ABSTRACT BOOK

SCIENTIFIC SUMMITS

WSEPCM-2024

November 14-16, 2024 | Rome, Italy

WORLD SUMMIT AND EXPO ON

POLYMERS & COMPOSITE MATERIALS

FOREWORD

Dear Colleagues,

It is my pleasure to cordially invite you all to join the "World Summit and Expo on Polymers and Composite Materials (WSEPCM-2024)" which will be held in Rome, Italy during November 14-16, 2024.

WSEPCM-2024 is the ideal opportunity for research scientists, academics, industrial engineers and students working on Polymers and Composite Materials to discuss their cutting-edge innovations, ideas and recent achievements. The meeting will cover both Polymers and Composite Materials, Composite Materials in Aerospace Applications, Self-healing Composite Materials, Poly-Nanoparticles and Nanomaterials, 3D Printing Polymers, Ceramic and Carbon Matrix Composites, Biomaterials and Tissue Engineering, Biopolymers and Bio plastics, Recycling and Waste Management of Bio-polymers and Thermo set Composite Materials and other topics.

WSEPCM-2024 will be a three-day event that gathers together key players of the Polymers and Composite Materials and related sectors. This event aims to attract global participant's intent on sharing, exchanging and exploring new avenues of Polymers and Composite Materials related scientific and commercial developments.

The wide-ranging scientific program will consist of plenary lectures, keynote lectures, invited lectures, parallel sessions, as well as poster sessions for young scientists covering all topics in Polymers and Composite Materials. This conference provides a wonderful opportunity for you to enhance your knowledge about the newest interdisciplinary approaches in Polymers and Composite Materials. Moreover, the conference offers a valuable platform to create new contacts in the field of Polymers and Composite Materials, by providing valuable networking time for you to meet great personnel in the field.

We look forward to seeing you at WSEPCM-2024 in Rome, Italy.

Yours Sincerely

Dr. Thomas J. Webster
Conference Chair| WSEPCM-2024.
Hebei University of Technology, China
Nominee for Nobel Prize in Chemistry

Samit Roy

Prof. Samit Roy
Conference Co-chair
University of Alabama, USA

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PLENARY ABSTRACTS

ENVIRONMENT-ASSISTED DEGRADATION OF FIBRES IN FIBRE REINFORCED POLYMER COMPOSITES FOR ADVANCED CONCRETE STRUCTURES

Prof. Raman Singh

Department of Mechanical & Aerospace Engineering, Department of Chemical & Biological Engineering Monash University, Victoria, Australia

ABSTRACT

Common concretes use considerable amounts of fresh water and river sand, and their excessive use has serious implications on environment. In this respect, seawater and sea sand concrete (SWSSC) is a very attractive alternative, since it addresses the increasing shortage of fresh water and dredging of river sand. A major concern with reinforced SWSSC is the severe corrosion of the steel reinforcements by sea water (that has a very high content of chloride which is very corrosive), thereby seriously impairing the strength of such concrete. Fibre reinforced polymer (FRP) can be a suitable alternative to replace steels as reinforcement. However, there has been little systematic work to understand the degradation kinetics and mechanisms of FRP in the chloride-containing alkaline SWSSC environment. This presentation will provide an overview of the degradation of FRP composites in chloride-containing alkaline SWSSC environment, as well as provide a pathway to systematic experimental approach to understanding such degradation, particularly by using scanning electron microscopy (SEM) and Fourier transform infrared spectroscopy (FTIR). Underpinned by this fundamental understanding of the degradation of FRPs due to the complex SWSSC environment, the presentation will also make a comprehensive assessment of the influence of environment-assisted degradation on mechanical properties of FRPs.

Keywords: Seawater sea sand concrete; Concrete reinforcement; Fibre reinforced polymers

BIOGRAPHY

Professor Raman Singh's primary research interests are in the relationship of Nano-/microstructure and Environment-assisted degradation and fracture of metallic and composite materials, and Nanotechnology for Advanced Mitigation of such Degradations. He has also worked extensively on use of advanced materials (e.g., graphene) for corrosion mitigation, stress corrosion cracking, and corrosion and corrosion-mitigation of magnesium alloys (including for the use of magnesium alloys for aerospace, defence and bioimplant applications). Prof Singh is a senior professor at Monash University, Australia. He is a Guest Professor at ETH Zurich, Switzerland (2020, 2023, 2024), US Naval Research Lab, Indian Institute of Science, and University of Connecticut. He worked as a scientist at Indian Atomic Energy and as a post-doc fellow at University of New South Wales, Australia. Prof Singh's professional distinctions and recognitions include: Guest Professor of ETH Zurich, Editor of a book on Cracking of Welds (CRC Press), Lead Editor of a book on Non-destructive Evaluation of Corrosion (Wiley), Editor-in-Chief of an Elsevier and two MDPI journals, leader/chairperson of a few international conferences and numerous plenary/keynote lectures at international conferences, over 270 peer-reviewed international journal publications and 15 book chapter, and several competitive research grants (that includes 4 Discovery, 7 Linkage and one ITRH grants of Australian Research Council). Prof Singh has supervised 58 PhD students. His vibrant research group at Monash University comprises of PhD students from different disciplines (Mechanical, Chemical, Materials and Mining Engineering, and Science) as well as from different cultural backgrounds (Australian, Middle-eastern, Chinese, Malaysian, Indian, African, North American and Israeli).

INTELLIGENT IN-SITU SELF-HEALING OF DAMAGE IN POLYMER COMPOSITE STRUCTURES

Dr. Samit Roy

William D. Jordan Professor of Aerospace Engineering and Mechanics
University of Alabama, U.S.A.

