machinery of prion formation and propagation is important for both counteracting amyloid diseases and understanding the role of protein-based inheritance in adaptation to environmental conditions. (Supported by grants 1817976 from NSF and RF1AG079256 from NIH.)

Biography:

Yury Chernoff is a geneticist and molecular biologist, studying protein aggregation, yeast models for amyloids and prions, and protein-based inheritance. He has discovered the prion induction by protein overproduction and the crucial role of chaperones in prion propagation. Dr. Chernoff has graduated from St. Petersburg State University, Russia, performed postdoctoral research at Okayama University, Japan, and University of Illinois, Chicago, USA, and joined Georgia Institute of Technology, Atlanta, USA in 1995 (currently a full Professor). He serves as Editor-in-Chief of the journal Prion, and is a Fellow of the American Association for the Advancement of Science.

Materials for Chiral Polymer Photonics: Design, Development, and Modulation Strategies for Chiroptical Properties

Jojo P. Joseph¹, Shema R. Abraham², Avisek Dutta¹, Alexander Baev¹, Mark T. Swihar^{t2}and Paras N. Prasad^{1*}

¹Institute of Lasers Photonics and Biophotonics and Department of Chemistry, State University of New York at Buffalo, United States; ² Department of Chemical and Biological Engineering, State University of New York at Buffalo

Abstract:

Chiral photonics is an actively developing/emerging area of photonics that encompasses enantioselective polarization control of linear and nonlinear optical functions and holds great potential in optical signal processing, sensing, and imaging. Advancing the emerging area of chiral photonics demands new chiral material design and amplification strategies to enhance optical activity and associated optical rotatory dispersion. Herein, we developed a series of chiral fluorenebased polymers copolymerized with varying thiophene comonomer PF8TS-PF8TTTS where the varying number of conjugation units within the monomer building block shows specific influence on the resulting trend of chiroptical activity. Our design concept delineates an underexamined approach: the concept of tuning backbone conjugation and helicity within the main chain to enhance the optical activity of chiral polymer systems. In advance, we demonstrate versatile strategies to further enhance chiroptical properties in the poly-fluorene-thiophene system via supramolecular softener (PEM-OH) additive and in-situ plasmonic doping. Finally, spatiotemporal control over chiroptical properties via in-situ photopolymerization in chiral peptide based diacetylene system is demonstrated. In addition, selective chiral based plasmonic enhancement in chiroptical properties is demonstrated in this system over photopolymerization via chiral plasmonic doping. Thus precise approaches to utilize chirality in enantiopure conjugated polymers are exhibited which are anticipated to be significant for a wide range of applications in chiral photonics, metaphotonics, and optoelectronics.

Biography:

Jojo Paruvaparampil Joseph earned his undergraduate and master's degrees in pharmacy from Kerala University, India. He attended Institute of Nanoscience and Technology, Mohali, India for his Ph.D. in Polymer Chemistry and Nanoscience where he worked with Prof. Asish Pal to develop acrylate polymers and amyloid based peptides for biomimetic applications. He is currently A Postdoctoral researcher with Prof. Paras N. Prasad in the Department of Chemistry at State University of New York at Buffalo. His current work focuses on the design and development of chiroptical polymeric materials for photonics applications. He authored several research articles in reputed international journals.

Functional Biomaterials for Applications in Environmental Remediation

Priyanka Sharma

Assistant Professor ,Department of Chemical and Paper Engineering WESTERN MICHIGAN UNIVERSITY,Floyd Hall,

1 Campus Dr., Kalamazoo, Michigan

Abstract:

There is a vast amount of underutilized biomass sources in our community. For example, millions of tons of wood waste are generated annually from tree and brush trimming and natural disasters. The conventional process is to treat this waste by processing it into compost and mulch or dispose of it in non-sustainable ways that are damaging to the environment by contaminating the groundwater and GHG emissions. In this talk, I will showcase my developed Nitro-oxidation process from an idea to a scaleup process and the pros/challenges of using this process to upcycle such biomass waste. Additionally, I will show my future research plan on developing sustainable chemical ways to upcycle unutilized plant biomass, including agricultural residues, into valuable products such as plant-based hydrogels and sponges to tackle the food-water nexus issues and to promote the circular economy.

Effect of Co-Grinding on the Dissolution Behavior of Urapidil, Which Forms a Pentahydrate During Dissolution, and the Water-Soluble Polymer HPC-SSL

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Faculty of Pharmaceutical Sciences, Tokyo University of Science, 2641 Yamazaki, Noda, Chiba, Japan

Abstract:

Co-milling with water-soluble polymers is known as one of the methods to improve the solubility of poorly water-soluble pharmaceuticals.

Recently, hydroxypropyl cellulose grade "SSL" (HPC-SSL), a low molecular weight water-soluble polymer, has been developed. However, its application to co-milling has rarely been investigated.

In the present study, we focused on this HPC-SSL and used the adrenergic α 1-receptor antagonist urapidil (UPD) as a model for drugs that form hydrates when dissolved, and performed co-milling in a ball mill. When a physical mixture was prepared by adding HPC-SSL to UPD in a mortar and then co-milling it with a ball mill, it was found that the UPD became amorphous and formed a solid dispersion. In addition, no recrystallization of UPD was observed during the dissolution process in the dissolution test, indicating that the UPD was effective in inhibiting agglomeration. In the co-milling with 50% (w/w%) UPD and 50% HPC-SSL, no improvement in dissolution rate was observed, but the sample with 40% UPD and 60% HPC-SSL showed an increase in dissolution rate.

Biography:

Hanawa has been engaged in research and education as a professor in the Faculty of Pharmaceutical Sciences at Tokyo University of Science since 2012. His research area of expertise is formulation engineering, and he is using this expertise to study methodologies for the nanoparticulation of poorly water-soluble pharmaceuticals using a simple method of pulverization. In recent years, he has also focused on hydrogel formulations to develop semi-solid formulations for wound healing.

Artificial Biomembrane Models using Giant Vesicles of Amphiphilic Diblock Copolymers

Eri Yoshida*

Department of Applied Chemistry and Life Science, Toyohashi University of Technology, Japan

Abstract:

Artificial models of biomembranes using synthetic polymer vesicles help better understand the biomembrane based on their similarities in structure, morphology, and stimuli-responsive behavior. This study investigated the fabrication of dynamic morphologies of the biomembranes using giant polymer vesicles to elucidate the intrinsic membrane properties from polymer science and engineering aspects.

Poly(methacrylic acid)-block-poly(n-butyl methacrylate-random-methacrylic acid), PMA-b-P(BMA-r-MA), underwent a human erythrocyte-like morphology transformation in response to temperature changes. The copolymer produced spherocyte-like spherical vesicles with a dimple by the photopolymerization-induced self-assembly in a 70% aqueous methanol solution. The vesicles transformed into echinocyte-like crenate vesicles when heated in the solution. Increased vesicle concentration transformed the dimpled spherical vesicles into stomatocyte-like cup-shaped vesicles. Light scattering studies revealed that the transformations were reversible and repeatable, as are the erythrocytes. The transformation was also dependent on the methanol content in the solution. A 60% methanol content solution increased the number of discocyte-like and knizocyte-like vesicles among the stomatocyte-like vesicles. A decrease in the methanol content to 50% slightly produced stomato II-acanthocyte-like and torocyte-like vesicles. A lower content below 40% prevented the vesicles from transforming even at 50°C. These findings promote a better understanding of the intrinsic properties of the erythrocyte membrane on a molecular basis.

An artificial model for the neurite extension of neurons will also be reported.

Biography:

Eri Yoshida received her Ph.D. from the Tokyo Institute of Technology, Japan. After her Ph.D. completion, she joined the Kyoto Institute of Technology as an Assistant Professor. She is an Associate Professor at the Toyohashi University of Technology. She was also a visiting scientist at the University of North Carolina at Chapel Hill and a faculty-exchange program member of the City University of New York, Queens College. Her research focuses on polymer designing using nitroxide-mediated controlled/living radical polymerization and CO2 capture technologies. She has been serving as an editorial board member of several international journals.

Charge Transport and Thermoelectric Properties in Electrochemically Doped Conducting Polymers

Hisaaki Tanaka^{1*}

¹Department of Applies Physics, Nagoya University, Japan

Abstract:

Conducting polymers have been attracting much interest in terms of both scientific and technological viewpoints. Owing to the highly sophisticated material designs, various new high-mobility polymers

have been synthesized with the transistor mobility approaching, or even exceeding, 1 cm2/Vs. Carrier doping on such state-of-the-art polymers can thus cultivate various new applications such as wearable thermoelectric generators. However, charge transport mechanisms in these polymers have not been fully understood yet, especially in their doped states, due to the highly complicated film structure consisting of both crystalline domains and domain boundaries.

In the present talk, we introduce our recent studies on the charge transport and thermoelectric properties of electrochemically-doped semicrystalline polymers [1]. We adopt an electrolyte gating method to sensitively control the doping level up to high concentration regions by applying external gate voltages. We observed that a typical semicrystalline polymer PBTTT underwent a macroscopic metal-like transition upon doping, associated with a peak of the thermoelectric power factor, consistent with the recent theoretical studies. From the magnetoconductance measurements, we found some localization effects, such as weak localization occurring within the crystalline domains and variable-range hopping occurring at the domain boundaries, as the temperature was lowered [2]. The structural optimization by DFT calculations revealed that the planarity of the polymer backbone was improved by the doping, promoting the inter-domain charge transport, which should be a key to realize macroscopic metal-like charge transport in semicrystalline polymers.

We will also introduce our recent study on a less-crystalline donor-acceptor-type polymer, which has highly-planar backbone structure [3].

Design of Phase Separating Peptide and Peptide-Based Regulation of Phase Separation of Drug-Target Disordered Proteins

Kiyoto Kamagata*

Institute of Multidisciplinary Research for Advanced Materials, Tohoku University, Japan

Abstract:

Artificial phase-separating (PS) peptides can be used in various applications such as microreactors and drug delivery; however, the design of artificial PS peptides remains a challenge. This can be attributed to the limitation of PS-relevant residues that drive phase separation by interactions of their pairs in short peptides and the difficulty in the design involving interaction with target PS proteins. Recently, we proposed a rational method to design artificial PS peptides that satisfy the requirements of liquid droplet formation and co-phase separation with target PS proteins based on the target PS protein sequence (Sci. Rep. 2023). As a proof of concept, we designed artificial PS peptides from a model PS protein p53, and tested their phase separation and target-recruiting capabilities experimentally. Our results highlight the designability of the artificial PS peptide droplets.

Intrinsically disordered regions (IDRs) of proteins are involved in many diseases. However, the flexible IDRs hinder the use of 3D structure-based drug design methods. Liquid droplets of aggregation-prone proteins with IDRs, which become hydrogels or form amyloid fibrils, are a potential target for drug discovery. In this presentation, I will introduce a rational design method to obtain a peptide that can bind an IDR using only protein sequence information (Sci. Rep. 2019; 2021; 2022). We applied the method to the disordered disordered domains of a tumor suppressor p53 and demonstrated the regulation of liquid droplet formation and DNA-binding function. The sequence-based design may be useful in targeting IDRs for therapeutic purposes.

Biography:

Kiyoto Kamagata is a biophysicist. He developed single-molecule fluorescence microscopy and related technologies, and are studying the dynamic physical properties and functions of DNA-protein complex systems. Recently, he has started full-scale research on liquid-liquid phase separation of proteins and the design of molecules that control their functions. The latter is basic drug discovery research targeting naturally denatured proteins that do not have a specific three-dimensional structure. In particular, we are focusing on developing original technologies for "measurement", "control & regulation", and "design".

Alkyl Vinyl Imidazolium Polymers as Fuel-Binders for Photo-Curable Energetic Propellants

Yuval Zertal¹, Matthew Yong¹, Avishai Levi¹, Sagi Sevilia¹, Mauricio Dantus¹, Alex Tsoglin², Galit Parvari¹, Levi Gottlieb², Yoav Eichen^{1*}

¹Schulich Faculty of Chemistry Technion – Israel Institute of Technology Technion City, Haifa 3200008, Israel

²RAFAEL, Advanced Defense Systems LTD, POB 2250 Haifa, Israel

Abstract:

Polymers, made of energetic ionic liquid building blocks, are used as the fuel-binder components in propellant compositions. These compositions exhibit desired mechanical and energetic properties and may serve as photoactive feed for 3D printable propellants. Quaternary vinyl imidazolium perchlorate and nitrate energetic salts are used as monomers in fuel-binder polymers, while ammonium perchlorate is used as the heterogenous oxidizer in the composition. The vinyl groups on the heterocyclic cations provide covalent interconnecting sites for the construction of the polymer backbone and binding sites for in-chain plasticizers, enabling control over mechanical and initiation sensitivity properties in the cured composite product. The advantageous oxygen balance, OB, and heat of formation values of these ionic liquid monomers, along with their ability to photopolymerize, allows both the effective dispersion, and reduced ratios of the heterogeneous oxidizer content without compromising the energetic properties of the resultant propellant. Branching of the alkyl chains was shown to rule combustion properties of the finished propellants, allowing control of the way the propellant burns, simply by varying the ratio of different alkyl chains on the imidazolium skeleton. Pressure-independent burn-rates were achieved in compositions containing 2- ethoxyethyl acrylate plasticizer, thus avoiding the need for additional additives, stratification, and geometrical constraints on the burning bulk.

Antibacterial Activity of Arundinariinae Microfibre Reinforced Polyvinyl Alcohol

Che Wan Sharifah Robiah Mohamad

Universiti Malaysia Perlis, Malaysia

Abstract: Not Available

Review: Trends and Challenges of Biodegradable Plastics for Food Contact Applications

Namasivayam Navaranjan^{1*}, Prashad Navaranjan², Hamta Majd³, Mohan Edirisinghe³

¹Universiti Teknologi Brunei, Brunei Darussalam;

²University of Wollongong, Australia;

³University College London, UK *Email: nava.navaranjan@utb.edu.bn

Abstract:

Global plastic packaging market was USD 369.2 Billion in 2022 and forecasted to reach USD 492.3 Billion in 2030. Food and beverage packaging shared 51% of the market in 2022. The current trend in using environmentally friendly and single-use food packaging promotes an increase in the market of biodegradable packaging that has been forecast to reach to USD 9.13 billion by 2030. Polylactic acid (PLA), polyhydroxyalkanoates (PHA) and some starch-based polymers draw more attention as biodegradable plastics for food contact applications. Fossil-based biodegradable plastics such as polybutylene adipate terephthalate (PBAT) and polycaprolactone (PCL) are not cost effective to use for food packaging.

PLA has sufficient strength, transparency, and good barrier properties like fossil-based polyethylene (PE) and polyethylene terephthalate (PET). It has high density and low glass transition temperature, but costlier when comparing to PE and PET. PHA and starch polymers have inadequate strength and barrier properties.

Global legislation and regulation have provided guidance for selection and use of biodegradable polymers for food contact. Most importantly, polymers should not migrate any harmful substances to food and modify food composition. The contact polymers should have adequate mechanical, physical and barrier properties. They should not biodegrade during the supply chain of a food in contact from manufacturing to consumption. Most food manufacturers are reluctant to use expensive packaging and pass the increased cost to their customers. Therefore, careful tailoring of the manufacturing process and the development of new food packaging forming processes play a vital role.

Biography:

Navaranjan is currently the Dean School of Applied Sciences and Mathematics, Universiti Teknologi Brunei, and has over 30 years of academic, research and commercial experience. His major involvement was in food contact materials, and bio-based and hybrid materials for engineering and food packaging applications. He published over 35 refereed journal and conference papers and submitted over 50 scientific reports to government, clients and stakeholders. He involved as a team member and individual to obtain research grants nearly USD 50 million during his previous job in New Zealand. He also received a few prestigious awards.

Synergistically Enhancing Photore duction of $\mathrm{CO}_{_2}$ on CdS Quantum Dots Stabilized by Amphiphilic Metallopolymer

Wissuta Boonta¹, Waraporn Panchan², Kittipong Chainok³, Patchanita Thamyongkit¹, Teera Butburee⁴, and Junjuda Unruangsri^{*1}

¹Department of Chemistry, Faculty of Science, Chulalongkorn University, Thailand;

²National Metal and Materials Technology Center (MTEC), Thailand;

³Thammasat University Research Unit in Multifunctional Crystalline Materials and Applications (TU-MCMA), Thammasat University, Thailand;

⁴National Nanotechnology Center (NANOTEC), Thailand.

Abstract:

CdS quantum dots (QDs), acting as photosensitizers, or sometimes solo photocatalysts in CO2 reduction (CO2R), have offered a myriad of advantages including quantum confinement effect, surface functionalization, tunable redox potential, and photoreduction selectivity. However, CdS QDs are frequently compromised by thermal and oxidative instability, as well as photocorrosion, which restricts their practical applications. We propose an effective method endowing CdS QDs by assembling with amphiphilic metallopolymer (Re-IL) to enhance their stability and synergistic activity. Electrostatic interaction facilitated the spontaneous self-assembly of Re-IL onto thioglycolic acid-capped cadmium sulfide quantum dots (TGA-CdS QDs) facilitating photo-induced electron transfer (PET) from TGA-CdS QDs to vicinal bipyridyl Rel(CO)3CI derivatives in water and a mixture of DMF/water. All hybrid catalysts (Re-IL/TGA-CdS QDs) demonstrated synergistically boosting photocatalytic CO2 reduction to yield CO with over 90% selectivity in 25 mL DMF/water (4:1 v/v), under LED 370 nm irradiation. For example, CdS/P(5% Re-IL) was the optimum catalyst in our system showing the highest CO production rate of 38.3 mmol g-1 h-1 and selectivity of 93.8% within the first 2 h with no induction period, which is ranked among the top state-of-the-art CO2R photocatalysts in mixed organic-water media.