ABSTRACT

This abstract describes the in-situ self-healing of composite structures using an array of smart sensors that can detect the damage and activate self-healing using the same network of sensors through a control module. Laminated composites are highly susceptible to delamination, and delamination due to fatigue loading is one of the most critical damage modes in composite structures that may lead to a catastrophic failure. Hence, it is paramount to investigate and quantify the delamination crack growth behavior due to fatigue loading and explore methods to heal the delamination. To this end, double cantilever beam (DCB) specimens of carbon fiber-reinforced polymer (CFRP) composite containing thermoplastic healants and "smart" shape memory polymers (SMP) were manufactured, and the Mode-I fatigue delamination experiments were carried out for the virgin case, and seven healing cycles using in-situ macro fiber composite (MFC) sensors. The motivation for using MFCs as actuators for self-healing is because the same network of MFCs can be used as sensors in the structure to detect localized damage and then perform the healing. The primary purpose of using thermoplastic healants- polycaprolactone and shape memory polymer - is to heal the cracks formed during fatigue loading and regain load-carrying capacity of the composite structure. From the fatigue test data for the virgin and healed specimens, Paris law parameters were extracted, and the results obtained from different specimens were found to be similar. Furthermore, the delamination crack growth rate retardation factor for the healed specimens was found to be in the range of 14% ~ 24% of that for the virgin specimen, thereby suggesting good healing performance of the specimens under fatigue loading. In addition, the in-situ healing performance of Mode-I interlaminar fracture of CFRP composites subjected to fatigue loading for seven healing cycles was investigated. The in-situ healing was carried out by activating the macro fiber composite actuators attached to the DCB specimen to generate heat after 5000 cycles of loading, once crack growth was detected. For the fifth, sixth, and seventh healing cycle, the crack closure observed after in-situ healing was significant, with 200% improvement in fatigue life after in-situ healing. Recent results indicate that the self-healing concept works even under high vacuum and cryogenic conditions,

simulating the harsh environment of outer space.

Keywords:
Smart sensors network, in-situ healing, Mode-I fatigue, thermoplastic healant, repeatable self-healing.

BIOGRAPHY

Dr. Samit Roy received his Ph.D. in Engineering Science & Mechanics from Virginia Tech in Blacksburg, Virginia. He is currently the William D. Jordan Endowed Professor in the Department of Aerospace Engineering and Mechanicsat University of Alabama (UA). Dr. Roy's research interest is directed towards multi-scale modeling and life-prediction of fiber reinforced polymer composites and structural adhesives subjected to aggressive environmental conditions. He is also actively involved in the application of nanostructured reinforcements in enhancing performance of composite materials. He has developed structural health management concepts that include sensor placement optimization for structural weight and cost reduction, as well as smart materials for non-autonomous self-healing. He has authored over 200 peer-reviewed journal articles and book chapters. He was elected Associate Fellow of the American Institute of Aeronautics and Astronautics (AIAA) in 2004, elected Fellow of ASME in 2010, andFellow of American Society for Composites (ASC) in 2022. He was elected Chairman of the ASME NanoEngineering for Energy and Sustainability (NEES) steering committee in 2014, and Division Chair, Emerging Composite Technologies Technical Division, of theAmerican Society for Composites in 2022. He is the recipient of the ASC Outstanding Researcher Award in Composites in 2019 and again in 2023.

ADVANCED NANOCOMPOSITE MEMBRANES FOR CLEAN ENERGY AND CLEAN WATER APPLICATIONS

Prof. (Neal) Tai-Shung Chung

Honorary Chair Professor, 玉山學者, Graduate Institute of Applied Science and Technology, National Taiwan University of Science and Technology (NTUST); Emeritus Professor, National University of Singapore (NUS); Fellow, Academy of Engineering Singapore

ABSTRACT

Clean water, clean energy, global warming and affordable healthcare are four major concerns globally resulting from clean water shortages, high fluctuations of oil prices, climate changes and high costs of healthcare. Clean water and public health are also highly related, while clean energy is essential for sustainable prosperity. Among many potential solutions, advances in membrane technology are one of the most direct, effective and feasible approaches to solve these sophisticated issues. Membrane technology is a fully integrated science and engineering which consists of materials science and engineering, chemistry and chemical engineering, separation and purification phenomena, environmental science and sustainability, statistical mechanics-based molecular simulation, process and product design. In this presentation, we will introduce and summarize our efforts on nanomaterials for membrane development in the fields of clean water and clean energy production. Various material and fabrication strategies to enhance membrane performance will be discussed, especially for water reuse, seawater desalination, H2 production and CO2 capture.

BIOGRAPHY

Prof. Neal Tai-Shung Chung is a Jade Mountain Chair professor at Graduate Institute of Applied Science and Technology, National Taiwan University of Science and Technology (NTUST), Taiwan. Before joining NTUST, he was a Provost's Chair Professor at the ChBE dept of National University of Singapore in 2011-2021. His research focuses on polymeric membranes for clean water, clear energy and pharmaceutic separation. In 2005-2008, he worked as a Senior Consultant for Hyflux, led and built its membrane research. He became a Fellow in the Academy of Engineering Singapore in 2012 and received IChemE (Institute of Chemical Engineers, UK) Underwood Medal for exceptional research in separations and Singapore President's Technology Award in 2015. He was No. 6 worldwide in the Chemical Engineering field by the list of "the top 2% scientists in the world" published by Stanford University in 2023 and the top 0.1% of scholars on Water Purification over the past 10 years, as "World Expert" by Expertscape in 2021, Water Purification: Worldwide - Expertscape.com. His H-index = 127 (Scopus) or 147 (Google Scholar). He is an editorial board member of more than 20 journals including Desalination, J. Membrane Science, Env. Sci. & Tech., AIChE J, Separation & Purification Techno., and many others.