Biography:

Junjuda Unruangsri received her M.Chem degree in Chemistry in 2010, and DPhil in Inorganic Chemistry from the University of Oxford in 2015 under the supervision of Prof. Philip Mountford. After graduation, she joined the research group of Prof. Charlotte K. Williams at Imperial College London in 2015-2016. After, she came back to Thailand and joined the Department of Chemistry, Chulalongkorn University in 2016, where she is now an assistant professor. Her research interests include organometallics, polymer synthesis, catalytic materials, and green catalysis.

Poster Presentation

Sustained Administration of Chitosan-Tripolyphosphate-DNA Nanoparticles Expressing Fish Codon-Optimized Caenorhabditis Elegans FAT-1 Increase Omega3 Fatty Acid Production in the Liver of Gilthead Seabream (Sparus Aurata)

Yuanbing Wu^{1*}, Ania Rashidpour¹, Anna Fàbregas², María Pilar Almajano³, Isidoro Metón¹

¹ Secció de Bioquímica i Biologia Molecular, Departament de Bioquímica i Fisiologia, Facultat de Farmàcia i Ciències de l'Alimentació, Universitat de Barcelona, Spain;

² Mimark Diagnostics S.L., Spain;

ABSTRACT BOOK

³ Departament d'Enginyeria Química, Universitat Politècnica de Catalunya, Spain

Abstract:

Eicosapentaenoic acid (20:5n-3, EPA) and docosahexaenoic acid (22:6n-3, DHA) are long-chain polyunsaturated fatty acids (LC-PUFA) that belong to the omega-3 family, and which have numerous health benefits, including prevention of atherosclerosis, stroke, obesity, type-2 diabetes, inflammation, and autoimmune disease. Marine fish and shellfish are major sources of n-3 LC-PUFA in the human diet and acquire pre-formed LC-PUFA by trophic transfer. However, substitution of fish oil with vegetable oils in aquafeeds is currently reducing the n-3 LC-PUFA content in cultured fish, while increasing proinflammatory n-6 fatty acids. To induce sustained production of n-3 LC-PUFA in cultured fish, chitosan-tripolyphosphate (TPP) nanoparticles encapsulating plasmids expressing fish codon-optimized Caenorhabditis elegans FAT-1 desaturase were obtained by ionic gelation and intraperitoneally administered to gilthead seabream (Sparus aurata) every 4 weeks (3 doses in total). After 70 days of treatment, real-time guantitative RT-PCR assays showed that nanoparticle administration significantly increased the expression of the exogenous enzyme (FAT-1) in the liver. Fatty acid methyl esters assay revealed that FAT-1 expression significantly increased the hepatic production of EPA, DHA, and total n-3 LC-PUFA, while reduced the n-6/n-3 ratio. In conclusion, besides being an alternative methodology that does not involve obtention of genetically-modified organisms, the present study shows that chitosan-TPP-DNA nanoparticles are efficient to enable sustained expression of fish codon-optimized C. elegans FAT-1 and produce cultured fish rich in n-3 LCPUFA.

Biography:

Yuanbing Wu has completed his PhD degree in April 2023 and he is currently performing a postdoctoral stay at the University of Barcelona (Spain). His main research interests are focused on application of polymer nanoparticles to aquaculture, and unraveling fish intermediary metabolism with emphasis on the production of omega-3 long-chain polyunsaturated fatty acids.

Plenary

Polymeric Biomaterials for Biomolecule Delivery and Tissue Regeneration

Peter X Ma

University of Michigan, Ann Arbor, MI

Abstract: Not Available

Conjugated Polymers and Carbon Macromolecules for Clean Energy and Environmental Remediation

Liming Dai

University of New South Wales, Australia

Abstract: Not Available

Keynote

Zeolite-based Nitric Oxide Delivery Platforms for Treatment of wound Infections by Drug-Resistant Bacteria

Pradip Mascharak

Department of Chemistry and Biochemistry, University of California, Santa Cruz, CA

Abstract:

Emergence of multi-drug resistant bacteria has raised serious concern in hospitals around the globe. These stubborn pathogens have recently shown to undergo cell death upon exposure to nitric oxide (NO). We have recently reported a water-soluble photoactive metal-nitrosyl complex that could be incorporated in a variety of polymer platforms that could thwart chronic infections by both Gram-positive and negative bacteria. The antibiotic (NO) delivery can be conveniently controlled by exposure to visible light of low-intensity. Rapid diminution of bacterial loads by two such NO delivery platforms will be presented in this talk.

Biography:

Pradip K. Mascharak received his Ph. D. from the Indian Institute of Technology, Kanpur. He did his post-doctoral research work at Stanford, Harvard, and Massachusetts Institute of Technology before joining the University of California, Santa Cruz in late 1984. He is currently a Distinguished Professor of Chemistry and Biochemistry at UCSC. His major focus of research includes (a) modeling of active sites of metalloenzymes, (b) catalysts for "Green Chemistry" and (c) syntheses of photoactive NO- and CO-donating drugs for chemotherapy of infection and malignancies. His research is supported by the National Science Foundation and the National Institute of Health.

Polycarbolong Chemistry: Main-Chain Metals-Containing Conjugated Polymers

Shiyan Chen, Dafa Chen, Haiping Xia*

Shenzhen Grubbs Institute and Department of Chemistry, Southern University of Science and Technology, Shenzhen, China.

Abstract:

The inclusion of transition metals with d orbitals into the skeletons of conjugated polymers results in $d\pi$ -p π conjugated polymer systems, which may exhibit intriguing properties and applications. In 2020, we reported a new addition reaction of alkynes and metal carbynes. Subsequently, this efficient reaction was developed as a new polymerization reaction that leads to the main-chain metals-containing conjugated polymers, also called polycarbolongs. Recently, a double-monomer polymerization methodology was developed. This synthetic strategy enjoys the advantages of flexible selection of spacers, short synthetic procedures, good functional-group tolerance and high efficiency. The facile route can not only enrich the polymer structures but also tune the polymer properties, thereby broadening their application scopes. These metallopolymers could open up significant opportunities for preparation of functional materials.

Biography:

Haiping XIA obtained his B.S. in Chemistry in 1983, M.S. in Polymer Science in 1986, and Ph.D. in Chemistry in 2002, all from Xiamen University, where he was promoted as a Full Professor in 1999. In 2018, he moved to Southern University of Science and Technology as a Chair Professor, and has been appointed as the Executive Dean of Shenzhen Grubbs Institute since 2019. He has won many awards, such as the "Chinese Chemical Society Huang Yao-Zeng Award in Organometallic Chemistry", and the second prize of "the National Natural Science Award" of China in 2020.

Research Progress and Industrialization in Polymer Materials of SINOPEC

Yang Ling

SINOPEC Tech Houston LLC, Houston, TX

Abstract: Not Available

Directed Assembly of Functional Polymer Films for Energy and Sustainability

Alamgir Karim^{*}, Maninderjeet Singh, Kshitij Sharma

William A. Brookshire Department of Chemical and Biomolecular Engineering, University of Houston, TX

Abstract:

Our research is focused on developing polymer films for functional applications in the energy and sustainability space. To this end we have developed nanostructured polymer and block copolymer films for multiple applications for energy storage and in the separations of immiscible liquids, nanoparticles, and biomolecules. We show that the dielectric strength of glassy and entangled polymer films increases sharply as an inverse power-law of the film thickness h for "ultrathin" films below a micron in thickness. The dielectric strength enhancement in these polymer films can reach values as large as ≈ 2 GV/m in films thinner than 100 nm, but this large "finite-size" effect depends strongly on the polymer mass and sample aging time. Likewise, directed assembly to obtain parallel morphology of block copolymer was used for dielectric energy storage applications. In contrast, vertical morphology of cylinder and lamellae forming block copolymer films, whose selective domains were etched for separations applications. Oil-water mixtures were separated with high efficiency due to capillary wettability effects, nanoparticles and biomolecules based on shape, aspect ratio and chemical interactions.

Biography:

Alamgir Karim is Dow Chair Professor and Director of the Materials Engineering Program. He obtained his PhD in Physics from Northwestern University with a post-doctoral in Chemical Engineering at University of Minnesota. He is Fellows of American Physical Society, American Association for the Advancement of Science, and Neutron Scattering Society of America. His areas of interest and research include polymer thin films, surfaces and interfaces. He has published over 220 papers with an h-index of 68 and edited several books in these areas of polymer research, and organized several international conferences on these topics.

Surface and Thin Film Characteristics of Polymer Melts from All-Atom Molecular Dynamics Simulations

Do Y Yoon

Stanford University, Stanford, CA

Abstract: Not Available

Oral Presentations

Parallel Session-1

Construction of Dielectric Constant Prediction Models and Design of Monomers for Polymer Materials Using Machine Learning

Yuya Shiraki^{1*}, Yuko Kawanami, Kenichi Shinmei², Hiromasa Kaneko¹

¹ Department of Applied Chemistry, Meiji University, Japan;

²Corporate R&D Center, SEKISUI CHEMICAL Co.,Ltd., Japan

Abstract:

Many electronic devices such as smartphones and computers include polymer materials. To reduce energy loss in such electronic devices, materials with low dielectric constant are in demand. However, finding materials with low dielectric constants requires many experiments and takes a long time to be developed. Therefore, we have attempted to solve this problem by using machine learning to construct prediction models between chemical structures of monomers in polymer materials and dielectric constants of the materials. To construct the prediction models, molecular descriptors calculated using RDKit software were used as explanatory variables x, and log-transformed values of the dielectric constant measured at 1 GHz were used as objective variables y. Additionally, to consider composition ratios of monomers for copolymers, the geometric mean was calculated from descriptors and used as x. Then, Gaussian process regression was used to construct the model y=f(x). A number of virtually generated monomer structures were input into the constructed model to predict the dielectric constant at 1 GHz. In addition, the probability of achieving the target values of the dielectric constant was calculated simultaneously. Monomer structures with lower dielectric constant values than the minimum dielectric constant of the existing dataset could be provided with the proposed method, and we could design monomer structures with target values of dielectric constant.

Modeling the Time-dependent Pvt Behavior of Amorphous Thermoplastics Using the Interrelation of Shear and Bulk Retardation Spectra

Felix Baumgärtner* and Christian Bonten

University of Stuttgart, Institut für Kunststofftechnik, Germany

Abstract:

The rheological behavior, consisting of shape-changing and volume-changing deformation, and the mechanisms involved in solidification are directly linked by the macromolecular structure of plastics. The macromolecular structure causes a pronounced process dependency of the solidification process, through which the internal state of the material is influenced. The timedependent solidification process can be described by means of the pressure, specific volume and temperature behavior (pvT). When considering material models for describing pvT behavior, it can be seen that the methods used still have sufficient potential for improvement. Time-dependent effects cannot be considered with the conventional Tait model. In the scientific literature, there are some approaches for modeling pvT behavior under process-near conditions, such as the KAHR model. However, a closer look reveals that these approaches are either unable to account for important effects encountered under real process conditions, such as the pressure dependent retardation process. Or, the determination of the material specific model parameters still requires too much experimental effort. Both factors contribute to the fact that these approaches have not been transferred into engineering practice. The present work shows a possible faster way to determine model parameters. For this purpose, a combination of shear rheological investigation methods is used in both the melt and solid temperature ranges. This allows the description of a temperature invariant master curve, which was shown in this work using polystyrene as an example. The retardation behavior is mapped over a temperature range of 40-240 °C depending on the velocity of loading.

A Novel Method for the Initial Expansion and Deformation Behavior Analysis Within the Bead Foam Extrusion Process

Tobias Schaible* and Christian Bonten

Institute of Plastics Engineering/University of Stuttgart, Germany

Abstract:

The knowledge of the initial expansion and deformation behavior in dependency of the polymer. the blowing agent concentration, and the process conditions is crucial for the determination of the elongational viscosity during foaming and thus the development of new and advanced polymers for foaming applications. Therefore, this study presents a novel method for the observation and analysis of the initial expansion and deformation behavior within the bead foam extrusion process. For this purpose, a borescope equipped with a camera was integrated into the water box of an underwater pelletizer for bead foaming. As a blowing agent, nitrogen was injected into the polymer melt within the extrusion process. The camera is controlled by a developed trigger by means of angular step signals of a rotary encoder on the cutter shaft of the underwater pelletizer. Thus, images can be taken at any time during the foaming process depending on the cutter position to the die outlet. It is shown, that the method provides reliable results and that the differences of the initial expansion and deformation behavior can be analyzed in dependency of real foaming process conditions and the blowing agent concentration. Thus, the influence of the polymer, the blowing agent concentration and the process parameters on the initial expansion behavior of the blowing agent can be investigated and characterized within the real foam extrusion process. In addition, the deformation data is used to determine the equibiaxial elongational viscosity during the initial expansion of bubbles by use of the molecular stress function model.

Biography:

Tobias Schaible done PhD-Thesis (finished 2022): Inline characterization and prediction of the viscosity and initial bubble growth behavior during foaming of blowing agent loaded polymer melts. Tobias Schaible is a PhD-Student and researcher at the Institut of Plastics Engineering (IKT) at the University of Stuttgart from 2017 until now. Research fields: Rheology and Foaming. He has M.Sc. Mechanical Engineering with a specialization in plastics engineering at the University of Stuttgart and at the University of Connecticut from 2014 to 2017

Numerical Simulation of Particle-laden Flow in Single-screw Extruders by Means of CFD-DEM Considering Melting of Thermoplastics

Celik, A.1*; Bonten, C.1

University of Stuttgart, Institut für Kunststofftechnik, Germany

Abstract:

ABSTRACT BOOK

The single-screw extruder is one of the most important plastics processing machines. In order to improve the design of the machines and in order to predict relevant process variables, computeraided approaches as three-dimensional simulation are increasingly coming to the fore. Depending on the process zone, different modeling approaches are used. For the feed zone, the so-called Discrete Element Method (DEM) is becoming increasingly important. For the melting zone, Computational Fluid Dynamics (CFD) is predominantly used with sub methods like the Finite Volume Method (FVM). However, to date, no method has been explored that allows joint consideration of the feed zone and the melting zone. In this paper, building on the authors' recent work, a novel approach is presented and validated, that allows a joint consideration of these zones. The approach explored is based - for the first time in the case of the single-screw extruder - on a coupled CFD-DEM method. The approach pursued represents a three-phase model. It is based on the Volume of Fluid (VoF) Method and couples it with DEM. In this work, the melting process in the single-screw extruder is simulated using the new approach with joint consideration of the feed zone and the melting zone. To calculate the melting process, a melting model recently published by the authors is used. The results are compared with experimental investigations

Biography:

He worked as Research Assistant from 2017-2021: at IKT and form 2022-today: he worked as Head of Plastics Processing Department at IKT

Key Topics: Modeling and numerical simulation of plastics processing processes

Investigation of the Material and Processing Influences on the Weld Seam Quality of a Combined Thermoforming and Welding Process

Dominik Müller^{1*}, Christian Bonten¹

¹Institute of Plastics Engineering, University of Stuttgart, Germany

Abstract:

During thermoforming, heated plastic sheets are formed into three-dimensional parts. This allows the production of large-area components. But compared to injection molding, thermoforming has a limited design freedom and is restricted to shell-like parts without individualized design elements. Part-specific design elements such as ribs or screw domes have to be added in a further processing step (welding or adhesive bonding). A combined thermoforming and welding process developed at the University of Stuttgart allows to integrate design elements into the thermoforming process. Therefore, a design element is first placed into the thermoforming mold, heated separately and then welded to the sheet during the forming process. Since thermoforming is performed in the thermoelastic state and welding is performed in the thermoplastic state, the welding procedure in this combined process is done at lower temperatures than usual. According to state of the art, the resulting weld seam quality is not only influenced by the process parameters but also by the material properties. For this reason, plastics with special material properties were produced. During the material development, the focus was on the adjustment of the viscosity in order to compensate the low processing temperature. To investigate the influence of the specific material modifications on the weld seam quality, welding tests were carried out under thermoforming parameters. Due to the modification and combination of the materials, it was possible to achieve a high weld seam quality even under very untypical welding conditions.

Biography:

Dominik Müller has done his PhD Since 2018 until now: at the Institute of Plastics Engineering (IKT) at the University of Stuttgart in the Department of Processing Technology, Thermoforming Division with the topics: process development and material modification for thermoforming, material characterization for thermoforming simulation. He studied Master's degree from 2016: in mechanical engineering with a specialization in plastics technology at the University of Stuttgart. He

done Apprenticeship from 2011: as a mechanical technician and studies in mechanical engineering at the University of Applied Sciences in Ulm.