IMPROVING CARBON CAPTURE: INSIGHTS FROM NANOSTRUCTURED TO HYBRID INTEGRATED MEMBRANES

Prof. Richard J. Spontak, Ph.D., dr. h. c., FRSC, FIMMM, FPMSE

Departments of Chemical & Biomolecular Engineering and Materials Science & Engineering
North Carolina State University, Raleigh, NC 27615, USA

ABSTRACT

While various carbon-capture efforts are being developed around the world to help mitigate the adverse effects of global climate change, advances in membrane technologies that combine improved CO2 separation efficacy with low cost, facile fabrication, upscaling and implementation, and mechanical robustness are still needed. Initial studies identified the utility of polyether-containing membranes generated from chemically-crosslinked homopolymers to physically-crosslinked block polymers. The transport properties of these materials are promising, but are restricted by the upper bound. For this reason, we considered charged polymers that self-assemble and produce hydrophilic nanochannels. While their CO2 selectivity does not change substantially, the CO2 permeability of such amphiphilic polymers can be physically enhanced. With promising structure-property relationships in hand, we nanoengineeredunique multifunctional polymer systems. In this spirit, we have successfully introduced an integrated membrane strategy wherein a high-permeability thin film is functionalized with a highly CO2-philic patch-like surface layer. In this nanofabrication scheme, a low-diffusivity, high-solubility mechanism relies on enrichment of CO2 in the surface layer hydrated by the water vapor present in all targeted gas streams, followed by fast CO2 transport through a highly-permeable support substrate. Integrated multilayer membranes prepared in this fashion are not diffusion-limited and retain high CO2 permeability while their CO2 selectivity is increased by over ~150x, far exceeding the upper bound that reflects the trade-off between gas permeability & selectivity. This new design paradigm shows tremendous promise that nanofabricated membranes can exhibit the necessary functionality to achieve significantly improved carbon capture.

BIOGRAPHY

Richard J. Spontak, a Distinguished Professor at NC State University, received his Ph.D. from UC Berkeley and pursued post-doctoral research at Cambridge University before joining P&G in 1990 and NC State in 1992. He has published over 300 peer-reviewed journal papers and 40 book chapters and invited works, and delivered over 400 invited presentations worldwide. He has received numerous research awards including the NC State Holladay Medal for Excellence, the ACS-PMSE Tess Award, the SPSJ International Award, the IChemE Underwood Medal and Global Award, the ACS-RUBB Chemistry of Thermoplastic Elastomers Award, the SPE International Award, and the IOM3 Colwyn Medal and Medal for Excellence. A fellow of IOM3, ACS-PMSE, APS and RSC, he is a member of the Norwegian Academy of Technological Sciences and holds an honorary doctorate from NTNU.

30,000 ORTHOPEDIC IMPLANTS AND COUNTING: NO INFECTION, NO INFLAMMATION, AND NO FAILURES

Prof. Thomas J. Webster

1School of Health Sciences and Biomedical Engineering, Hebei University of Technology, Tianjin, China; School of Engineering, Saveetha University, Chennai, India
CSO and co-founder, 12 start-up companies, Mansfield Bioincubator, Mansfield, MA, USA

ABSTRACT

Nanomedicine is the use of nanomaterials to improve disease prevention, detection, and treatment which has resulted in hundreds of FDA approved medical products. While nanomedicine has been around for several decades, new technological advances are pushing its boundaries. For example, this presentation will present an over 25 year journey of commercializing nano orthopedic implants now in over 30,000 patients to date showing no signs of failure. Current orthopedic implants face a failure rate of 5 – 10% and sometimes as high as 60% for bone cancer patients. Further, Artificial Intelligence (AI) has revolutionized numerous industries to date. However, its use in nanomedicine has remained few and far between. One area that AI has significantly improved nanomedicine is through implantable sensors. This talk will present research in which implantable sensors, using AI, can learn from patient's response to implants and predict future outcomes. Such implantable sensors not only incorporate AI, but also communicate to a handheld device, and can reverse AI predicted adverse events. Examples will be given in which AI implantable sensors have been used in orthopedics to inhibit implant infection and promote prolonged bone growth. In vitro and in vivo experiments will be provided that demonstrate how AI can be used towards our advantage in nanomedicine, especially implantable sensors. Lastly, this talk will summarize recent advances in nanomedicine to both help human health and save the environment.

BIOGRAPHY

Thomas J. Webster's (H index: 122; Google Scholar) degrees are in chemical engineering from the University of Pittsburgh (B.S., 1995; USA) and in biomedical engineering from RPI (Ph.D., 2000; USA). He has served as a professor at Purdue (2000-2005), Brown (2005-2012), and Northeastern (2012-2021; serving as Chemical Engineering Department Chair from 2012 - 2019) Universities and has formed over a dozen companies who have numerous FDA approved medical products currently improving human health in over 20,000 patients. His technology is also being used in commercial products to improve sustainability and renewable energy. He is currently helping those companies and serves as a professor at Brown University, Saveetha University, Vellore Institute of Technology, UFPI, and others. Dr. Webster has numerous awards including: 2020, World Top 2% Scientist by Citations (PLOS); 2020, SCOPUS Highly Cited Research (Top 1% Materials Science and Mixed Fields); 2021, Clarivate Top 0.1% Most Influential Researchers (Pharmacology and Toxicology); 2022, Best Materials Science Scientist by Citations (Research.com); and is a fellow of over 8 societies.Prof. Webster is a former President of the U.S. Society For Biomaterials and has over 1,350 publications to his credit with over 55,000 citations. He was recently nominated for the Nobel Prize in Chemistry. Prof. Webster also recently formed a fund to support Nigerian student research opportunities in the U.S.

KEYNOTE ABSTRACTS

ADVANCING IN VITRO TISSUE ENGINEERING: EXPLORING BIOMATERIALS AND DEVELOPMENTAL BIOLOGY

Dr. Udi Sarig

Dr. Miriam and Sheldon G. Adelson School of Medicine, Ariel University, Ariel, Israel.
Department of Chemical Engineering, Ariel University, Ariel, Israel.