Application of Systems Dynamic Simulations in the Preparation and Characterization of Novel Functionalized Casein Microparticles and Casein Microgels

Ronald Gebhardt^{1*}, Md Asaduzzaman¹

Soft Matter Process Engineering, Aachener Verfahrenstechnik, RWTH-Aachen University

Abstract:

Caseins are the main protein component of milk, which exist under natural conditions as casein particles (so-called casein micelles). They are natural nano-carriers for insoluble calcium phosphate and are used as nano- or microcarriers for bioactive substances due to their good swelling properties. We use pectin-induced depletion flocculation and subsequent film drying as a structure-preserving preparation method. The microparticles produced in this way swell quickly and repeatable, which also makes them interesting for ion-sensitive biosensor applications [1]. We use systems dynamic modelling techniques to simulate and predict the expansion and shrinkage behavior of the microparticles as well as the elastic properties that occur after conversion into microgels. We vary the process and environmental conditions and apply pre- and post-treatment strategies to target the swelling properties [2]. We show that a subsequent temperature treatment similar to enzymatic cross-linking converts the microparticles into casein microgels, so that stable equilibrium swelling values can be achieved by suitable process control [3]. The new chemical and physical contacts lead to characteristic features such as overshooting in the swelling curves. Our systems dynamic, parallel modelling approach separates this new elastic component from the contribution of the uncross-linked protein and allows detailed investigations of microgel formation and microstructure engineering to optimize properties.

Biography:

Ronald Gebhardt has been professor and head of the Chair of Soft Matter Process Engineering within Aachen Process Engineering at RWTH Aachen University, Germany since the beginning of 2017. He started his scientific career as post-doctoral researcher and later junior scientist at the European Synchrotron Radiation Facility, ESRF in Grenoble, France where he worked on the fine structure of biopolymers. He then moved to the Chair of Food Process Engineering at Technische Universität München, Germany as group leader where he investigated structure-function-process relationships in food. Before moving to Aachen, he was professor at the Friedrich-Alexander University of Erlangen-Nuremberg, Germany in biotechnology.

Modification of Nonlinear Viscoelastic Properties for Biomass-Based Plastics

Masayuki YAMAGUCHI*

Japan Advanced Institute of Science and Technology, Japan

Abstract:

Addition of high-molecular-weight fraction and incorporation of long-chain branches are the

promising methods to modify the nonlinear viscoelastic properties under elongational flows. However, it is not so convenient for commercially available biomass-based plastics. In this presentation, we will introduce some novel methods to provide the strain hardening in transient elongational viscosity for poly(lactic acid) (PLA) to improve the processability at various processing operations such as foaming, blow-molding, tubular-blown film, and thermoforming: (1) addition of flexible nanofibers, (2) addition of long-chain branched polymer, and (3) addition of another biomass-based polymer. Since all methods are quite simple, i.e., just mixing with PLA in a molten state, they can be available for industrial applications. Moreover, mechanical properties in the solid state can be also improved by the specific method.

Moreover, we will introduce the modification method of rheological properties under shear flow for cellulose acetate (CA). CA having high molecular weight shows good processability at injection molding and extrusion processing by the addition of appropriate plasticizer.

Biography:

M. Yamaguchi got his master degree in 1989 and PhD in 1999 at Kyoto University. Before joining JAIST, he has been working at Tosoh Corporation from 1989 to 2005. The main topic of his research is applied rheology of polymeric materials. He is a full professor and the director of Research Center for Carbon Neutral in JAIST.

Rapid Polymerization of Thin Film Thermosetting Polymers Using Pulsed Light

Kurt A. Schroder*, Vahid Akhavan, and Vikram S. Turkani

PulseForge, Inc. Coupland,TX

Abstract:

A new commercial process for the rapid polymerization of thin film thermosets such as polyimides and epoxies is presented. This process, which is based on photonic curing, uses an industrial, pulsewidth modulated flashlamp to thermally process thin-film thermosetting polymer precursors. Ordinarily, when curing in an oven, the time to process is about two hours. With this new process, a full cure can be attained in about 20-30 seconds. The resulting films are defect free and crosslinking was verified with FTIR. This new process complements the existing family of flashlampbased non-equilibrium heating processes including photonic curing, photonic debonding, and photonic soldering which are used to fabricate flexible hybrid electronics and complement the semiconductor industries.

Biography:

Kurt A. Schroder is CTO of PulseForge, Inc. He has Physics degrees from MIT and the University of Texas at Austin and is a two-time winner of the R&D100 award which is given to the top 100 inventions in the US each year. He was named Inventor of the Year for the state of Texas for the development of photonic curing and has 41 US patents primarily in the fields of printed electronics and nanotechnology.

Online Sensing of Polymer Properties and Process Design with Machine Learning

Rinta Kawagoe^{1*}, Kazutoshi Terauchi², Fumiya Hamada², Toshinori Yamaji², Hiromasa Kaneko¹

¹Department of Applied Chemistry, Meiji University, Japan

²DIC Corporation Production Engineering Dept. Core Process Engineering Development Group, Japan

Abstract:

In our life, we usually use polymer materials, for example, PET bottles, tires, and organic electroluminescence. When a polymer material is produced, polymerization is conducted in a reactor. Reaction process includes 1. Input monomers, 2. Heat a reactor, 3. Drop an initiator, 4. Maintain reactor temperature, 5. Add some additive, and 6. Cool a reactor. To appropriately stop the reaction or the process, a reactant is sometimes samples and its properties are analyzed. However, it is difficult to monitor the properties online by the analyzers and to appropriately control the temperature and the addition of additive. In this study, our objective is online sensing on polymer properties and the design of profiles of temperature and additive. By using a dataset of measured polymer properties, near-infrared and Raman spectroscopy, initial conditions, and time-series data of temperature and additive, two machine learning models are constructed. One model predicts polymer properties from the spectra and is used for online monitoring of the properties. The other model predicts polymer properties from initial conditions and time-series data of temperature and additive and is used to design the conditions and the profiles of temperature and additive for polymerizing the product with target values of the properties. Linear and nonlinear regression analysis methods were compared to construct the models, and we achieved the online monitoring and the process designs of the constructed models.

Embedded Carbon Nanotubes in the Hydroscopic Hydrogel for the Environmental Water Harvesting

Nasrollah Hamidi*

Department of Biological and Physical Sciences/1890-Research, South Carolina State University, Orangeburg, SC

Abstract:

Freshwater is one of the main components of life and innovative activities such as industrial, agricultural, rural developments, and defense endeavors, and its resources are depleting quickly. One of the proposed solutions for this problem is harvesting water from the environment which may contain as much as 13 trillion tons of vapor distributed worldwide with fast replacement. Emerging technology could harvest vapor as freshwater from any environment, including arid regions, land-locked areas, and remote communities. Materials that absorb fast vapor at room temperature and release it as a liquid at a slightly higher temperature are the critical components for atmospheric water collecting. One of the promising materials is the flexible hybrid photothermal water sorbents composed of hygroscopic salt and hydrogel that possesses superior water sorption capacity even in low-humidity air. In these devices, the deliquescent salt, adsorbed to the hydrogel body, maintains its solid form after a significant amount of water is condensed in the structure.

The condensed water could be released at temperatures below the boiling point of water (70 to 90 °C), a temperature that is achievable under sunlight via the photothermal effect. A sample of hygroscopic hydrogel with the embedded carbon nanotube was fabricated and tested under laboratory conditions. It absorbed up to 60% of its weight water and its maximum rate of water release was within 70 to 90 °C, a temperature achievable under direct sunshine. Environmental harvesting water devices made of these materials could become a complemental resource to reduce freshwater stresses.

Microcellular Foaming Technology

S.W Cha^{1*}, K.H Kim² and Jin Hong²

^{1,2}Yonsei University, South Korea

Abstract:

In modern industry, plastic is the widely used material in everyday life, such as electronic devices, automobile parts, and household goods. Also, since the corona pandemic, plastic use is being done in more places. The development of plastics began at the Massachusetts Institute of Technology in the United States, and in the 1980s, the microcellular foaming process that enabled the significant growth of plastics was completed.

The microcellular foaming process uses an inert gas and rapid pressure and temperature differences to form the fine and dense cells inside the plastic base material. The process changes the foam properties by several factors, mainly solubility and glass transition temperature. The benefit of this process is that a wide variety of plastic products can be manufactured by minimizing the amount of material used and maximizing the strength and lightweight of the product.

The microcellular foaming process includes batch process, injection molding process, reaction injection molding process, and extrusion process. Each process has its unique technique and advantages. In addition, this process is an environmentally friendly method, and the micro-sized cells produced by applying the process have excellent heat insulation, sound insulation, optical properties, and more.

In the ongoing research, we plan to continue researching the overall contents of the foaming factors of the microcellular foaming process, research and development of new microcellular foams that are developing in various ways, and future applications.

Biography

Sung Woon Cha received Ph.D. from MIT in 1994. From 1994 to 1996, he worked as a project manager at MIT and as a chief scientist at Trexel Inc. on the development of microcellular foaming process technology. Also, he holds US patents related to the microcellular foaming process. Since 1997, he has been a professor at the Department of mechanical engineering at Yonsei University, researching the microcellular foaming process, axiomatic design, and developing new materials and manufacturing processes. In addition, he introduced creative classes at Yonsei University and is striving to develop the creativity of many younger students.

Parallel Session-11

Graphene Oxide Reinforced Vinyl Ester Polymer Matrix Composites

Andre Lee^{*1}, David F. Vogelsang1 and Robert E. Maleczka Jr.²

¹Michigan State University, Dept. of Chemical Engineering and Materials Science, USA; ²Michigan State University, Dept. of Chemistry, USA

Abstract:

Graphene oxide (GO) nanoplates are 2-D nanomaterials that offers the potential to reduce moisture uptake and provide mechanical benefit to polymeric materials such styrene vinyl ester (VE) resins. However, it has been demonstrated the dispersion of GO in VE is a significant challenge. In this work, a high thermal stability coupling agent with isocyanate and styrene on the opposite ends was used to modify the surface chemistry of GO. This surface modification can significantly improve the dispersion of GO in VE, while provide covalent bonds between GO and VE network. Using this approach, VE network containing 0.2 wt% of GO had a 100% improvement on the flexural strength over the neat VE network (105 MPa versus 55 MPa) and 100% improvement on the flexural fracture strain (3.5% vs. 1.6%). In the presentation, synthesis of the coupling agent used, characterization of GO surface modification, mixing details, and mechanical and thermal behavior of GO reinforced cured VE networks will be discussed in detail.

Biography:

Andre Lee is currently a professor in the Department of Chemical Engineering and Materials. In the past 20+ years, he has been working various silsesquioxane chemistries and developing their engineering application for used in high-performance thermosetting materials. He is recognized as a pioneer in developing engineering sigificant silsesquioxanes.

High Energy-Density Energy Storage Capacitor in Multi-Layer Polymer and 2D Nanofiller Composites

Nihar R Pradhan^{1*} Sumit Bera¹, Rukshan Thantirige¹, Priyanka Das¹, Maninderjeet Singh², Alamgir Karim²

¹Jackson State University, MS, United States

²University of Houston, TX, United States

Abstract:

Polymer nanocomposites are a promising concept to improve energy storage density of capacitors, but realizing their hypothetical gains has proved challenging. Introduction of high permittivity nanofillers in a traditional dispersion method often leads to reduction in breakdown strength

at higher concentration of fillers. In this talk we will introduce a new method of preparing heterostructure of polymer-nanofillers composites using two-dimensional materials such as h-BN, Mica, MoS2 as fillers to enhance the dielectric and breakdown strength. A dramatic enhancement of breakdown strength can achieve using the 2D fillers, which yields high energy density ~75 J/ cm3 using 2D-Mica nanofillers is the highest among the observed energy density of the polymer-nanocomposite based dielectrics.

Biography:

Pradhan currently serving as an Associate professor of Physics at Jackson State University, Mississippi, USA. He received his PhD degree in Physics from Worcester Polytechnic Institute, Massachusetts, USA and did postdoctoral work at National High Magnetic field Laboratory, Florida before joining as an Assistant professor at Jackson State University. His current research interest is studying dielectric properties of polymer-based nanocomposites, transport properties twodimensional materials and exploring their low temperature physics.

Biodegradable Electrospun Scaffold of PLA/PBS Reinforced with Cellulose Nano Fibril for Tissue Engineering

Hamad A. Al-Turaif* and Usman Saeed

Chemical and Materials Engineering Department, King Abdul Aziz University, Saudi Arabia

Abstract:

Today, tissue engineered scaffolds made by electrospinning are becoming a focus of research due to their ability to assist native tissue recovery. Compared to a single material, multifunctional composite scaffold could provide more suitable microenvironment for the tissue regeneration. In this study, electrospun composite scaffolds are developed by reinforcing a matrix of poly (lactic acid) (PLA) and poly (butylene succinate) (PBS) by cellulose nano-fibrils (CNFs). Initially, PLA/ PBS fibrous scaffolds with different ratio were prepared. The best properties and bioactivity of the scaffolds were obtained at equal ratio of PLA and PBS. Overall performance of electrospun scaffolds improved greatly by introduction of CNF into the PLA/PBS scaffolds. The developed composite scaffolds showed a uniform fibrous structure with desirable size dimension, cell-friendly surface characteristics, sustainable biodegradation behaviour and sustainable mechanical property compared to native tissue. Overall the developed composite scaffolds demonstrated their potency for vascular tissue engineering application

Biography:

Hamad A. Al-Turaif obtained his Doctor of Philosophy degree in Chemical Engineering from the University of Maine in the United States of America in 1999. Directly after that, he joined the Chemical and Materials Engineering Department at King Abdulaziz University (KAU) in Jeddah. He established the surface science and coatings laboratories at the KAU. He worked as a technical advisor for the foam laminates factory. Prof. Al-Turaif is a member of different Saudi and international societies. He published and presented his work in many international journals and conferences. Professor Al-Turaif served in the university in different positions, such as director of Central Labs and director of House of Expertise. Now, he is the Vice Dean of Graduate Studies and Scientific Research in college of engineering at KAU.

Polymer-Ceramic Nanocomposite Electrolyte for Solid-State Battery Applications

Yuepeng Zhang^{1*} and Sanja Tepavcevic¹, Jungkuk Lee¹, Michael J. Counihan¹, Wooseok Go², Pallab Barai¹, Michael Tucker², Marca Doeff², Venkat Srinivasan¹

¹Argonne National Laboratory, USA

²Lawrence Berkeley National Laboratory, USA

Abstract:

Composite ceramic lithium conductor and polymer membranes are promising candidates for solidstate lithium battery electrolytes. Upon establishing an effective transport network, the composite membrane electrolyte is expected to show a high room-temperature Li-ion conductivity that is contributed by the lithium ceramics and an improved mechanical integrity at the electrodeelectrolyte interface during charge-discharge cycling provided by the soft polymer matrix. In this study, we report the synthesis of Al0.25Li6.25La3Zr2O12 (LLZO) nanofibers and the LLZOpolyethylene glycol (PEO) composite membranes and their electrochemical properties.

Biography:

Yuepeng Zhang is a Principal Materials Scientist at Argonne National Laboratory. She has a Ph.D. in Materials Science and Engineering from McMaster University in Canada. Yuepeng's current research areas include nanomaterial and membrane development and scale-up for battery and fuel cell electrolyte and electrode applications. Before joining Argonne, Yuepeng worked as a Principal Engineer for Western Digital Corporation in San Jose, California.

High Capacity Polypyrrole Membrane as Energy Storage Material

Ze Zhang^{1,2*}, Zahra Roohi^{1,2}, and Frej Mighri¹

¹Université Laval, Canada; ²CHU de Québec – Université Laval, Canada

Abstract:

Polypyrrole (PPy) is a heterocyclic and intrinsically conductive polymer showing poor mechanical property and processability. PPy is also electroactive owing to its redox property and has been actively investigated as an energy storage material for supercapacitors. We have developed a unique interfacial polymerization method, through which free-standing and nano-fibrous PPy membranes were synthesized. Such a PPy membrane is very light in weight, and can be cut into different shapes and assembled together. The electrochemical properties of the PPy membrane were characterized by cyclic voltammetry and electrochemical impedance spectroscopy. Membrane chemistry and morphology were analyzed with X-ray photoelectron spectroscopy, infrared spectroscopy, and scanning electron spectroscopy. It's thermal stability was studied with thermogravimetric analysis. The electrodes made of the PPy membrane showed ultrahigh areal specific capacity and fairly good cyclic stability. The high specific capacity was found closely related with the morphology of the membrane. The membrane morphology was controlled by the polymerization method, and was significantly affected by the type of dopant. Such a polymer membrane could be a good candidate to construct supercapacitors.

Biography:

Ze Zhang received his Bachelor and Master degrees in Engineering from Chengdu University of Science & Technology in 1982 and 1984, and a PhD degree in Experimental Medicine from Université Laval in 1993. After postdoctoral training at the AIST in Japan, he returned to Canada and entered the Saint-François d'Assise Hospital Research Center as a researcher. He then became a professor at Université Laval and a senior researcher in the Division of Regenerative Medicine of the Centre de recherche du CHU de Québec–Université Laval. He studies materials and devices in medicine, and conductive polymers as energy storage materials.

Rheological Property Recovery and Stability of Recycled Polymers

Guinevere Tillinghast, Jonathan P. Rothstein, H. Henning Winter*

University of Massachusetts Amherst

Abstract:

The research project aims to improve the effectiveness of plastic recycling processes, focusing on both mechanical and chemical recycling of plastic waste collected from different regions in the United States. We are particularly interested in enhancing the mechanical properties of recycled plastics, as defined by rheology, which is the study of how materials deform and flow.

To assess the thermal stability of the polymers, consecutive frequency sweeps were repeated over an hour under isothermal conditions, supported by time-resolved rheology analysis (Mours M, Winter HH, Rheologica Acta 33:385–397, 1994) using the IRIS Rheo-Hub software (IRIS Development LLC). Small Amplitude Oscillatory Shear (SAOS) experiments were performed on the Kinexus rheometer (Netsch). Under stable conditions, steady shear viscosity experiments were conducted across a wide range of shear rates. To detect changes that may not be apparent in shear rheology, we also employed extensional rheology (Chellamuthu M, Arora D, Winter HH, Rothstein JP, J. Rheol 55:901–920, 2011), which is highly sensitive to variations in molecular weight and cross-link density. This allows for a more comprehensive understanding of the rheological properties of the recycled plastics.

Furthermore, the research includes work on application-specific polymers, where the aim is to identify rheology criteria that are ideal for different molding processes

The research is supported by the US Department of Energy under award # DE-EE0009285 and is in collaboration with research groups led by G. Huber (U Wisconsin Madison) and K. Vorst and G. Curtzwiler (Ohio State University Ames).

Functional Modification of Macromolecular Systems For nano-generators

Unnikrishnan Gopalakrishna Panicker

National Institute of Technology Calicut, India

Abstract:

The utilization of materials with piezoelectric/triboelectric characteristics for micro- or nano-

scale device fabrication has been examined by scientists for many years. The features of various individual polymeric systems or their derivatives have been identified as extremely promising in this regard. However, the energy harvesting efficacy of many of them has been found to be inferior compared to most of the inorganic substances in this domain. This aspect can interestingly be addressed to a great extent through various modification protocols.

The present work initially covers the examinations to modify the piezoelectric features of poly(vinylidene fluoride) [PVDF]. The embedding of suitable nanofillers within PVDF matrix is a possible strategy for modulating the β phase of PVDF with piezoelectric characteristics. Thus, hybrid nanocomposites have been developed with tio2 and sio2 as nucleating agents, through the first part of this work. The characterization has been done by employing X-ray diffractometry, FTIR, TGA and DSC. The hybrid filler incorporation approach has been found to cause considerable increase in peak voltage compared to the performance of PVDF alone.

The second part of the work presents the development of piezoelectric polymer mats, from ethylene vinyl acetate- millable polyurethane-nanohydroxy apatite (EVA-MPU/nha) composite systems, by an electrospinning technique. The evaluation of in-vitro bio-compatibility features of the EVA-MPU/nha systems has been done for their possible utilization in the bio-medical field. The physiological motion of human body parts has subsequently been used as the input for triggering tribo-piezoelectricity, and for developing LED sensors/ buzzers.

Biography:

Unnikrishnan is a Professor in the Department of Chemistry of NIT Calicut. His current research interests include nano- materials, polymer blends for bio-medical applications, tribo-piezoelectric materials etc. He was a visiting researcher at the Department of Chemistry, University of Leeds, UK. He had combined research programmes with Lunghwa University, Taiwan. His post-doctoral experience includes the assignment as an Environmental Specialist at Abu Dhabi, related to petroleum related operations. He is a Fellow of Royal Society of Chemistry and a Member of ACS and IUPAC. He is the current President of the Calicut Chapter of Society for Polymer Science (India).

Water Electrospray with Polymer Micro Nozzles and its Applications

Seung Seob Lee

KAIST, South Korea

Abstract: Not Available

Advances in Nanocomposite Power Scavenging Technologies

David L. Carroll*

Center for Nanotechnology and Molecular Materials and Department of Physics Wake Forest University, Winston Salem NC

Abstract:

Carbon nanotube based polymer composites possess several properties that make them ideal

for use in the low-power waste heat recovery applications not suitable to inorganic crystalline materials. The favorable thermoelectric properties of the carbon nanotubes with moderate Seebeck coefficients and potentially large electrical conductivities result in modest power factors, while the low thermal conductivity of the polymer host aids in maintaining a temperature gradient across the composite, thereby providing a reasonable figure of merit. Although the thermoelectric performance of these composites is lower than that of standard crystalline thermoelectrics, their light weight and flexible physical structure makes them more ideal for use in the utilization of waste heat for personal and portable electronics. In order to effectively utilize a thermoelectric material in a practical application, it must be combined in a thin film device structure consisting of alternating p-type and n-type elements that are connected electrically in series and thermally in parallel. Recently we have introduced a device structure that combines both these thermoelectric modalities of power scavenging with piezoelectric power scavenging simultaneously. The device performance is then a combination of intrinsic thermoelectric properties and piezoelectric properties. However, surprisingly, the total power output is more than the simple addition of these two components. In this presentation we will show that there is a third, synergistic effect, which results from the combination of piezo and thermoelectric functionalities into a single structure. We call this effect, the "T/PEG effect" and show that it can result in significant power gains for organic power harvesters, bringing them to the threshold of commercial viability

Biography:

Carroll got his PhD. at Wesleyan University, and postdoctoral experience at UPENN as well as a three year stay at the Max-Planck Institut in Stuttgart. He is currently professor of Physics at Wake Forest University and director of the University's Nanotechnology Research Center. Professor Carroll is widely published in the area of polymer composites with more than 400 papers in journals, 37 different patent families, and several books. He is a Fellow of the APS.

Advancing Understanding of Composite Polymer Electrolytes with LLZO Nanofibers

Sanja Tepavcevic^{*}, Michael Counihan, Jungkuk Lee, Pallab Barai, Justin Connell, Venkat Srinivasan, Yuepeng Zhang

Materials Science Division, Argonne National Laboratory, S Cass Ave, Lemont, IL, USA

Abstract:

Ceramic Li6.55Al0.2La3Zr2O12 (LLZO) is one of the most attractive electrolyte materials for solid-state batteries that combined with metallic Li anodes holds the promise for safer and more energetically dense battery, but its performance is limited by the increases in electrolyte-electrode interfacial resistances upon cycling. The combination of Li+-conducting ceramics and polymers offers a new pathway to create better electrolytes with both high ionic conductivity and good (electro) mechanical interfacial properties. We optimized two-step annealing processing conditions for the fabrication of cubic-LLZO nanofibers and Li2CO3 removal. Using industrially relevant roll-to-roll electrospinning and slot-die coating, we fabricated thin composite membranes with reproducible thickness down to 20 microns. We investigated PEO based composite polymer electrolyte (CPE) with a high, 50 wt% loading of Al-doped LLZO nanofibers in comparison with nanofiber-free PEO electrolyte. XPS measurements show that LLZO is not present at the composite electrolyte surface, and solid electrolyte interphase (SEI) formation is dictated solely by PEO and LiTFSI when reacting with Li metal. Electrochemical SEI formation, studied by cyclic voltammetry, shows SEI formation is

identical with and without up to 75 wt% LLZO in the electrolyte. Galvanostatic cycling with lithium symmetric cells shows that the critical current density (CCD) can be tripled by including 50 wt% LLZO, but half cell cycling reveals this comes at the cost of CE. Varying the LLZO loading shows that even a small amount of LLZO drastically lowers the CE, from 88% at 0 wt% LLZO to 77% at just 2 wt% LLZO. Mesoscale modelling reveals that the increase in CCD cannot be explained by an increase in the macroscopic or microscopic stiffness of the electrolyte; only the microstructure of the LLZO nanofibers in the PEO-LiTFSI matrix slows dendrite growth by presenting physical barriers that the dendrites must push or grow around. This tortuous lithium growth mechanism around the LLZO is corroborated with mass spectrometry imaging. Electrochemical impedance spectroscopy (EIS) analysis showed comparable bulk ionic and interfacial resistances with and without nanofibers, indicating that PEO dominates Li+ transport and interfacial chemistry. The total Li-ion conductivity of the composite is still governed by the polymer matrix due to high interfacial resistance between the garnet particles and the PEO/LiTFSI matrix. This work highlights important elements to consider in the design of CPEs for high-efficiency lithium metal batteries.

Biography:

Sanja Tepavcevic is a Material Scientist at Materials Science Division at ANL. She has more than 15 years of experience in advanced materials for beyond Li-ion electrochemical energy storage. She is PI and lead experimentalist on current VTO solid-state battery projects focused on studying solid-electrolyte/anode and solid-electrolyte/cathode interfaces. She developed and exploited a variety of ex situ and in situ experimental surface sensitive techniques and spectroscopic and electrochemical methods to explore and explain bulk and interfacial properties of ceramic and glass materials for solid electrolytes.

Polyazole Based Polymer Materials Development for Challenging Applications

Husnul Maab*, Azra Touheed, Bashir Iqbal, Hussain Ahmad

Affiliation (National Engineering & Scientific Commission Islamabad, Pakistan & university of Buner KPK, Pakistan)

Abstract:

A series of fluorinated polytriazole polymers based on hexafluoroisopropylidene (HFA) on the main polymer back-bone with different fluorinated aniline derivatives as side chain were synthesized by polycondensation method in the lab followed by gas transport properties of single and mixed gas system including CH4, CO2, N2, C2H6 and Helium (He) through the dense and symmetric membranes prepared by solution casting technique from chloroform solvent. The gas performance of the polymer membranes such as permeability and selectivity values were found mainly depending on the bulky fluorinated aniline derivatives (4-fluoroaniline, 2,5-difluoroaniline, 4-bromo-2,5-difluoroaniline, 2,3,4,5,6-pentafluoroaniline and 3-(trifluoromethylaniline)) groups as a side chain of the polymer back-bone. The membranes exhibited high mechanical stability with no plasticization effect under a high range of pure CO2 feed pressure from100 to 800 PSI at room temperature. The polymers synthesis protocol is very simple and reproducible, high solubility of polymers in common organic solvents (Chloroform, THF, NMP, DMF, DMAc etc.) and easily scalable for commercial production. The membranes materials developed in this work, exhibited a high permeability for carbon dioxide (CO2) and Helium (He) gases as compared to other gases such as methane (CH4), nitrogen (N2) and ethane (C2H6) under a high range of operating feed

pressure upto 800 PSI. Based on the separating gas performance results, the polymers membranes materials developed in this work, can be considered as promising novel polymer materials for gas purification and separation technologies, more specifically for CO2 removal and helium (He) recovery from the natural gas stream under high field processing pressure. (800 PSI). This work demonstrates the testing of the novel fluorinated polytriazole polymer membranes (dense and symmetric) under different experimental conditions of feed pressure (100 - 800 PSI) at room temperature to investigate their mechanical and chemical stability for potential industrial and commercial application of high pressure processing natural gas.

Biography:

Husnul Maab currently working as General Manager (Technical chemistry) in the Research & Development Center of National Engineering & Scientific commission, Islamabad and as a visiting Associate Professor (Chemistry) at the University of Buner, KPK, Pakistan. He holds a PhD degree in Engineering Sciences from Faculty of Engineering, Christian Albrecht University of Kiel, Germany. Dr. Husnul Maab worked in Germany and Saudi Arabia on the development of polymer materials for separation and purification technology in water & Energy sectors. His scientific achievements have been protected in international patents including USA, EP & WIPO with publication of research articles in international journals of high impact factors.

Orals

Metal-Like Lustrous Materials using Oligo(3-Alkoxythiophene) Dyes

Satoru Tsukada*

Department of Materials Science, Graduate School of Engineering, Chiba University, Japan

Abstract:

Metallic colors, especially metallic gold, are expensive. Thus conventional metal-like luster paints comprise metal effect pigments, namely fine powders of flaky aluminum or zinc dispersed in a binder resin solution containing colorant. However, metal flakes cause problems such as corrosion and shielding electromagnetic waves. Under this background, metal-free organic solids that exhibit metal-like lusters have been discovered. These organic materials have attracted considerable attention because they have the potential to solve various issues associated with paints that contain metal flake pigments.

We have developed a gold-like luster film based on the high-molecular-weight oligomer, oligo(3methoxythiophene) (O3MeOT), obtained via chemical polymerization of 3-methoxythiophene. O3MeOT is soluble in several polar solvents and can be used to produce a gold-like luster coating with good film-forming properties and excellent aging stability on various substrates. In this study, we synthesized oligo(3-alkoxythiophene) with linear or branched chain and investigated the effect of substituent structure on film properties. Depending on the slight difference in the substituents, we were able to obtain metallic glossy films with different color tones.

Biography:

Satoru Tsukada was born in Tokyo, Japan, in 1983. He graduated from Saga University in 2007 and received his Ph.D. degree from The University of Tokyo in 2012 under the supervision of Prof. Hiroshi Nishihara. Then he was appointed an assistant professor at Tokyo University of Science, working with Prof. Takahiro Gunji. In 2017, he moved to Hiroshima University. Since 2019, he has been an assistant professor of Graduate School of Engineering at Chiba University, joining Prof. Hoshino's group. His current research interest lies in creation of metal-like luster materials without metal flakes and functional materials using organic synthesis techniques.

Toughening of Poly(ionic liquid)-based Ion Gels by Adding Nanomaterials

Takaichi Watanabe^{1*}, Yuna Mizutani¹, Yume Tao¹, Carlos G. Lopez², Tsutomu Ono¹

¹Okayama University, Japan; 2RWTH Aachen University, Germany

Abstract:

lon gels are a class of ionic liquid (IL)-based soft material consisting of a three-dimensional crosslinked polymer network and an IL as a solvent. Recently, ion gels can be applied to electrochemical devices, sensor and actuators, and carbon dioxide separation membranes. However, low mechanical strength of ion gels hinders their practical application. In this study, a tough and thermally stable ion gel was developed using a partially-clustered nanomaterial network and a hydrophobic poly(ionic liquid) (PIL) network with a large amount of free IL. Rheological studies of IL dispersions containing nanomaterials (such as silica nanoparticles, cellulose nanofibers, and alumina particles) showed shear thinning behavior and that zero-shear viscosity increased with increasing nanomaterial concentration. These results suggest that nanomaterials form physically cross-linked gels in IL. It was found that the addition of nanomaterials to PIL ion gel increased the mechanical strength of ion gel. Especially, alumina/PIL ion gel had 40 times and 3 times higher fracture stress than PIL ion gel (SN) and silica nanoparticle/PIL ion gel. These behaviors suggest that the improved mechanical properties would be due to an energy dissipation mechanism. We envision that these tough PIL-based ion gels can be used as electrochemical devices, sensors and actuators, and carbon dioxide separation membranes.

Biography:

Takaichi Watanabe received his Ph. D. from Okayama University (Japan) in 2014. He was a JSPS postdoctoral fellow at Okayama University in 2014, and a project researcher with Prof. Shoji Takeuchi at the University of Tokyo from 2015 to 2016. In 2016, he joined Okayama University as an assistant professor, and was appointed a research associate professor in 2021. He is also a visiting scientist at RWTH Aachen University (Germany) from 2022 to 2024. He studies about the design of soft materials using poly(ionic liquid)s and process development of well-defined polymer particles using microfluidics.

Wetting Behaviour of Poly(ethylene oxide)-Grafted Silica Surfaces in the Presence of Free Homopolymers

M. Natália D. S. Cordeiro^{1*}, Zuzana Benková²

¹LAQV-REQUIMTE, Department of Chemistry and Biochemistry, Faculty of Sciences, University of Porto, Rua do Campo Alegre, Porto, Portugal

²Polymer Institute, Slovak Academy of Sciences, Dúbravská cesta 9, Bratislava, Slovakia

Abstract:

Polymer-grafted surfaces offer tuneable properties and have wide-ranging applications in technology, biomedicine, and biochemistry. By coating surfaces with chemically identical polymer chains, surface interactions can be manipulated in the presence of free polymer chains. A system consisting of a single polymer-grafted surface within a matrix of homopolymers is equivalent to a system with two opposing polymer-grafted surfaces, allowing us to deduce the behaviour of the latter.

In this communication, we move a step forward and present results of fully atomistic molecular dynamics simulations (MD) to investigate the conditions under which free poly(ethylene oxide) (PEO) chains are prevented from penetrating a layer of PEO chains end-grafted on an amorphous silica surface. The grafting density of anchored PEO chains and the molar mass of free PEO chains were varied parameters. Density distributions, grafted layer height, overlap parameters, and orientation order parameters were calculated, analysed, and compared to the theoretical phase

diagram. The results indicate that a high grafting density of ca. 3.5 chains/nm2 is needed to expel free PEO chains from the grafted PEO layer on the silica support. Furthermore, when exposed to bulk free PEO chains with comparable molar masses, two opposing PEOgrafted surfaces do not adhere. The behaviour of the grafted layer resembles immersion in either a good solvent or a Θ -solvent, depending on the molar mass of the free PEO chains.

These MD results contribute to a more comprehensive theoretical understanding of wetting phenomena and offer valuable insights for synthesising polymer-functionalised surfaces with the "grafting to" approach.

Biography:

M. Natália D.S. Cordeiro is a Professor of Theoretical Chemistry at the University of Porto, Portugal. She leads the Cheminformatics and Materials research group at the Associated Laboratory for Green Chemistry. Her group's research spans a wide range of areas, including polymers, nanomaterials, electrochemistry, catalysis, and drugs/materials design, with the goal of advancing their applications. Equally varied as the research topics are the methods employed to study them, which involve molecular simulations as quantum-mechanical calculations and even machine learning tools. She has authored over 350 SCI works and contributed to more than 25 book chapters.

Design of Soft Materials: Where Theory, Simulations and Experiments Meet

Andrey V. Dobrynin

Department of Chemistry, University of North Carolina, Chapel Hill, NC

Abstract:

During the last decade, our understanding of soft matter has been transformed through the synergistic consolidation of theory, computer simulations, and experiments into a materials design engine (platform). In this talk, I will describe how this approach has guided synthesis towards programmable molecular architectures to yield novel functional materials with well-controlled physical properties. In particular, I will demonstrate how theory and computer simulations have empowered the design of polymeric networks capable of replicating the unique self-assembly, mechanics and temporal evolution of living tissue. These synthetic tissue mimics are vital for biomedical device engineering and embody significant implications for decoding a multitude of cellular processes including proliferation, locomotion, and differentiation.