ABSTRACT

Tissue Engineering (TE) is an interdisciplinary field that applies the principles of life sciences and engineering to develop biological substitutes that restore, maintain, or improve tissue function. The principal tissue engineering dogma relies on tissue-specific stem or progenitor cells to provide biological functionality, often supported by a biomaterial scaffold, of either natural or synthetic origin, and by dedicated bioreactor engineering— mimicking the physiological conditions in vitro. I will present my work on natural extracellular matrix (ECM) derived biomaterials focusing on the intricate and reciprocal cross-talk between these biomaterials, and various multi- and pluripotent stem and progenitor cells in vitro and in vivo. Collectively, the presented findings suggest that a biomimetic approach is imperative in order to overcome the challenges of generating functional complex tissues and organs. I will finally discuss the possible clinical and commercial applications for such a biomimetic approach in the context of my current research focus on synthetic and applied developmental-biology-inspired tissue engineering at Ariel University.

Keywords: Tissue Engineering, Biomaterials, Extracellular matrix (ECM), 3D Bioprinting, Applied Developmental Biology.

BIOGRAPHY

Dr. Sarig is a Senior Lecturer and Deputy Chair of the Department of Medical Studies at the Dr. Miriam and Sheldon Adelson School of Medicine and is co-affiliated with the Department of Chemical Engineering at Ariel University. He received his Ph.D. in Biotechnology and Food Engineering from the Technion-Israel Institute of Technology and completed postdoctoral training at Nanyang Technological University (NTU) in the School of Materials Science and Engineering. Dr. Sarig's current research focuses on 3D bioprinting of engineered synthetic barrier tissue-mimicking biochips inspired by developmental biology, as well as models of synthetic human morphogenesis and organogenesis. With over 15 years of experience in tissue engineering, regenerative medicine, synthetic and developmental biology, and stem cell research, Dr. Sarig has authored more than 20 publications in internationally recognized peer-reviewed journals and scientific conference proceedings.

BIOMIMETIC BIOPOLYMERS IN BIOMEDICAL APPLICATIONS

Dr. Aharon (Roni) Azagury

Head, Noninvasive Biomimetic Drug Delivery Systems Lab, The Department of Chemical Engineering and Biotechnology, Ariel University, Israel

ABSTRACT

In the last decade, there has been a tremendous increase in research focused on biomimicry and bioinspiration. Herein, I will start by reviewing these exciting fields and concentrate on biomimetic drug delivery systems (DDS). Biomimetic DDS have been developed using various biomaterials (e.g., proteins and polysaccharides), plants (e.g., corn), organelles (e.g., exosomes), organisms and cells. These novel biomimetic DDS have been utilized due to their inherent biodegradability, biocompatibility, and non-immunogenicity. Then, I will present results from my lab, where we develop biomimetic algal-based DDS specifically designed for noninvasive administration. We focus on utilizing the natural bioadhesion of nature-derived nanovesicles, as bioadhesion was shown to increase residence time and systemic uptake when given orally. To measure the bioadhesion of these vesicles, we have developed a customized in vitro model comparable to the traditional use of ex vivo tissues.

Our nanoparticles (NPs) from specific algae types (80-200 nm with a surface charge of -10 to -30 mV) possess a bioadhesion force of up to 7-fold stronger than common bioadhesives. Moreover, these algal NPs achieved 100% cellular uptake.

BIOGRAPHY

Aharon (Roni) Azagury is an Assistant Professor in the Department of Chemical and Biotechnology Engineering at Ariel University. He received a Bachelor’s (2007), Master’s (2009), and PhD (2014) Degrees in chemical engineering (2007) from Ben Gurion University of the Negev. His current research focuses on developing novel noninvasive biomimetic and bioinspired drug delivery systems.

CIRCULAR ECONOMY AND SUSTAINABLE INNOVATION: BIOPOLYMERS AND THEIR COMPOSITES TOWARDS THE DEVELOPMENT OF MULTIFUNCTIONAL SYSTEMS

Dr. F. Luzi

Department of Science and Engineering of Matter, Environment and Urban Planning, Polytechnic University of Marche, Ancona, Italy

Light field 3D display is an import true 3D display technology. However, the performance of the traditionallight field 3D display needs to be improved. We proposed and developed a large-viewing angle tabletop light field 3D display based on integral imagingtechnology and a high-resolution light field 3D displaybased on super-view technology. The structure, principle and performance of the light field 3D displays will be introduced in the talk.

ABSTRACT

Academic research and engineering activities have shifted toward the development of sustainable and environmentally benign polymers to reduce environmental pollution, mainly due to the high impact of plastic wastes and plastic leakage into ecosystems. Biobased and biodegradable polymers show some limitations respect to traditional ones. Therefore, the development of composites/nanocomposites and polymeric blends represents a valid approach to modulate/increase the physical and functional properties of neat polymers. In terms of materials' processability, solvent and melt compounding were applied as useful processing techniques for the realization of the biocomposites to be applied in many different sectors, food packaging application, medical and pharmaceutical areas and automotive applications.

Keywords: Biodegradable polymers, food-packaging application, biomedical sector, active systems

REFERENCES

R. Cerdá-Gandia, Á. Agüero, M. P. Arrieta, & O. Fenollar, Polymers,

F. Luzi, I. Tortorella, A. Di Michele, F. Dominici, C. Argentati, F. Morena, L. Torre, D. Puglia, S. Martino, Nanomaterials

BIOGRAPHY

Associate Professor of Science and materials technology (IMAT-01/A: Science and materials technology). She has gained considerable experience in: development and characterization of innovative and multifunctional polymeric systems for industrial and biomedical applications and revalorization of lignocellulosic materials. Her research activity is witnessed by more than 100 documents (papers, book chapters etc.) and 15 oral and/or posters contributions to national and international conferences and workshops. Total citations 3862, H index 35 (from Scopus database).