Biography:

ANDREY DOBRYNIN is Mackenzie Family Eminent Distinguished Professor of Chemistry at University of North Carolina at Chapel Hill. He received his B.S. (1987) and Ph.D. (1991) degrees in Polymer Physics from the Moscow Institute of Physics and Technology, Moscow, Russia. He is a fellow of APS, AAAS and POLY Division of ACS. His research is focused on computationally driven materials design, polymer networks and gels, wetting and adhesion at the nanoscale, associating polymers, polyelectrolyte solutions and gels, charged polymers at surfaces and interfaces, electrostatic interactions in biological systems, time programmable materials, 3D printing, active matter, and soft-matter physics and biophysics.

Spanning From the Nano-Scale to Individual Polymer Chains: A Chemical Perspective on the Glass Transition

Armand Soldera*

Université de Sherbrooke, Canada

Abstract:

The glass transition stands as one of the most enigmatic physical properties of polymers. Occurring over a temporal spectrum spanning from mere nanoseconds to several years (as seen in aging), this transition demarcates two domains of investigation distinguished by their disparate viscosities and mechanical characteristics, all while retaining an amorphous nature. A novel avenue of inquiry has unfurled through molecular simulation, aiming to delve into the atomic intricacies. It has metamorphosed into a fullyfledged technique that navigates the confluence of experimentation and theory. Its application to the scrutiny of the glass transition proffers a captivating avenue for advancement. When the values of Tg (glass transition temperature) harmonize with empirical observations, an opportunity arises to unveil its molecular genesis, paving the way for a chemical interpretation of this transition. However, this also begets a cluster of additional queries. For instance, what precisely does this glass transition signify? How is it precisely manifest in simulated dilatometry? Can one speak of a glass transition intrinsically tied to a solitary polymer chain? The purpose of this presentation is to furnish hints to these intriguing interrogations. It endeavors to furnish a chemical perspective on this extraordinary phase change.

Biography:

Armand Soldera presently holds the position of a professor at the Université de Sherbrooke, Canada, since 2002. He also serves as the Vice-Dean Partnerships within the Faculty of Sciences. His research endeavors revolve around exploring the intricate relationship between micro and macro scales within the realm of soft matter, which encompasses polymers, liquid crystals, and organic glasses. To navigate this intricate terrain, he employs a holistic approach that combines simulations and experimental investigations, embracing a multi-scale methodology. A testament to his expertise and contributions, he coedited a book titled "Advanced Materials," which was published in 2020 by de Gruyter.

Metabolic Pathways Involved in The Biopolymer / Polyhydroxyalkanoates Production by Pseudomonas Sp. LFM046

Juliana Cardinali Rezende^{*a,b,c}, Mariana G. Ferrarini^d, Luiziana F. Silva^c, Marie-France Sagot^d, José Gregório^c. Gomez^c , Alexander Steinbüchel^b

^aCenter for Natural and Human Sciences, Federal University of ABC, Santo André, SP, Brazil

^bWestfalische Wilhelms-Universitat Munster, Institut fur Molekulare Mikrobiologie und Biotechnologie, Munster, Germany

^cUniversity of São Paulo, Institute of Biomedical Sciences, São Paulo, Brazil.

^dERABLE, Inria, 43, Bd du 11 Novembre, Villeurbanne, France.

Abstract:

Polyhydroxyalkanoates (PHAs) containing medium-chain-length 3-hydroxyalkanoates are produced from renewable resources by Pseudomonas sp. LFM046, isolated from sugarcane crop soil. The PHA monomer constituents will determine the mechanical properties and fields of application of this polymer. The complete genome sequence of this strain was obtained. The transcriptome analysis was carried out in order to understand which genes are differentially expressed when using fructose or glucose as sole carbon source. LFM046 strain was cultured in 400 mL of MSM containing 15 g I-1 of glucose or fructose, at 30°C and 150 rpm for 72 h. PHA accumulation increased with the time and differed in quantity and monomer composition between conditions (glucose and fructose). RNASeg was performed by Illumina HiSeg (2500) platform and 75% of the reads obtained were successfully mapped to the LFM046 genome. 166 differentially expressed genes was observed, being 99 up-regulated and 67 down-regulated in fructose (in comparison to glucose). COG enrichment analysis showed that up-regulated genes (active in fructose growth) were correlated with energy production and conversion while down-regulated genes with secondary metabolites biosynthesis, transport and catabolism. Pathway enrichment analysis showed that upregulated genes were related to carbon metabolism conversion, while down-regulated genes in fructose were involved in benzoate degradation and fatty acid metabolism. This study is essential to understand the cellular response at gene level, since it will predict changes in metabolism and evaluate the rationality of the successful PHA production in Pseudomonas sp. LFM046. Financial support: 2014/08061-1 and 2016/24290-6, São Paulo Research Foundation (FAPESP).

Biography:

Rezende is Biologist, Specialist in Microbiology, MSc and PhD in Genetics. Professor at Federal University of ABC and coordinator of the Genetics and Metabolic Engineering Laboratory (LGEM). Dr. Rezende developed post-doctoral project at the Bioproducts Laboratory (University of São Paulo) and was gest researcher at the Technical Institute of the University of Lisbon (Portugal) and in the Institute of Molecular Microbiology and Biotechnology, University of Münster (Germany) under the supervision of Prof. Alexander Steinbüchel. Dr. Rezende has developed activities involved in different projects whose main objective is to optimize the generation of bacterial PHAs using of renewable carbon sources.

Adhesive Bonded Joints in the Automotive and Transportation Industry: Experimental and Numerical Aspects

Pierre Jousset^{1*}

¹OST, Eastern University of Applied Sciences, Switzerland

Abstract:

Adhesive bonding is an innovative solution for assembling different parts together. Depending on the nature of the polymers used in the adhesive, the adhesive can resist either high loads or strong deformations. The use of adhesive is therefore suitable for many industrial applications where the mechanical loadings are of different nature. In the specific case of the automotive and transportation industries, bonding enables the assembly of lightweight material combinations such as aluminum and composites, thus helping to reduce CO2 emissions. Bonding is also useful where conventional methods such as welding cannot be applied. The use of bonding to accurately design products and structures in industry requires reliable material constitutive models that can effectively predict the mechanical behavior of polymers in finite element analysis. Validation of vehicle designs in procedures such as crash tests require describing the contribution of the adhesive from its undeformed state to full damage and failure.

The present work presents a procedure including experimental testing, parameter calibration, and numerical simulation to account for the behavior of adhesives in complex loading situations met in the automotive and transportation industry, where the adhesive damages and fractures.

The procedure is fast to use, has excellent results accuracy and can be perfectly integrated into industrial design processes.

Biography:

Pierre Jousset, 45, is for 8 years professor at the OST in Rapperswil, Switzerland He heads the department of joining technologies at the IWK, Institute for materials technology and plastics processing. Previously, Pierre worked for 10 years at Sika Technology in Zurich, Switzerland as a principal scientist in the field of simulation of bonded products and structures. Prior to that, Pierre worked for 3 years as a computer engineer in Munich/Germany for the automotive and aerospace industry. Pierre holds a PhD in structural mechanics from the UTC in France and lived in Paris until he was 20 years old.

Molecular Design and Understanding of Multifunctional Hydrogels from Fundamentals to Diverse Applications

Jie Zheng

Professor, Dept. of Chemical, Biomolecular, and Corrosion Engineering The University of Akron

Abstract:

Hydrogels, as versatile materials, hold tremendous potential for a wide range of applications. This work delves into the molecular design and comprehensive understanding of multifunctional hydrogels, covering fundamental principles and exploring their diverse applications. Through a combination of theoretical models, experimental investigations, and computational simulations, we unravel the intricate molecular interactions and structural properties of hydrogels. Additionally, we highlight the development of innovative strategies to tailor hydrogels for specific applications, including wound dressing, smart soils, antifreezing materials, antifouling coatings, actuators, sensors, and bioelectronics. I will also highlight the interplay between theory, experiments, and design in our research approach. By bridging the gap between molecular design and practical applications, this research aims to unlock the full potential of multifunctional hydrogels in various fields.

Biography:

Jie Zheng is Professor and Department Chair of Chemical, Biomolecular, and Corrosion Engineering at the University of Akron. He received his B.S. degree in Chemical Engineering from Zhejiang University, China in 1995 and Ph.D. degree in Chemical Engineering from University of Washington in 2005. He was a research scientist at NCI, NIH, before joining the faculty at U. Akron in 2007. He was then promoted to Associate Professor in 2012, Full Professor in 2016, and Departmental Chair in 2021. Zheng is the recipient of the NSF CAREER Award (2010), 3M Non-Tenure Faculty Award (2008), and Anton Award from National Resource for Biomedical Supercomputing (2010). He received the multiple times of Outstanding Research Award and Louis A. Hill Faculty Award at U. Akron. His main research interest focuses on design of better bio-inspired, bio-functional, and bio-mimetic soft materials for engineering and biomedical applications. He is author of 270+ journal papers, with a total citation of 20000+ times and an h-index of 75.

An Epoxy Silicon Hybrid Coating as a Solution to Lower Ice Adhesion Strength on Metallic Structures

Akré Simone Anne Adja^{1*}, and Sarah Sobhani^{1*}, Gelareh Momen^{1*}, Issouf Fofana^{1*}, Julie Carrière^{2*}

¹University of Quebec At Chicoutimi, Canada;

²Northern institute for research in occupational health and safety. Organization, Canada

Abstract:

Ice adhesion cause severe problems to outdoor infrastructures that may promote corrosion issues with time. In this contribution, a new icephobic epoxy-silicone based coating with additives is proposed to lower the ice adhesion strength on steel structures. Laboratory tests including ice adhesion strength, push off method, centrifugal adhesion along with durability using QUV-ageing machine show promise for real life applications.

Biography:

Akré Simone Anne Adja is graduated from a prestigious engineering school in Cote d'Ivoire (National polytechnique Institute Felix Houphouët-Boigny, Simone Anne Adja pursued her study in Canada and obtained a Master science degree chemical process where she specialized process modelling. Years later, she is now about to complete a phD in chemical engineering where she worked on functional materials namely coatings to address icing problems in artic environment. As a thirsty spirit of knowledge, she will never stop to learn new ways to address our daily concern in engineering.

Towards Biomimetic Polymers for Protein Recognition

lan A Nicholls^{1*}

¹Department of Chemistry & Biomedical Sciences, Linnaeus University, Kalmar, Sweden

Abstract:

Antibody-peptide/protein interactions are critical for many processes in the pharmaceutical and biotechnology industries, and as important tools for biomedical and biochemical research. Recently developed methods for synthesizing molecularly imprinted polymer nano-particles displaying antibody-like recognition of peptides and proteins can offer the possibility for substituting antibodies with these robust materials in applications where the structural integrity and function of antibodies can otherwise be compromised, e.g. by temperature, pH, solvent, etc..

The state-of-the-art of and future perspectives on the development of molecularly imprinted peptide and protein targeted antibody-mimicking nanoparticles shall be presented. Examples

based upon novel solid phase synthesis approaches which demonstrate sub-nanomolar binding shall be in focus. The value of rational design strategies employing all-atom, full-system molecular dynamics shall be highlighted, along with the use of fluorescence and quartz crystal microbalance (QCM) detection techniques for studying antibody-like recognition behavior.

Biography:

Ian A Nicholls is Professor of Chemistry and Dean of the Faculty of Health & Life Sciences at Linnaeus University (Sweden). After his BSc(hons) and PhD at Melbourne University (Australia, 1981-89), a lectureship at Victoria University (Australia, 1989), then post-doctoral positions at Cambridge University (UK, 1990-92) and Lund University (Sweden, 1992-1994), he held a series of lectureships at Lund (1994-1995) and Kalmar/Linnaeus University (1995-1999), he was appointed associate professor at Lund (1998), and professor of chemistry (Kalmar, 2000). His research is founded on an interest in molecular recognition and has a strong focus on biomimetic polymer development and application.

Birefringence Control of Photoalignable Liquid Crystalline Polymers and Application to Polarization Optical Devices

Nobuhiro Kawatsuki^{1*} and Hiroshi Ono²

¹Department of Applied Chemistry, Graduate School of Engineering, University of Hyogo, Shosha, Himeji, Japan

²Department of Electrical Engineering, Nagaoka University of Technology, 1603-1 Kamitomioka, Nagaoka, Japan.

Abstract:

Photoalignment is a promising technique for fabricating birefringent optical films and polarization sensitive diffraction devices. Photosensitive polymeric films are frequently used to attain anisotropic film-surfaces based on the polarization axis-selective photoreaction, which is combined with uniaxial or patterned alignment of curable liquid crystalline materials on them. On the other hand, we have carried out systematic study of photoalignable liquid crystalline polymers (PLCPs), which directly attain molecularly oriented structure of their own by the use of photo-exposure and thermally stimulated self-organization. In these cases, generated birefringence of the photoaligned film is one of the important issues to fabricate thinner optical birefringent devices. Herein, we present our PLCPs and their application to optical devices, which include high photoreactivity and controllability of the generated birefringence.

The photoinduced molecularly reorientation in liquid crystalline co(poly)methacrylates, which contains mesogenic side groups of a 4-oxycinnamic acid (CA), 4-oxybenzoic acid (BA), and 4-oxyphenyl aldehyde (PA), is explored using linearly polarized (LP) 313-nm light irradiation. Cooperative molecular reorientation can be achieved after annealing the exposed films. Then, in situ condensation reaction with oriented PA side moleties using phenylamine derivatives that exhibit higher inherent birefringence of the PLCP film, where the great improvement of the generated birefringence from 0.12 to 0.2 and more is achieved. Additionally, polarization optical devices such as polarization gratings and polarization Fresnel lenses using PLCPs are demonstrated.

Biography:

Nobuhiro Kawatsuki done BS in 1982 at Kyoto University, in 1984 done his MS in Kyoto University, he done his PhD in1994 at Kyoto University, He worked in 1984-1994 at Central Research Labs, Kuraray Co. Ltd. He became Assistant Professor in 1994, Himeji Institute of Technology (University of Hyogo), He worked as Associate Professor in1997 at U. of Hyogo, He worked as Professor in 2007 at U. of Hyogo, He became Dean of Graduate School of Engineering from 2015-2021 at U. of Hyogo.

Nanostructured Multi-Responsive Coatings for Tuning Surface Properties

Suzanne Giasson^{*1,2}, Alberto Guerron²

^{1,2}Laboratory of Engineering and Dynamics of Stimuli-Responsive Surfaces, Faculty of Pharmacie1 and Department of Chemistry2), Université de Montréal, Québec, Canada. *

Abstract:

Responsive polymer coatings can be used as functional elements in nanotechnologies such as valves in microfluidic devices, substrates for culture of biological tissues or in developing nanomaterials for targeted therapies in different diseases. However, such coatings usually suffer from major shortcomings such as lack of selectivity and poor environmental stability. The talk will present multi-responsive hierarchical polymer-based coatings aiming to overcome some of these limitations.

Two-dimensional arrays of thermo-responsive PNIPAM-based microgels and surface-functionalized with non-responsive or pH-responsive polymers, was covalently grafted to substrates to tune independently the surface chemistry and the swelling of the coatings using different stimuli. The ability of these microgels to independently control the swelling and surface properties using temperature and pH was investigated in aqueous suspension and as coatings using DLS and Surface Forces Apparatus. Polymer chain grafting did not impede the ability of cationic PNIPAM microgels to undergo a volume phase transition above the PNIPAM microgel transition temperature (VPTT), either in suspension or immobilized on a substrate. The microgels functionalized with PEG exhibited the most promising behavior. Indeed, their thermo-triggered swelling did not give rise to changes in the microgel surface properties (surface potential and adhesion) within a wide range of pH values. The immobilized microgel-co-PEG undergo a volume transition without change in adhesion, suggesting that the surface of the thermo-responsive microgels remains rather hydrophilic above the VPTT. This work confirms the possibility of tuning the swelling behavior of microgels without changing the adhesive properties.

Biography:

Giasson's current research program is on the development and investigation of responsive micro/ nano-structured surfaces and coatings whose physical properties and surface chemistry can be tuned independently and reversibly. Such responsive nanostructured materials are obtained by approaches using surface chemistry, polymer sciences and self-assembly. They enable significant advances in biomedical surface engineering and microfluidics. Her research efforts have led to the completion of several papers in refereed journals (PNAS, Nature, Soft Matter, Macromolecules, Langmuir, J. of Physical-Chemistry, J. of Pharmaceutical Science, J. Physics: Condensed Matter and others).

Developing Polypropylene for Extrusion-Based 3D Printing

Hans-Werner Schmidt*

Macromolecular Chemistry I and Bavarian Polymer Institute, University of Bayreuth, Germany

Abstract:

Polymer materials or material formulations specifically tailored towards extrusion-based additive manufacturing are of great interest. In this context, a miniature small-scale material processing and testing approach was developed as a screening method to evaluate novel polymer materials for fused deposition modeling (FDM). This approach is suitable for a small material input of less than 10 g using a mini compounder in combination with an injection molding machine to manufacture short rods, usable as FDM feedstock. Compared to conventional continuous filament extrusion, in which typically 2 – 10 kg are required. In order to demonstrate the approach, semi-crystalline commercial grades of polypropylene and polypropylene/ethylene random copolymer (raco PP) are processed into rods and compared to commercially available filaments. Most important is the optimization to reduce warp deformation caused by shrinkage without sacrificing interlayer bonding. In the technology field of additive manufacturing, the broad property profile of polypropylene offers enormous potential and is becoming increasingly important for the manufacture of 3D-printed products. For successful industrial 3D printing of polypropylene using established extrusion-based processes such as Fused Filament Fabrication (FFF), Fused Deposition Modeling (FDM) or Fused Granular Fabrication (FGF), three critical components are essential. First, the 3D printed material should have low warpage and high interlayer bonding strength. Second, the 3D printing build surface must allow reliable 3D printing of PP parts and non-destructive and residue-free removal of the product without need of additional adhesives. Third, a support material is needed to print more complex structures.

Biography:

Hans-Werner Schmidt studied chemistry at the University of Mainz (Germany) and ETH Zurich (Switzerland) and received his PhD in macromolecular chemistry from the University of Mainz. After a stay at DuPont Central Research in Wilmington (USA), he moved to the University of Marburg (Germany) to obtain his Habilitation. He was Assistant and Associate Professor with tenure at the Materials Department, College of Engineering at the University of California, Santa Barbara (USA). Since 1994 he is Full Professor for Macromolecular Chemistry at the University of Bayreuth. In 2018 he co-founded the PPprint GmbH, concentrating on 3D printing of polypropylene.

Extrusion Processes of Acrylonitrile Butadiene Styrene During the Material Extrusion Additive Manufacturing

Department of Mechanical and Aerospace Engineering, University of Texas, Arlington, TX

Abstract:

In material extrusion additive manufacturing, solid polymer filaments are fed into extruders to generate extrudates needed to build 3D plastic parts. There is a finite gap between the inner surface of an extruder and the edge of a filament, which facilitates the insertion of the filament inside the extruder. It is still not clear how this gap is filled during the extrusion. On the other hand, it is important to know this information, for example, to model the distributions of temperature

and pressure during the extrusion. In this work, the gap-filling processes of Acrylonitrile Butadiene Styrene (ABS) filaments are directly observed through a heated glass tube. The gap filling inside an extruder is found to be affected by curved profile and buckling deformations of the filament, conical geometry of the nozzle, and temperature of the extruder. When the extrusion reaches a steady state, the distributions of temperature and pressure inside the extruder are further explored. The corresponding results provide a better understanding of the extrusion process, which is important in choosing printing parameters.

Biography:

Cheng Luo obtained his PhD degree in May 2000, from the Department of Mechanical Engineering at the University of California at Berkley. Since September 2011, he has been a full professor in the Department of Mechanical and Aerospace Engineering at the University of Texas at Arlington. His research is related to solid mechanics, fluid mechanics, and manufacturing. His recent research focuses on polymer 3D printing. To date, he has published over 100 peer-reviewed papers in technical journals and conference proceedings.

In Situ Investigation of Polymer Structure Evolution with Neutron Scatteringa

Yingrui Shang^{*1}, Tyler Guin², George K. Larsen², Gergely Nagy¹, Carrie Gao¹, and Wei-Ren Chen¹

¹Neutron Scattering Division, Oak Ridge National Lab, Oak Ridge, TN

² National Security Directorate, Savannah River National Lab, Aiken, SC

Abstract:

Neutron scattering techniques are widely used for studying the conformational changes in polymer chains. Owing to the incoherent scattering inherent in hydrogen atoms within these chains, a mixture of fully deuterated and hydrogenated chains is commonly employed. This approach can facilitate the exploration of polymer chain conformation within bulk materials, utilizing neutron scattering methods. Traditionally, the fully deuterated macromolecules are synthesized from polymerization of deuterated monomers. This process, however, is not only costly but also timeintensive, thus limiting the application of neutron scattering techniques for studying alkene chain structures. While solutions with polymer chains in deuterated solvents are possible, the behavior of chains in dilute solutions can significantly deviate from their behavior in bulk. To address these challenges, a novel approach is proposed. The deuterated mineral oil as a solvent for alkene polymers is prepared. Polyethylene and polypropylene solutions within deuterated mineral oil and xylene are scrutinized using small-angle and ultra-small-angle neutron scattering at Oak Ridge National Laboratory. The results affirm that the behavior of PE and PP chains within this deuterated mineral oil solution mimics their behavior in bulk. By combining the power of deuteration and neutron scattering techniques, this approach emerges as a promising avenue for investigating the conformational evolution of polymer chains within bulk materials.

Biography:

Yingrui Shang's research interests focus on computational materials science with synergy of numerical modeling and polymer science. He is also responsible for the software development of drtSANS and other software projects for small angle neutron scattering at ORNL. Dr. Shang got his

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Ph. D. in polymer engineering from University of Massachusetts at Lowell. He joined Prof. Simon Billinge's research group at Columbia University and then was appointed as Associate Professor at Tianjin University, Tianjin China. He joined the SANS group as a Computational Instrument Scientist at ORNL in 2021.

Recent Progress on the Revolutionary Mechanical Recycle and Environmentally Friendly Molding based on Physical Degradation / Physical Regeneration Theory

Shigeru Yao*

Institute for Creation of Functional and Structural Materials, Fukuoka University, Japan

Abstract:

Mechanical recycling is an indispensable technology to solve the problem of the environmental load of waste plastics and to establish a resource circular economy. However, conventionally, waste plastics have been irreversibly deteriorated in mechanical properties due to chemical degradation accompanied by molecular chain breakage, and it has been said that they can be applied to almost onetime downgrade recycling.

On the other hand, from the basic investigation, we have found that the main cause of this deterioration of mechanical properties is physical degradation due to structural deformation inside of the plastic, and it is possible to improve the mechanical properties by optimizing the molding method. According to this investigation, we proposed the Physical Degradation / Physical Regeneration Theory. Furthermore, it has been clarified that this theory can extend to the environmentally friendly molding.

This presentation is based on results obtained from a project, JPNP20012, commissioned by the New Energy and Industrial Technology Development Organization (NEDO).

Biography:

Shigeru Yao, Doctor of Engineering, now is a Professor of Department of Chemical Engineering, Fukuoka University. He got his B Eng., M Eng., and Engineering Doctor's degree at Kyoto University. He worked at Ube Industries, Ltd. and Mitsubishi Research Institute, Inc.. From 2011, he is working at Fukuoka University. Currently Dr. Shigeru Yao is investigating focus on mechanical recycle process of waste plastics based on "Physical degradation and Physical regeneration theory". He also focuses on self-organization mechanism of polymer and especially the crystalline supramolecular interaction between side chain crystalline block copolymer and crystalline polymer.

Multivalent-Type Compounds Remarkably Enhance the Biological Activities

Koji Matsuoka*

^aDivision of Material Science, Graduate School of Science and Engineering,

^bMedical Innovation Research Unit (MiU), Advanced Institute of Innovative Technology (AIIT), & cHealth Sciences and Technology Research Area, Strategic Research Center, Saitama University, Sakura, Saitama, Japan

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Abstract:

Glycoproteins, glycolipids, and proteoglycans are known as glycoconjugates and these are generally existing on cell surfaces. In biological events, the glycoconjugates play roles not only as carriers of information in cell-cell interactions but as markers of cellular differentiation, aging, malignant alteration, and so on. The oligosaccharide chains of glycoconjugates are, therefore, the third chains of biomacromolecules next to nucleic acids and proteins. Since the saccharide chains have highly complex structures, functions of the glycoconjugates were not completely investigated.

Affinity of a monomeric saccharide chain against the appropriate protein, such as a carbohydratebinding protein, a lectin and an enzyme, is not so high, usually it is in the mM range. In the 70's, Lee reported remarkable enhancement of the binding affinity by means of multivalent-type sugar substrates, so-called "sugar clustering effect".1) The clustering effect has been expanded to other bioactive substances.2) In this presentation, our recent progress on design, synthesis, and biological evaluation of our multivalent-type substances will be discussed.

Biography:

Koji Matsuoka is a Professor of Material Science, Graduate School of Science & Engineering, Saitama University (SU), Saitama, Japan. He received a Bachelor degree from Seikei University in 1990 and a Ph.D. from Hokkaido University (with Prof. S.-I. Nishimura) in 1995. He did his postdoctoral research at RIKEN, Saitama, Japan. He joined Department of Functional Materials Science, Faculty of Engineering, Saitama University in 1995 as an assistant professor, and was promoted an associate professor in 2001 and professor in 2011. He has published more than 100 research articles and book chapters in organic chemistry and polymer chemistry field.

3D Printing of Bone Scaffolds Based on Starch and Active Hydroxyapatite

Bianca Chieregato Maniglia^{1*}, Pedro Augusto Invernizzi Sponchiado², Maryanne Trafani de Melo², Samile Bezerra de Aguiar², Pietro Ciancaglini², Ana Paula Ramos²

¹São Carlos Institute of Chemistry Universidade de São Paulo, Brazil

²Faculty of Philosophy, Sciences and Letters at Ribeirão Preto, Universidade de São Paulo, Brazil

Abstract:

3D printing enables the production of personalized bone scaffolds, and one potential biomaterial for this purpose is starch, a natural polymer that is biocompatible and biodegradable [1]. By incorporating hydroxyapatite nanoparticles (HA) replaced by strontium ions, these scaffolds can promote bone formation and reduce bone reabsorption [2]. In this way, this study aimed to explore the bioactivity of 3D-printed bone scaffolds using starch hydrogels and hydroxyapatite nanoparticles (HA) substituted with strontium ions (0, 50, and 100%). The HA nanoparticles were synthesized following a modified methodology based on Nassif et al. [3]. The scaffolds were printed using a BioedPrinterV4 3D printer (Bioedtech, Brazil). Various tests were conducted to evaluate swelling, biodegradability, cytotoxicity (using MC3T3-E1 pre-osteoblast cells and macrophages), and mineralization ability. Results showed that the HAp_100 scaffold exhibited the highest biodegradability, with 70% of degradation within 14 days. All scaffolds demonstrated significant swelling within 2 hours, but the swelling subsided afterward. Cytotoxicity tests revealed no negative effects on cells, with the HAp_100 scaffold showing positive results in cell proliferation. Scaffolds

containing HA nanoparticles displayed enhanced mineralization, which further improved with increased Sr2+ substitution. These findings highlight the potential of 3D-printed bone scaffolds incorporating starch and HA nanoparticles with varying Sr2+ levels. The scaffolds exhibited improved biodegradability, favorable cell response, and increased mineralization capacity. The 3D printing technology combined with the use of a cheap and widely available source, starch, added with an active additive, shows promise for effective application in bone regeneration in a personalized way.

Immunoactive Polysaccharides of Natural Origin - Complex Mechanisms of Immunomodulatory Activity

Jadwiga Turło^{1*}, Marzenna Klimaszewska¹, Beata Kaleta², Aleksander Roszczyk²

¹Department of Drug Technology and Pharmaceutical Biotechnology, Medical University of Warsaw, Poland

²Department of Clinical Immunology, Medical University of Warsaw, Poland.

Abstract:

Polysaccharides of natural origin are among the best known and strongest macromolecules with anti-cancer and immunomodulatory properties.

Although the structure-activity relationship (SAR) among polysaccharides is not clear, it is assumed that the determinants of their immunomodulatory activity are (among others) monosaccharide composition, water solubility, molecular weight, degrees of branching (DB) and triple helix conformation - with whereby the uncertainty of structural data at the atomic level makes this task much more difficult.

The literature reports show that the modification of the structure of polysaccharides carried out by biotechnological or chemical methods may cause a significant change in their biological activity.

In our earlier works we described the biosynthesis, isolation and immunomodulatory activity of selenium-containing polysaccharide fractions isolated from Basidimycota mycelial cultures. In our assumption, they were supposed to be selenium-containing analogues of the immunostimulating drug - lentinan. The results of structural studies were unexpected and showed that the obtained selenated polysaccharide fraction was a mixture of high molecular weight polysaccharides, structurally completely different from the leading structure. The results of preliminary studies on immunomodulatory activity were also surprising: the effect of Se-polysaccharides on the proliferation of human blood lymphocytes showed their selective immunosuppressive effect, opposite to the immunostimulating effect of most polysaccharides of fungal origin. In-depth studies of receptor binding, however, indicate a more complex mechanism of action and do not exclude some mechanisms of activation of the immuno suppressants, there is no simple and obvious answer yet.

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Development of Poly (lactic acid)/Poly (ethylene glycol)-Poly(propyl glycol)- Poly(ethylene glycol) Blended Nanofiber Membranes for Fog Collection

Mohammad Rezaul Karim

King Saud University, Saudi Arabia

Abstract: Not Available

Construction of Amino-Thiol Functionalized Ion-Imprinted Chitosan for Lead (II) Ion Removal

Jawza Sh Alnawmasi*

Department of Chemistry, College of Science, Qassim University, Buraydah, 51452, Qassim, Saudi Arabi

Abstract:

Ion-imprinting technique was used to create a lead ion-imprinted sorbent from an amino-thiol chitosan derivative (Pb-ATCS). First, 3-Nitro-4-sulfanylbenzoic acid (NSB) unit's amidized the chitosan, and then the -NO2- residues were selectively reduced to -NH2. Imprinting was accomplished by cross-linking with epichlorohydrin and removing the Pb (II) ions from the across-linked polymeric complex formed from the amino-thiol chitosan polymer ligand (ATCS) and Pb (II) ions. The synthetic steps have been investigated by nuclear magnetic resonance (NMR) and Fourier transform infrared spectroscopy (FTIR), and the sorbent was tested for its ability to selectively bind Pb (II) ions. The produced Pb-ATCS sorbent had a maximum capacity of roughly 300 mg/g, and it showed a greater affinity for the Pb (II) ions than the control NIATCS sorbent particle. The pseudo-2nd-order equation was also consistent with the adsorption kinetics of the sorbent, which were quite rapid. This demonstrated that metal ions were chemo-adsorbed onto the Pb-ATCS and NI-ATCS solid surfaces via coordination with the introduced amino-thiol moieties.

Residence Distributions Methodology an Approach to Modeling Stress History and Pharmaceutical Properties

David I Bigio

Mechanical Engineering Department, Advanced Manufacturing Laboratory, University of Maryland

Abstract:

Twin Screw Extruders (TSE) are traditionally used to compound base polymers with additives to improvise the properties of the extrudate. Quantification of mixing in the TSE is essential towards understanding the influence of screw configuration and geometry on the properties of the extrudate. The Residence Stress Distribution (RSD) is an in-line, experimental method to quantify the stress in a melt that induces dispersion. The RSD method uses the percent break-up (%BU) of stress-sensitive micro-beads to quantify the stress history in a twin-screw melt at any set of operating conditions. Using the %BU information across an operating condition domain, a predictive equation is generated to estimate the stress level in a melt as a function of operating

conditions. Various studies have shown the capability of the RSD approach to quantify the stress history of different screw geometries, and extruder diameters. Furthermore, predictive equations are generated with the variables of screw speed, specific throughput, and barrel temperature. Results show that increases in screw speed and specific throughput increase the %BU, while increases in barrel temperature decrease the percent break-up. In addition, the effect of screw speed and specific throughput is lessened as the barrel temperature increases. These equations allow for prediction and control of a twin-screw compounding process with three separate operating conditions. Numerical simulations are used to validate and illuminate the findings.

The effect of extrusion on degradation of an active pharmaceutical ingredient is considered, as well as the effect on water content of the extrudate. These properties were measured across an operating condition range of screw speed, specific throughput, and barrel temperature. From the property response, predictive equations for degradation and water content were generated as a function of the significant operating conditions. Results showed that barrel temperature increases the degradation and decreases the water content of the extrudate. Conversely, specific throughput decreases degradation and increases water content. When designing a pharmaceutical extrusion process, the tradeoffs between these two properties must be evaluated by examining the magnitude of the barrel temperature and specific throughput effects across the operating domain.

Biography:

David Bigio has been engaged in the field of polymer processing for over 30 years. He received his Ph.D. from M.I.T. in 1986. His research focused on mixing phenomena in extruders in which he studied the nature of mixing in a co-rotating twin screw extruder. He holds 4 patents and has published fifty journal papers and over one hundred conference papers. Since joining the faculty of the University of Maryland at College Park, he has established the Polymer Processing Laboratory which is engaged in research dedicated to the quantification of mixing as a basis for extruder performance evaluation. The concept has been applied to various polymer processes like reactive extrusion, devolatilization, and blend compatibilization for both individual companies and the Polymer Mixing Program - an Industrial Partnership. He was the PI for two NSF-Goali programs - one focused on establishing a novel controls approach to extrusion processes and one involved with a novel design for the next generation of injection molding machine. The first GOALI project supported the creation of a Twin Screw Injection Molding Extruder -(TIME) a device which performed compounding and injection molding in one process. The device and process has received two patents and is being licensed for manufacture. The second NSF-Goali award was with duPont as our partner. The concept was to create a physics based approach to understanding residence distributions as a function of operating conditions, materials and screw design. The goal of the project is to design and implement a control system using a peroxide initiated degradation in the polymer extruder to regulate specific product viscosity. This work has led to a comprehensive study of transient behavior and controls of polymer processes. His overarching theme has been exploring the question, "Is there an overriding kinematic approach to modelling the mixing in a twin-screw extruder that can be applied to specific processes?" This has led to the development of the RxD and RSD Methodologies for modeling extruder performance.