BREAKING THE MOLD: EXPLORING THE POTENTIAL OF BIODEGRADABLE POLYMERS IN SUSTAINABLE INNOVATION

Prof. S.Sabbatini, P. Stipa, E. Laudadio and F. Luzi

Department of Materials, Environmental Sciences and Urban Planning, Polytechnic University of Marche, Ancona, Italy

ABSTRACT

The increasing environmental concerns associated with conventional plastics have prompted a significant shift towards the exploration of biodegradable polymers as a viable solution for sustainable innovation. This presentation delves into the potential of biodegradable polymers to break the mold of traditional plastic applications, emphasizing their role in reducing plastic waste and minimizing ecological impact. We examined various types of biodegradable polymers, including polylactic acid (PLA), polyamide 6 (PA), and Poly(lactic-co-glycolic acid) (PLGA), and we studied their applications, particularly in food packaging, automotive and medical field. Molecular Dynamics (MD) simulations, ATR-FTIR spectroscopy, and Scanning Electron Microscopy (SEM), have been carried out for their characterisation.

Keywords: Biodegradable polymers, food-packaging, drug delivery systems, FTIR spectroscopy, Molecular Dinamics (MD) simulation

REFERENCES

C. Minnelli, R. Galeazzi, P. Stipa, T. Armeni, S. Sabbatini, B. Romaldi, P. Mengucci, A. Celli, G. Mobbili, E. Laudadio, European Polymer Journal 182, 111723 .
C. Minnelli, P. Stipa, G. Mobbili,S. Sabbatini, B. Romaldi, T. Armeni,E. Laudadio, ACS Omega 8, 48292- 48303

BIOGRAPHY

Associate Professor of Chemistry (CHEM 06/A: chemical foundations of technologies). She has gained considerable experience in the characterization of materials through FTIR infrared spectroscopy. She coordinates research activities in: characterization of biological material, microplastics, bitumen and inert materials, synthesis and spectroscopic characterization of biomaterials and biodegradable polymers. Her research activity is witnessed by more than 70 papers, 2 book chapters and about 70 posters and/or oral contributions to national and international conferences and workshops. Total citations 1501, H index 23 (from Scopus database).

TOWARDS A MOLECULAR LEVEL UNDERSTANDING OF POLYETHYLENE GLYCOL AS A SOLVENT

Prof. Markus M. Hoffmann

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ABSTRACT

Interest in using polyethylene glycol (PEG) as a green chemical solvent is growing because of its low toxicity, biodegradability and interesting solvent characteristics. 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 PEG200, a polydisperse mixture of ethylene glycol oligomers with an average molar weight of 200 g/mol. Insights from these simulations with particular focus on hydrogen bonding will be presented. To the best of our knowledge these simulations are the first ones reported for a polydisperse mixture of ethylene glycol oligomers.

BIOGRAPHY

Prof. Hoffmann studied chemistry as an undergraduate at the Technical University (TU) 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. Since 2015, he has been a “Mercator Fellow” supporting him as a guest researcher at his alma mater TU-Darmstadt with the groups of Prof. Buntkowsky and Prof. Vogel.

DEVELOPMENT OF FUNCTIONAL HETEROSTRUCTURED NANOCATALYSTS FOR GREEN HYDROGEN GENERATION

Prof. Tokeer Ahmad

Department of Chemistry, Jamia Millia Islamia, Jamia Nagar, New Delhi, India.

ABSTRACT

Functional nanostructures based photochemical and photoelectrochemical water splitting is an ultimate source of hydrogen generation as renewable green energy for tackling the ongoing fuel crisis. g-C3N4 is an ideal candidate for overall water splitting as a result of the excellent alignment of its band edges with water redox potentials. However, a single catalyst with a limited number of active sites does not exhibit significant photo/electrocatalytic activity for hydrogen production. Therefore, we have developed the semiconductor heterostructures of g-C3N4 with CuFe2O4 , Cu2O, CdSe, CdS and MoS2 NPs and QDs as the highly efficient nanocatalysts for enhanced hydrogen evolution reactions. The monophasic heterostructures have been designed in different weight ratios with fairly uniform distribution of nearly spherical particles and high specific surface area which creates an interfacial charge transfer between two semiconductors. As prepared heterostructures showed significant hydrogen evolution which is evident by observing high apparent quantum yield, low onset potential, lower overpotential and high electrochemical active surface area that will be presented in detail.

BIOGRAPHY

Prof. Tokeer Ahmad is graduated from IIT Roorkee and Ph.D. from IIT Delhi. Presently, he is full Professor at Department of Chemistry, Jamia Millia Islamia, New Delhi. Prof. Ahmad has supervised 15 PhD's, 77 postgraduates, 9 projects, published 175 research papers, one patent and three books with research citation of 6215, h-index of 47 and i10-index of 127. Prof. Ahmad is active reviewer of 149 journals, delivered 150 Invited talks, evaluated 50 external doctoral theses and presented 128 conference papers. Prof. Ahmad is the recipient of MRSI Medal, SMC Bronze Medal, ISCAS Medal, Inspired Teacher's President Award, DST-DFG award, Distinguished Scientist Award, Maulana Abul Kalam Azad Excellence Award of Education, Teacher's Excellence Award and elected as Member of National Academy of Sciences India. Prof. Ahmad has been figured in World Top 2% Scientists for consecutive four years since 2020 in both coveted lists including career long by Stanford University, USA. Prof. Ahmad has been recently admitted as Fellow of Royal Society of Chemistry (FRSC), UK.