Compatibilization of Polyolefins through Dynamic Covalent Crosslinking

Yinghua Jin^{1*}, Wei Zhang², and Rong Long³

¹RockyTech, Ltd.; ²University of Colorado, Boulder, USA

Abstract:

Plastics have become an indispensable component of modern society, driving unparalleled advancements in both technological domains and everyday conveniences. Since the invention of synthetic polymers, over 9.5 billion tons of plastics have been produced globally. However, less than 10% of this vast amount has been recycled, with the majority ending up in landfills, posing severe threats to the environment and our ecosystems. A primary hurdle in plastic recycling is the challenge of sorting. Different types of plastics aren't compatible, and frequently, multiple plastics are combined in a single product, complicating the sorting process. For example, polyethylene (PE) and polypropylene (PP), together constituting over 60% of synthetic plastic production, share similar chemical compositions and densities and frequently coexist in diverse product designs, making their separation challenging. Unfortunately, blends of these two plastics are incompatible and result in diminished mechanical properties and stability. In this study, we present a compatibilization technique of PE and PP using dynamic covalent chemistry. This approach aims to upcycle mixed blends of PE and PP by enhancing their mechanical properties, viscosity, and molecular weight.

Biography:

Yinghua Jin obtained her Ph.D. from University of Illinois at Urbana-Champaign (UIUC) in 2006. She is the co-founder and CTO of RockyTech. Her research focuses on the development of soft materials including polymers, composites, biomaterials, and nanosized discrete molecules. She published over ~120 peer-reviewed journal articles, edited one book, and holds four US/ International patents in the related area.

Extraction and Characterization of Cellulose Nanocrocrystals from Corn Husk Wastes and its Application in Film Preparation.

Sergio Mayta^{*a, b}, Ronny G. Huamani-Palominoa , Bryan M. Córdovaa , Ernesto Riverac and María Quintanab

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Abstract:

Corn is the most cultivated cereal in the world; however, only 20% of the total plant mass

corresponds to the edible part, leaving the rest as wastes whose valorization is still a challenge. In particular, in Peru, corn crop residues are generally disposed of by open-air burning, impacting the soil and releasing greenhouse gases. Under this context, this research focuses on the valorization of Peruvian corn wastes into cellulose nanocrystals (CNC) using both mechanical (drying, milling, and sieving) and chemical treatments (alkaline treatment, bleaching, acid hydrolysis, dialysis, and ultrasonication) combined. Cellulose was extracted by a novel bleaching agent (peracetic acid), with a yield of 79.4%, and a purity of 70.3%. The average hydrodynamic diameter of the isolated CNC was determined by dynamic light scattering. The nanocrystal dimension was found to be 423 nm, furthermore, for comparison purposes, commercial CNC was also prepared and the dimension was found to be 218 nm. At the same time, the effect of lowfrequency ultrasonication was also studied, varying the time lapse in the range of 5 to 30 minutes, it was found that even the shortest period decreased the average size up to almost half the original size (234 nm), while the higher produced particles with a diameter of 204 nm. Finally, CNCs films were obtained by casting method. These films were highly transparent and brittle. Simultaneously it was verified that they had good resistance to acid (sulfuric acid) and alkali (sodium hydroxide) up to concentrations of 25% and 40%, respectively.

Biography:

Sergio Mayta received his bachelor's degree in chemical engineering at Universidad Nacional de Ingenieria, Peru with the highest honors. As an undergraduate, he investigated the extraction of cellulose from crop wastes. After graduation, he followed specialization studies in quality, safety, and environmental management and joined to the Center for the Development of Advanced Materials and Nanotechnology of the same university. Currently, he is a grad student, and his research focuses on the development of strategies for the valorization of lignocellulosic biomass into bio-based (nano)materials. Sergio has organized a bunch of academic events and has also participated in several congress around Peru, Brazil and the U.S.

Effect of NMP on the Holographic Data Storage of a Photosensitive Polymer

Junchao Jin¹, Po Hu1, Jinhong Li¹, Jie Liu¹, Mingyong Chen¹, Zuoyu Zhang¹, Junhui Wu¹, Zeyi Zeng¹, Qingdong Li¹, Li Wang¹, Yuhong Ren^{1,2}, Xiao Lin^{1,2}, Xiaodi Tan^{1,2*}

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Abstract:

Photopolymer are considered as the most promising holographic storage materials due to their high resolution, real-time recording, low cost and easy preparation. Traditional organic recording materials such as phenanthraquinone-doped poly(methyl methacrylate) (PQ/PMMA) have low diffraction efficiency and low photosensitivity, which greatly limit the storage capacity and recording speed of holographic data storage. Currently reported methods to improve holographic performance include doping nanoparticles (such as aluminum, silica, graphene oxide, etc.), changing the type of photosensitizer, increasing the copolymer, etc. We were surprised to find that holographic storage materials with high sensitivity, high diffraction efficiency and negligible

volume shrinkage were successfully prepared by the introduction of organic solvent NMP. The photosensitivity, diffraction efficiency and volume shrinkage reaching 2.06 cm/J, ~ 82% and ~ 0.1%, respectively. Further analysis showed that NMP had a certain anti-polymerization effect, and increased the content of C=C by reducing the molecular weight of PMMA, so as to improve the photosensitivity. Additionally, during exposure, there is an interaction between NMP and the photosensitizer PQ that speeds up the formation of PQ free radicals. Finally, collinear holographic systems with NMP-PMMA/PQ have the potential for quick and low bit error rate holographic information storage.

Keyword Holographic date storage, high diffraction efficiency, high sensitivity, photopolymer

Biography:

Xiaodi Tan is a professor at the College of Photonic and Electric Engineering in Fujian Normal University. His doctoral thesis was completed at the University of Tokyo in 2001. He was a Senior Engineer in Optware Corporation and later worked for Sony Corporation as a Senior Technology Analyst and Optical Technology Manager of Core Device Development Group. His overall research area is information optics and photonics with a focus on holographic storage, optical information display, and optical devices.

Novel Chain Extenders for Polyester

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Abstract:

The main goal of this work is to develop novel chain extenders that enable the use of recycled polyester for value-added applications. The proposed work will offer a closed-loop approach to polyester recycling. Commercial epoxy chain extenders (CEs) such as Joncryl ADR have various disadvantages, including the side reactions (branched/crosslinked reaction) and presence of styrene monomers resulting from depolymerization of polystyrene at higher temperatures which affecting the central nervous system. Moreover, the presence of glycidyl methacrylate (GMA) is potentially carcinogenic at high concentrations. This study aims to create polystyrene and/or GMAfree CEs that allow using polyester for additional-value applications. The new CE was prepared by free radical polymerization and characterized by 1H NMR spectroscopy, intrinsic viscosity, size exclusion chromatography, differential scanning calorimetry and Thermogravimetric analysis. The polyester, such as polyethylene terephthalate or polylactic acid, was blended with the new CE (very small amount) using reactive melt extrusion and injection molding techniques. The mechanical and thermal characteristics of polyester prepared with the new CE were estimated and compared with those of corresponding polymers prepared with the commercial chain extender. The outcomes displayed in this work open new opportunities for enhancing cost-effective polyester for packaging applications.

Biography:

Mohamed A. Abdelwahab was completed his undergraduate degree in Chemistry at Tanta University, Egypt. He has a M.Sc. in Polymer Chemistry from Tanta University, Egypt. In-2012, he continued his studies at Pisa University, where he received his Ph.D. degree in Biomaterial.

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He joined Tanta University Chemistry staff in 2012 as an Associate Professor. Dr. Abdelwahab worked as a Post-Doctoral at University of Guelph, Canada. Currently, Dr. Abdelwahab works as a Research Associate in the School of Packaging, at Michigan State University, USA. His main research interests are polymer science, nanocomposites, biopolymers, and sustainable materials.

Structural and Bioinformatic Studies of the Cellulose Synthase CESA5 Of Physcomitrium Patens and its Product – In Vitro Synthesized Cellulose Microfibrils.

B. Tracy Nixon^{*1}, Mark A. Frank¹, Lynn A. Massenburg^{1,2,} Sung Hyun Cho¹, Matthew T. Swulius³, Hui Yang¹, Andrew F. Neuwald4, Hugh O'Neill², Frank Deligey⁵, Alex Kirui⁵, Frederic Mentink-Vigier⁶, and Tuo Wang⁵.

¹The Pennsylvania State University-University Park, USA; ²Oak Ridge National Lab, USA; ³The Pennsylvania State University – Hershey, USA; ⁴University of Maryland, USA; ⁵Louisanna State University, USA; 6National High Magnetic Field Laboratory, USA

Abstract:

Cellulose, the most abundant biopolymer, is a central source for renewable energy and functionalized materials. In-vitro synthesis of cellulose microfibrils (CMF) has become possible using purified cellulose synthase (CESA) isoforms from Physcomitrium patens and hybrid aspen. The exact nature of these in-vitro fibrils remains unknown. Here, we characterize in-vitro synthesized fibers made by CESAs present in membrane fractions of P. patens over-expressing CESA5 using cryo-electron tomography and Dynamic Nuclear Polarization (DNP) solid-state NMR. DNP enabled measuring two-dimensional 13C-13C correlation spectra without isotope-labeling of the fibers. Results show structural similarity between in-vitro fibrils and native cellulose microfibrils in plant cell walls. Intensity quantifications agree with the 18-chain structural model for plant CMF and indicate limited fibrillar bundling. The in-vitro system thus reveals insight into cell wall synthesis and may contribute to novel cellulosic materials. The integrated DNP and cryo-electron tomography methods are also applicable to structural studies of other carbohydrate-based biomaterials. Finally, based on cryoEM structure of CESA5 and bioinformatic analysis of its sequence using our two programs Deep Analysis of Residue Constraints (DARC) and Structural Properties Associated with Residue Constraints (SPARC), we map functionally crucial residues to the CESA5 structure that could be altered to change its function and potentially create novel properties in the synthesized cellulose microfibrils.

Molecularly Imprinted Polymers as Recognition Elements in Acoustic, Electrochemical or Optical Sensors to Detect Pesticides or Drugs in Water

Maria Teresa S. R. Gomes*; Alisa Rudnitskaya, Sílvia Reis, Marta Veríssimo

CESAM, Department of Chemistry, University of Aveiro, Aveiro, Portugal.

Abstract:

Sensitive selective and reliable sensors are needed for a variety of purposes and in all aspects of modern life. Controlling the quality of water is mandatory, and among the known threats are the presence of pesticide residues, employed to control pests on fruits and vegetables, or to control

weeds. Residues of medicines and their metabolites, as the ones found in aquaculture, are also a matter of concern. For each threat, chemists need to find a recognition element, with a high degree of selectivity regarding other possible interfering compounds.

Numerous examples of sensing layers for different applications can be found in the literature, ionophores for many metals are commercially available, and synthesis of molecular receptors are being regularly published. However, the so called "chemosensors" are often water soluble, and molecular receptors for many of the pesticides and drugs are not known. Molecularly imprinted polymers (MIPs) may be prepared by making the polymerization in the presence of a mold, the target molecule itself, and in the presence of a crosslinker that helps the final structure to retain its shape. After removing the target, a molecularly imprinting polymer with cavities and chemical groups compatible with the analyte were obtained. Practical examples of sensors based on MIPs and different transducers (piezoelectric, optical, and electrochemical) will be presented. Sensors performance and advantages and difficulties of using MIPs will be discussed.

Biography:

MTSR Gomes obtained a degree in Chemical Engineering at the University of Coimbra in 1983. She became a teacher assistant, until 1997, when she obtained a PhD at the University of Aveiro with the thesis "Development of sensors based on piezoelectric quartz crystals for CO2 and SO2". At the present she is an associate professor at the University of Aveiro. Her current scientific interests are in the areas of analytical chemistry and sensors. She published around 80 WOS papers, 30 other papers, 4 book chapters, and presented more than 100 communications. She is the president of lbersensor.

Fabrication and Characterization of Hydrogen Peroxide and Thymol Loaded PVA/PVP Hydrogel Coatings as a Novel Anti-Mold Surface for Hay Protection

Eyal Malka^{1*} Ayelet Caspi², Reut Cohen³ and Shlomo Margel⁴

^{1,3,4} Chemistry Department, Bar Ilan University, Institute for Nanotechnology and Advanced Materials (BINA), Israel; ²TAMA group, Israel.

Abstract:

Animal food source production is increasing due to the growing world population. Many sources (e.g., hay) are prone to mold development resulting in food degradation. This study proposes an environment friendly anti-mold fungicide comprising hydrogen peroxide (HP) and thymol entrapped in a polyvinyl alcohol/pyrrolidone (PVA/PVP) hydrogel (PVA is biodegradable and PVP is water soluble non-toxic) coated on a polyethylene (PE) film for preservative hay packaging. The hydrogel improved the thermal stability of the entrapped HP and thymol, resulting in a prolonged release into the hay thereby increasing anti-mold activity. The hydrogel composition and morphology, thymol and HP thermal stability, and release rates through indirect (gas phase) contact were investigated. Fungicidal capabilities were tested, indicating wide range efficiency against mold growth on hay with a clear advantage for the thymol-loaded hydrogels. No visual side effects were observed on hay exposed to the released fumes of HP and/or thymol. These results demonstrate the potential of thymol-loaded hydrogels as effective and safe post-harvest preservatives.

Biography:

Eyal Malka is a doctoral student in polymers chemistry, under the supervision of Professor Shlomo

Margel. My research focuses on polymers for the controlled release of agricultural pesticides. I have industrial solid background in analytical chemistry and microbiology. In my MSc, I researched the anti-bacterial Synergism of Nano metal oxides, under the supervision of Professor Aharon Gedanken. The research yielded a novel composite with synergistic anti-bacterial and anti-biofilm properties, which was written under patent and followed with an article. Later, the patent was commercialized by Sonovia company.

Mechanical Properties of a PU Foam for Vehicle Safety Design Guided by a Novel Approach for Foam Chemistry Optimization

Anindya Deb^{1*}

Indian Institute of Science, India

Abstract:

Polyurethane (PU) foam is widely used in various day-to-day products for its versatility, customizability, and high specific stiffness as well as strength. A type of PU foam referred to as 'rigid' or 'crushable' can play a crucial role in enhancing occupant safety in vehicle crashes by minimizing injury through impact energy absorption. Efficient design of safety countermeasures based on such a foam calls for proper estimation of its engineering properties. It is well-known that formulation of a PU foam is preceded by complex chemical reactions typically involving a polyol and an isocyanate in the presence of a catalyst and a blowing agent. The mixing ratio of the main compounds is a key parameter for ensuring the consistence of a closed-cell foam. In the current exposition, a novel approach is demonstrated according to which the most desirable mixing ratio for a PU foam is identified by experimentally maximizing stiffness and mean strength while maintaining density as constant. The link between mechanical behavior and PU foam chemistry is further confirmed through SEM micrographs of foam cells. Armed with the desired mixing ratio, the dependence of foam properties notably plateau strength on density is demonstrated through compression tests performed on cubical foam samples. Additionally, impact tests on foam samples are carried out in a drop-weight test setup for capturing the dependence of foam strength on strain rate which is required for robust numerical prediction of the behavior of a foam-based countermeasure subjected to impact as in vehicle crashes.

Biography:

Anindya Deb is a Professor in the Centre for Product Design and Manufacturing, Indian Institute of Science, Bangalore. He heads the CAR (Creative Automotive Research) and Impact Safety Engineering Laboratory which he founded. He has published more than 200 papers in journals and conferences, and has obtained 6 patents. He previously worked with Ford Motor Company, Michigan, SDRC, Ohio, and Tata Motors, Jamshedpur, India. He was an Adjunct Lecturer in the Department of Mechanical Engineering, University of Michigan at Dearborn. He is a Fellow of the Indian National Academy of Engineering, and is an SAE (Society of Automotive Engineers) Fellow.

Free-Standing Polymer Thin Films for Delivery of Drugs or Stem Cells

Shinji Takeoka*

Faculty of Science and Engineering, Waseda University, Japan

Abstract:

Free-standing polymer thin films with a thickness of 10 to several hundred nanometer can be easily prepared by the application of printing technology and have a unique property that they can be applied to biological surfaces without using adhesives or glues owing to their very low bending rigidity and high adhesive surface force. In addition, various functions can be introduced by layering a plurality of thin films with drugs or cells. We are conducting experiments to evaluate the effects of loading antibiotic crystals, stem cells and spheroids onto free-standing polymer thin films of biodegradable and biocompatible polymers with a thickness of tens to hundreds of nm. We are immobilizing them on the wound areas in mouse models of infection and diabetes mellitus. I will talk from the introduction of free-standing polymer films (nanosheets) and porous nanosheets, antibiotic crystals-loaded nanosheets, porous nanosheets for cell transplantation, pristine nanosheets for spheroids transplantation, transplantation of spheroids with porous nanosheets for spheroids transplantation.

Application of Polymeric Scale Inhibitor Colloidal Materials for Oilfield Mineral Scale Control

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Department of Civil and Environmental Engineering, Faculty of Science and Technology University of Macau, Taipa, Macau

Abstract:

Mineral scale refers to the hard crystalline inorganic solid deposit from the water phase. Although scale formation is very common in natural environment, deposited scale particles can result in serious threats to the integrity as well as safety of various industries particularly oilfield productions. Scale deposition is one of three most serious water-related production chemistry threats in petroleum industry. The most commonly adopted engineering approach to control scale threat is chemical inhibition by applying scale inhibitor chemicals. Aminophosphonates and polymeric inhibitors are two major groups of scale inhibitors. To address the drawbacks of conventional inhibitors, scale inhibitor colloidal materials have been prepared as an alternative delivery vehicle of inhibitors for scale control. Quite a few studies have reported the laboratory synthesis and testing of scale inhibitor colloidal materials composed mainly of pre-precipitated metal-aminophosphonate solids. However, limited research has been conducted on the preparation of polymeric inhibitor based colloidal materials. In this study, we report the synthesis approach and laboratory testing of a novel polystyrene 2 sulfonate (PSS) based inhibitor colloidal material. PSS was selected in this study due to its high thermal stability and calcium tolerance with no phosphorus in its molecule. Both precipitation and surfactant surface modification methods were employed to prepare a barium-PSS colloidal inhibitor (BaPCI) material with an average diameter of several hundred nanometers. Experimental results indicate that the prepared BaPCI material has a decent migration capacity in formation medium and this material is superior to the conventional PSS inhibitor in terms of inhibitor return performance. The prepared novel BaPCI material has a great potential to be adopted for field scale control where environmentally friendly, thermal stable, and/or calcium tolerating requirements should be satisfied. This study further expands and promotes our capacity in fabrication and utilization of functional colloidal materials for mineral scale control.

Key words: mineral scale; scale inhibitor; polymer; colloid; transport

Engineering Nonconventional Lignin to Improve Biomass Saccharification

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Abstract:

Lignin is a complex heteropolymer that makes plant woody biomass processing difficult. Lignin bioengineering holds a promise to optimize plant feedstock with reduced recalcitrance. We have been designing different bioengineering strategies to alter lignin polymer structural and/ or physicochemical properties in energy crops. This includes to use one of our engineered monolignol 4-O-methyltransferases (MOMTs) to alter lignin composition and chain length. In fieldgrown poplar trees harboring expressed MOMT4, an approximately 80% reduction in syringyl lignin subunits and 45% increase in guaiacyl subunits occurred in their remaining lignin. Gel permeation chromatography analysis unveiled an increased Mw and decreased Mn in the biomass of transgenic poplars, which leads to a polydispersity index from 3.9 of the control sample to 5.6 of the transgenic wood. Meanwhile, NMR study revealed a 2~3-fold increase of lignin end group units (cinnamyl alcohols) in transgenic plants. These data implicate a hyper branching and more heterogenous lignin/cell wall biopolymer produced in the MOMT4 transgenic poplars. Moreover, expression of MOMT4 resulted in the production of novel flavanonols in planta that act as nonconventional monomers and incorporate into lignin polymer forming novel flavanonol-lignin. As consequence of alteration in lignin composition and physical property, the saccharification efficiency of transgenic woody biomass was increased up to 178%, and the fermentative ethanol yield with non-pretreated transgenic wood substantially exceeded that of the control wood even with intensive alkaline pretreatment. Our study suggests an applicable strategy for optimizing plant feedstocks to produce low-cost biofuels.

Biography:

Chang-Jun Liu, completed Ph.D. in plant biochemistry and molecular genetics, he is a Senior Scientist and Principal Investigator in Biology Department, Brookhaven National Laboratory, and he done a Scientific/ Project Lead in the U.S. Department of Energy's Bioenergy Research Centers. His research focuses on plant phenolic and lignin biosynthesis and plant cell wall biology.

Posters

Insitu Change of Polymer Glass Transition Temperature According to Gas Saturation by Temperature in High Pressure Vessel

Kwan Hoon Kim¹ and Jin Hong², Sung Woon Cha^{3*}

^{1,2,3}Yonsei University, Korea;

Abstract:

Polymer materials are widely used as substitute materials for metallic and ceramic materials. As the amount of polymer materials used increases, the development of a process capable of processing polymer materials is also developing. In order to apply a method such as an Microcellular foaming process technology using gas, it is necessary to predict a change in the mechanical properties of a

polymer according to the amount of gas dissolved. That is, if the change in the physical property value according to the gas solubility is not predicted, it is difficult to control and develop the process using gas. A typical property is the glass transition temperature.

There are several ways to measure the glass transition temperature, such as DSC, DTA, and DMA, but these methods cannot be measured under high pressure. Therefore, this research devised a device that can measure changes due to glass transition temperature by saturated CO2 gas in PMMA specimens in high pressure vessels, and conducted an experiment to measure changes in polymer in real time.

In fact, it can be confirmed that the glass transition temperature decreases as the solubility of gas increases. But the change due to the fluidity of the gas according to the temperature could not be confirmed. However, in this study, changes in glass transition temperature can be measured through real-time changes in polymer materials in gas flow according to temperature.

Tunable Heating Rate Sensitive Triple Shape Memory Polymer

Robert D. L. Jerusalem * and Frank Katzenberg, Michail Maricanov, Joerg C. Tiller

Biomaterials & Polymer Science, Department of Biochemical and Chemical Engineering TU Dortmund, 44221 Dortmund, Germany

Abstract:

Shape Memory Polymers (SMPs) are known to respond to multitude of external triggers, such as heat, light, solvents, and others. Powerful SMPs can be created by crosslinking a polymer to a degree of crosslinking right at the borderline between thermoplastics and elastomers. If done properly this creates an SMP with the properties of the original polymer. Dependent on the amount of phase changes, multiple temporary or intermediate shapes can be observed. In previous work, critically crosslinked x-sPP was tailored to realize the first heating rate sensitive triple shape memory polymer by exploiting the kinetics of the phase transition between two crystalline forms, where the height of the intermediate state correlates to the heating rate.[1] In this work we follow a new approach to SMPs by co-crosslinking two polymers. This allows us to specifically tailor the properties of the resulting co-network. Using a semi-crystalline polymer as a basis and adding a partially miscible amorphous polymer allows control over the crystallization kinetics in the co-network by altering the composition and/or degree of crosslinking and thus adapting the sensor to its potential application. [1] https://doi.org/10.1021/acsami.6b04177

R. Hoeher, T. Raidt, F. Katzenberg, and J. C. Tiller Biomaterials and Polymer Science, Department of Biochemical and Chemical Engineering, TU Dortmund, 44221 Dortmund, Germany

Biography:

Robert David Ludwig Jerusalem is a PhD student under Joerg C. Tiller at the chair of Biomaterials & Polymer Science in the department of Bio- Chemical- Engineering at the TU Dortmund. He studied Chemical Engineering in Dortmund.

Critical Crosslinking as a Tool for Innovative Polymer Properties

Frank Katzenberg* and Robert D. L. Jerusalem, Michail Maricanov, Joerg C. Tiller

Biomaterials & Polymer Science, Department of Biochemical and Chemical Engineering TU Dortmund, Dortmund, Germany

Abstract:

Cross-linking to a small degree right at the borderline between thermoplastics and elastomers, referred to as critical cross-linking, is a suited tool to render a thermoplastic into a smart material that shows at least a shape memory effect with storable strains up to 1000%. Dependent on kind of the chosen polymer this tool can be used to tailor other amazing properties – such as cold programmability, tuneablity of trigger temperature, multi-shape memory, heating rate sensitivity, shock- and energy-absorption capability, oriented crystallization beyond the possibilities of common crystallization kinetics – to commercial thermoplastics. A potpourri of smart and responsive properties will be demonstrated using the examples of critically crosslinked natural rubber (NR), polypropylenes (PP), polyethylenes (PE), polyvinylidene fluoride (PVDF), polyethylene terephthalate (PET) and others.

Biography:

First Author is the head of the polymer physics group at the chair of Joerg Tiller in the department of Bio- and Chemical Engineering at the TU Dortmund. He studied physics in Dortmund and did his dissertation there. After a stay as head of the resource thin film-technique at Fraunhofer IBMT in St. Ingbert, Germany, he returned to the TU Dortmund in 2001 and habilitated there. He is an expert in the area of shape memory polymers and known for critical cross-linking of thermoplastics.

Development of Biomedical Polymer Using Microcellular Foaming Process and Bacterial Cellulose

Jin Hong¹, Gukhyeon Yun², Kwan Hoon Kim² and Sung Woon Cha^{3*}

^{1,2,3}Yonsei University, South Korea

Abstract:

With the rapid growth of the high-tech convergence industry, research on new materials with high-added value is being actively conducted. Bacterial Cellulose (BC) is a biodegradable, non-toxic natural substance that can be obtained by culturing bacteria. It can be approached in various ways from physical, chemical, and biological points and is called a dream material due to its lightweight and stable thermal stability.

The microcellular foaming process was created using a technology based on the saturation of the polymer by supercritical CO2 and rapid decompression. An increase in saturation pressure leads to an increase in the molecular potential energy of CO2, which can be more easily compressed into the cellulose matrix.

This study is the friction and wear characteristics of microcellular foamed BC pellicle. Cellulose material is fabricated through physical foaming using a batch process. Specimen membranes produced by Komagataeibacter Xylinus were saturated with 10 MPa of CO2 for 4 h and foamed at

160 °C with saturation. And then on dry ice.

Friction and wear tests were performed using a pin-on-reciprocating type tribometer. After fixing the ball on the top of the device by applying a constant force with a 5 mm diameter stainless steel ball, microcellular foamed BC and non-foamed BC were fixed on the moving plate at the bottom, and the reciprocating motion was performed.

The microcellular foaming process significantly increased the wear characteristic and friction coefficient of BC. It can be used to scaffold the human body, especially artificial cartilage, and other biomedical polymer.

Potential Food Packaging Antibacterial Contact Surfaces: PLA dopped by Copper Double Salts

Olga Martin^{*1} Xiomara Santos¹, Diogo Videira², Juana Rodriguez², Francisco Guillen², Gemma Montalvo², Javier Pozuelo¹

¹Universidad Carlos III de Madrid, Spain

²Universidad de Alcalá, Spain

Abstract:

The globalization of the market, as well as the increasing world population, which requires a higher demand for food products, pose a great challenge to ensure food safety and prevent food loss and waste. In this sense, active materials with antibacterial properties are an important alternative in the prolongation of shelf life and food safety. In this work, the ability of copper (II) from doble salt hydroxy nitrate (DSN) or hydroxy phosphate (DSP) was evaluated inside a degradable polylactic acid, PLA, polymer film matrix. The antibacterial properties of films against Listeria monocytogenes and Salmonella enterica were evaluated by surface contact test, in which a bacterial cell reduction of at least 8 to 9 logarithmic units. The migration and cytotoxicity of the composites were evaluated, demonstrating the safety of these materials, which reinforces their potential use in food packaging applications.

Biography:

Dra Olga Martin Cádiz Ph in Physical-Chemistry at the University of Alcalá (Spain). Predoctoral research at Catalysis Department of Poitiers University (France), and Polymer Institute University of Akron (USA). Currently was a professor in Materials Science and Engineering at the University Carlos III of Madrid. In recent years, it has been leading a project of ecological transition in cooperation with a microbiology group at the University of Alcalá, forming biodegradable polymers with bactericidal properties generating several Q1 publications and 2 international Ph.D. theses, h-index=9.

Spray Deposited Functional Polymer Nanocomposites

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Abstract:

Polymer nanocomposites can combine the good processing properties of polymer and the functional properties of inorganic nanoparticles. Polymer nanocomposites have been widely used in optoelectronics, communication, packaging, and medical science and healthcare. our recent work, we have designed and developed functional coatings for varies application. For high k materials used in thin film capacitors, we have added surface modified TiO2 and BaTiO3 nanoparticles into PVDF matrix, the synergy of size effect and dielectric constant effect leads to the highest dielectric constant of 76.1 and a tangent loss of 0.01, measured at 1 kHz. For anti-icing/de-icing application, the superhydrophobic surface can delay ice formation due to its liquid repellence feature, but does not work very well under super cold temperatures; The electrothermal coating can effectively prevent ice formation, while it is very energy-consuming. In this work, a multilayered nanocomposite system that combined electrothermal layer (ET) with energy-saving superhydrophobic layer (SH) (SH@ET system) was fabricated to improve the energy efficiency of anti-icing/de-icing coatings.

Biography:

Mingqing Wang is a senior research fellow at Institute for Materials Discovery, University College London. She received her Ph.D. in Polymer Science and Engineering from Department of Chemical Engineering, Tsinghua University (China). Dr. Wang has rich experience in the design, processing, and characterization of solution processed semiconductor for thin film solar cells including polymer/CIGS/CZTS/perovskite solar cells. Except for thin film solar cells, Dr. Wang also expands her research on high k dielectric layer, low k interlayer, and thin film barrier coating for optoelectronics such as photoelectrochemical water splitting, photodetectors, X-ray detectors, self-powered photoelectrochemical biosensor, and active-matrix display through multidiscipline collaborations.

Preparation of Polymeric Membranes of P(VDF-Trfe) Containing a Tio2-Rgo Nanocomposite for the Photocatalytic Degradation of Organic Contaminants in Water, Under Solar Light

Eduarda B.H. Santos^{1*}, Valentina Silva¹, Leonardo Amaral² and Paula A. Marques³

¹Department of Chemistry and Centre for Environmental and Marine Studies (CESAM), University of Aveiro, Portugal; ²Department of Chemistry and Materials Research Centre CICECO, University of Aveiro, Portugal; ³ Department of Mechanics and Centre for Mechanical Technology and Automation (TEMA)

Abstract:

A major challenge in the application of nanocatalysts in photocatalytic water treatment is the post-treatment recovery of the catalyst nanoparticles. The toxicity of the nanoparticles remaining in treated waters rises some concern, and the loss of the nanocatalyst compromises its reuse and turns the process more expensive. In this work, a nanocomposite of TiO2 -rGO was prepared and the polymer P(VDF-TrFE) was used as support for the catalyst immobilization. The polymer was solubilized in an organic solvent and the nanocomposite was suspended in the solution. Two procedures were tested for the preparation of the polymeric membranes containing the nanocomposite: electrospinning and wet phase inversion. The second method is easier and less expensive and allowed preparing membranes which were easy-to-handle. Metoprolol, a drug for the treatment of cardiovascular diseases and an emerging water contaminant frequently detected

in rivers and effluents, was used for testing the efficiency of the polymeric membranes. Solutions of metoprolol containing a rectangular piece of membrane were irradiated in a solar simulator and the initial and final concentrations of metoprolol were determined by HPLC-UV. Both types of membranes exhibited a high photocatalytic efficiency, but those prepared by phase-inversion are easier to handle and reuse. They were reused several times and no loss of catalytic efficiency was observed.

Biography:

Eduarda BH Santos is an Assistant Professor in the Department of Chemistry at the University of Aveiro and is member of the research Centre for Environmental and Marine Studies (CESAM). She has developed research work in the area of Environmental Chemistry, with particular focus on studies of environmental photochemistry, namely, solar photodegradation of organic contaminants in water. In addition to other several publications, she has 52 articles published in journals indexed in Web-of-Science (WOS), most of which belong to the 1st quartile of the respective area, has more than 1720 citations and has an h-index of 26.

Improvement of Material Properties upon Tailoring the Morphology of Crosslinked Polyethylene

Michail Maricanov* and Robert D. L. Jerusalem, Joerg C. Tiller, Frank Katzenberg

Biomaterials & Polymer Science, Department of Biochemical and Chemical Engineering TU Dortmund, Dortmund, Germany

Abstract:

Innovation in the field of polymers is necessary to further optimize the energy sector in the future. In this context, it is ideal to use already existing polymers for new challenges. Cross-linked lowdensity polyethylene (XLDPE) is one of the most widely used polymers in the field of AC highvoltage cable insulation. In the future, however, high-voltage networks are to be converted to direct current, which in turn, among many positive aspects, leads to new material design challenges. One of the biggest problems is the accumulation of so-called space charges in the insulation material, which are injected into the material under a DC field. The accumulation of these space charges reduces the effective dielectric strength of the insulation material, which subsequently leads to faster aging of the material and consequently to electrical breakdown of the insulation. Initial results of this work showed that tailoring the morphology of XLDPE leads to a significant reduction of field enhancement. In other words, the electrical aging of the material is suppressed and a significant increase in the lifetime for the insulation is guaranteed. A major aspect of our work is to extend the structure-property relationships of thermoplastics through tailoring their morphology. Critical crosslinking is the perfect tool in this regard, because it enables the interplay between morphology and material performance by changing the orientation of polymers beyond the capabilities of common crystallization kinetics.

Biography:

Michail Maricanov is a PhD student under Frank Katzenberg at the polymer physics group at the chair of Joerg Tiller in the department of Bio- and Chemical Engineering at the TU Dortmund. He studied Chemical Engineering in Dortmund.

Structure and Properties of Isosorbide-Based Polycarbonate Containing Biobased Antiplasticizer

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Abstract:

Since isosorbide-based polycarbonate (ISB-PC) has been commercialized as a biomass-based transparent plastic, it is widely recognized as an excellent candidate to replace bisphenol-A polycarbonate (BPA-PC) and poly(methyl methacrylate) (PMMA). Most of the properties of ISB-PC, such as refractive index, mechanical properties, and thermal properties, are between those of PMMA and BPA-PC. Since ISB-PC is a new material, there is less information on its blends. In this study, dynamic mechanical properties including glass transition temperature, optical and tensile properties at room temperature, and rheological properties at processing temperature were measured to comprehend the performance of plasticized ISB-PC samples. Since the plasticizer employed in this study shows good biodegradability and non-toxic, it is a candidate to be employed as a modifier for various plastics including ISB-PC.

Biography:

Ruiqi Han is a PhD candidate in School of Materials Science at Japan Advanced Institute of Science and Technology. His research focuses on the modification of rheological properties for biomassbased isosorbide polycarbonate

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