LIGNINASA VERSATILE RENEWABLE POLYMERIN THE PRODUCTION OF INNOVATIVE MATERIALS

Dr. Biljana Bujanovic
USDA-FS-Forest Products Laboratory, Madison, WI, USA

ABSTRACT

Lignin is a main structural constituent of lignocellulosic biomass and the most abundant aromatic polymer on earth. It is readily available as a byproduct of the pulp and paper industry and increasingly from lignocellulosic biorefineries. The amount of lignin extracted from lingo cellulosics is estimated at ~70 million tons worldwide annually. Currently, a small fraction of this lignin (< 2 million tons) is used for high-value applications; most of the lignin is used as a low-cost fuel to produce heat and electricity due to its high heating value of 23.3-25.6 MJ/kg. Alternate commercial uses of lignin polymer are explored to take advantage of lignin's intrinsic properties, uniquely stemming from its polyphenolic structure, such as UV absorption, anti-oxidizing and antimicrobial properties, and thermal stability. However, the utilization of lignin for value-added applications, such as in the production of more sustainable innovative materials, presents considerable challenges due to the inherently heterogeneous nature of lignin. Lignin structure and properties are dependent on several factors, including its origin – related to species, location, morphological tissue, and age-and extraction/delignification and recovery process. Additional challenges are associated with contaminants incorporated into lign in during processing, suchassulfur. This report will focus on potential applications of sulfur-free lignins generated in hydrolytic and organosolv-based processes to produce thermoplastics, thermosets, and hydrogels to reduce their carbon footprint and improve their performance.

BIOGRAPHY

Biljana M. Bujanović holds degrees in Environmental Protection Engineering (BS, 1984) and Wood Chemistry (MS, 1993; PhD, 2000) from Belgrade University, Serbia, and in Paper Science and Engineering from Western Michigan University, MI, USA (PhD, 2003). She worked as an Assistant to Professor at the College of Forestry at Belgrade University (1986-1999), and an Assistant and then Associate Professor at the Chemical Engineering Department at SUNY-ESF, Syracuse, NY (2006-2020). She served as an Associate Chair at the same Department from 2016to 2020. She has held the title of SUNY-ESF Emeritus Associate Professor since 2020. At SUNY-ESF, she taught undergraduate and graduate courses in Introduction to Paper Making, Paper Properties, Paper Coating, and Transport Phenomena, established courses in Wood Chemistry and Biorenewable Products, and led research work in biorefinery operations/pretreatment and lignin isolation, characterization, and use. She has served as a Supervisory Research General Engineer at the USDA-FS-Forest Products Laboratory, Madison, WI, in the Fiber and Chemical Sciences Research group since 2020. Throughout her career, she has published >50 peer-reviewed manuscripts and book chapters, and presented >90 posterand oral presentations at national and international conferences (biljanabujanovic - Google Scholar). She is a member of ACS and TAPPI.

INVITED ABSTRACTS

CURRENT TRENDS AND FUTURE PERSPECTIVES OF POLYMER NANOCOMPOSITES CONTAINING CARBON-BASED NANO-FILLERS FOR ELECTROMAGNETIC INTERFERENCE SHIELDING

Prof. Marcelo Antunes

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ABSTRACT

Carbon-based materials and metals are two of the most used materials for Electromagnetic Interference (EMI) shielding, as they combine high electrical conductivity and effective wave reflection. As non-conductive materials, most polymers are less effective, unless when combined with other functional materials and/or components. Although their low conductivity may be solved by using conductive polymers, these polymers display reduced mechanical/thermal performances, limiting their uses. Thanks to the developments done on carbon-based nanofillers, their combination with non-conductive polymers has been considered as a strategy to obtain conductive polymer nanocomposites with enhanced EMI shielding performance. An important number of researchers have recently considered creating lightweight components based on such polymer nanocomposites through foaming, with the intention of further improving EMI shielding for the most varied applications, especially highly demanding ones such as aerospace or telecommunications. The advantages of foaming such materials are unquestionable, as foaming leads to even lighter structures and has been proven to effectively reduce nanofillers' electrical percolation threshold. Moreover, the generation of a controlled cellular structure promotes an absorption/multiple reflection-based EMI shielding mechanism, mitigating wave interaction with surrounding components. This presentation addresses the current trends in polymer nanocomposites, especially polymeric foams/porous structures, intended for EMI shielding applications, focusing on the following aspects control of the microstructure and cellular structure through supercritical CO2 foaming; importance of the type(s)of nanofiller(s) used, the combination of different nanofillers, and the selective distribution of said nanofillers in the formation of a conductive network; and the use of computational tools to characterize and tailor the EMI shielding performance. Finally, future perspectives are presented based on material/component development, the use of Artificial Intelligence and Machine Learning-based computational predictive tools, and more application-driven approaches.

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BIOGRAPHY

Marcelo Antunes obtained a degree in Chemical Engineering in 2005 (Instituto Superior Técnico, University of Lisbon) and a PhD in Materials Science and Engineering in 2010 (Technical University of Catalonia, UPC – Special Doctoral Award). Since 2015 he works as tenure-track 2 lecturer and develops his research in the Department of Materials Science and Engineering of the UPC. He is also member of the "Polyfunctional Polymeric Materials" (POLY2) research group, coordinating the research line in "Multifunctional polymer-based composite foams".

He has more than 65publications in recognized impact factor magazines, such as Progress in Polymer Science (first journal in the field of Polymer Science), Progress in Materials Science, Polymer or Carbon; thirteen book chapters in international editorials, such as Springer or CRC Press;six applied patents, four of them with their application field extended to EU countries and countries from South America and Asia; and has participated in more than 60 conferences. Likewise, he has co-directed PhD theses in the field of Materials Science and Engineering and has participated and participates in R+D public financing research projects (Spanish Ministry of Science and Innovation and Spanish Ministry of Economy and Competitiveness) in the field of the technology of polymer foams and multifunctional (nano) composites, and in R+D projects with plastics sector companies. He has also co-edited the Special Issues "Polymeric Foams", "Polymeric Foams II" and "Polymeric Foams III" in the journal Polymers (MDPI) and is currently member of the "Reviewer Board" of this journal, and has also co-edited the Topical Collections "Application of Graphene-Based Materials, 1st and 2nd volumes".

His research is mainly focused on the preparation and characterization of multifunctional polymeric (nano)composite foams, namely in the development of new multifunctional foams based on thermoplastics combined with different types of nanosized reinforcements, especially carbon-based such as graphene-based materials and/or carbon nanotubes, to be used as lightweight components in sectors like construction, packaging, electronics, automotive or aerospace. Particular relevance has been given to the process-structure-properties relationships of these novel foams, focusing on the optimization of the variables involved in foaming using different foaming processes, the cellular structure and microstructure of the developed (nano)composite foams, and their added functionalities, such as improved mechanical performance, fire behaviour or thermal/electrical conductivities, or enhanced EMI shielding efficiency.

MOST SIGNIFICANT PUBLICATIONS

- Antunes, M. Recent trends in polymeric foams and porous structures for electromagnetic interference shielding. Polymers, 16(2), 195, 1-23, 2024. doi: 10.3390/polym16020195.
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EFFECTS OF LAYERED NANOPARTICLES ON THE CELLULAR STRUCTURE, FLAMMABILITY AND RHEOLOGICAL PROPERTIES OF FLAME-RETARDANT ABS FOAMS

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ABSTRACT

The present work deals with the preparation and characterization of improved fire-retardant acrylonitrile-butadiene-styrene foams. A 25 wt% of ammonium polyphosphate (APP) and aluminium diethylphosphinate (AlPi) phosphorus flame retardant (PFR) system was added into the ABS matrix. As possible adjuvants, a 5 wt% of two different layered nanoparticles, a montmorillonite (MMT) and a layered double hydroxide (LDH), were also added to the ABS-PFR formulation. The different formulations were prepared by melt-blending the different components and the foams by a physicalone-step process using supercritical carbon dioxide (scCO2). The addition of PFR or PFR and MMT or LDH nanoparticles led to foams with slightly smaller cell sizes and higher cell nucleation densities than pure ABS foams.The presence of LDH nanoparticles changed the thermal decomposition of ABS-PFR formulation and increased the temperature associated to a 5wt% (T5%) and residue formation, being this difference more relevant in the foamed material. An increase of the glass temperature and specific loss modulus was also registered for the ABS-PFR/LDH foam respect to the ABS foam. Significant fire behaviour improvements were observed for unfoamed and foamed samples of ABS-PFR. Regarding PHRR's value, no significant differences for charring samples were noticed between unfoamed and foamed samples. Moreover, an improvement of the quasi-static HRR period, at the beginning of burning, was noticed when the LDH particles were present in the foamed sample.

Keywords: ABS foams, phosphorus-based flame retardants, montmorillonite, layered double hydroxide

BIOGRAPHY

Marcelo Antunes obtained a degree in Chemical Engineering in 2005 (Instituto Superior Técnico, University of Lisbon) and a PhD in Materials Science and Engineering in 2010 (Technical University of Catalonia, UPC – Special Doctoral Award). Since 2015 he works as tenure-track 2 lecturer and develops his research in the Department of Materials Science and Engineering of the UPC. He is also member of the "Polyfunctional Polymeric Materials" (POLY2) research group, coordinating the research line in "Multifunctional polymer-based composite foams".

He has more than 65publications in recognized impact factor magazines, such as Progress in Polymer Science (first journal in the field of Polymer Science), Progress in Materials Science, Polymer or Carbon; thirteen book chapters in international editorials, such as Springer or CRC Press; six applied patents, four of them with their application field extended to EU countries and countries from South America and Asia; and has participated in more than 60 conferences. Likewise, he has co-directed PhD theses in the field of Materials Science and Engineering and has participated and participates in R+D public financing research projects (Spanish Ministry of Science and Innovation and Spanish Ministry of Economy and Competitiveness) in the field of the technology of polymer foams and multifunctional (nano)composites, and in R+D projects with plastics sector companies. He has also co-edited the Special Issues "Polymeric Foams", "Polymeric Foams II" and "Polymeric Foams III" in the journal Polymers (MDPI) and is currently member of the "Reviewer Board" of this journal, and has also co-edited the Topical Collections "Application of Graphene-Based Materials, 1st and 2ndvolumes".

His research his mainly focused on the preparation and characterization of multifunctional polymeric (nano)composite foams, namely in the development of new multifunctional foams based on thermoplastics combined with different types of nano sized reinforcements, especially carbon-based such as graphene-based materials and/or carbon nanotubes, to be used as lightweight components in sectors like construction, packaging, electronics, automotive or aerospace. Particular relevance has been given to the process-structure-properties relationships of these novel foams, focusing on the optimization of the variables involved in foaming using different foaming processes, the cellular structure and microstructure of the developed (nano)composite foams, and their added functionalities, such as improved mechanical performance, fire behaviour or thermal/electrical conductivities, or enhanced EMI shielding efficiency.

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SELECTIVE ELECTROCHEMICAL DETECTION OF URIC ACID AND ASCORBIC ACID USING A POLY(BRILLIANT CRESYL BLUE)-MODIFIED GRAPHITE ELECTRODE

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ABSTRACT

Uric acid is the final product of purine metabolism in humans and serves as a valuable diagnostic marker when measured in body fluids, such as serum and urine Elevated uric acid levels are indicative of conditions like gout, hyperuricemia, or Lesch-Nyhan syndrome. Ascorbic acid (AA) (also known as vitamin C), a water-soluble nutrient found in citrus fruits, berries, and vegetables, is commonly used to prevent scurvy, combat the common cold, and address certain mental health issues. Both uric acid and ascorbic acid coexist in the extracellular fluids of the central nervous system and serum. Due to their similar oxidation potentials at most solid electrodes, distinguishing between them through electrochemical methods is challenging because of overlapping signals. Therefore, it is crucial to develop simple, rapid techniques for their selective detection in routine analyses

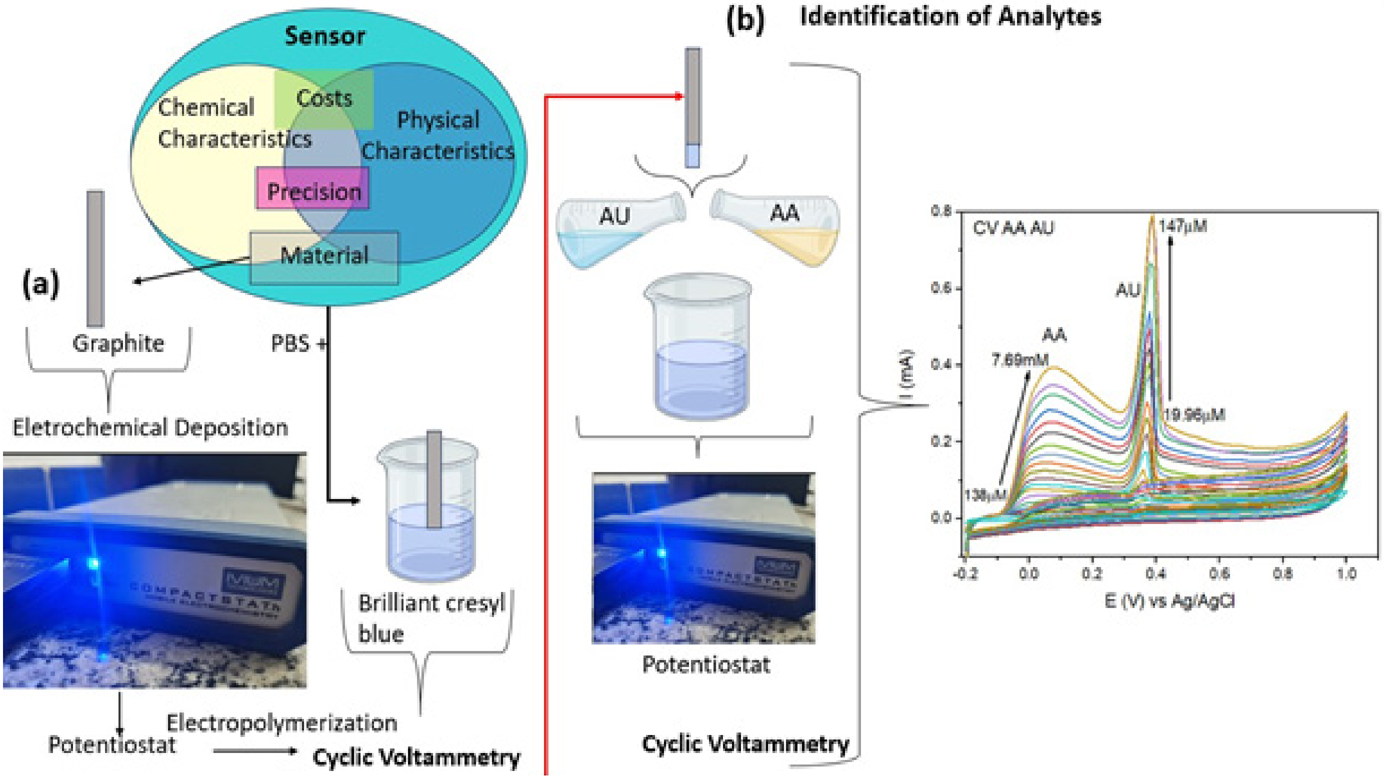

Fig. 1 (a) Electropolymerization of BCB at graphite electrode in 0.1M PBS (pH 7.0). (b) Detection of various concentrations of AA and UA in 0.1M PBS (pH 7.0) at the scan rate of 20 mV/s.

Traditional methods for detecting these biomolecules, such as chemiluminescence, chromatography, ultraviolet-visible spectroscopy, and capillary electrophoresis, are often complex, costly, and suffer from limitations in sensitivity, selectivity, and reproducibility [5]. To address these challenges, electrochemical techniques have been increasingly employed for biomolecules detection.

In this study, we demonstrated the simultaneous detection of ascorbic acid (AA) and uric acid (UA), as demonstrated in the graph in Figure 1, using a modified graphite electrode in a 0.1 M PBS (phosphate buffer solution) with pH 7.0 for the first time. The unmodified graphite electrode was unable to differentiate the voltametric signals of AA and UA. However, the PBCB-modified electrode successfully separated these signals, showing potential differences of 50 mV and 350 mV for AA and UA, respectively. This separation is likely due to the attraction of the anionic forms of AA and UA to the positively charged backbone of the PBCB film, resulting in enhanced peak currents for these analytes. The linear determination ranges of AA and UA were 138 M - 7.69 mM and 19.96 M - 147 M, respectively. The peak currents of them were increased with good correlation coefficient. The lowest detection limit was found to be 0.46 M and M, for AA and UA, respectively (S/N = 3).

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BIOGRAPHY

Ana Barros currently Full Professor the Federal Center for Technological Education Celso Suckow da Fonseca CEFET-RJ (2006-). She have experience in the following areas in Physics:

(i) Phenomenology in High Particle Energy Physics, (ii) Non-linear Optics and (iii) Atomic Physics collision and fragmentation of molecules, mass spectrometry and physics of surfaces at PUC-Rio, heavy ion collisions at GANIL (Grand Accelerator National d'Ions Lourds), Caen, France and photons at NASA AMES Research Center. At CEFET/RJ. She was the Coordinator of the Graduate Stricto Sensu Program in Electrical Engineering - PPEEL - master's degree (2013 - 2014). She is a coordinator of the PhD in Optics and Applied Instrumentation (PPGIO) - in association CEFET/RJ and UFF. Researcher, founder, and coordinator of the Laboratory of Experimental and Applied Physics (LaFEA) at CEFET since 2006.Currently Research Scientist -CNPq(301868/2017-4) and Scientist ofRio de Janeiro State - FAPERJ (Public Notice No. 09/2019).

The research activity of Ana Barros has been mainly devoted to experimental studies of chemical and physical modification induced by highly charged heavy ions, light ions, electrons, and photons on targets of astrophysical relevance, sputtering from solid surfaces, chemical modification, irradiation effects (cosmic rays, solar wind) when targets contain mixtures of hydrogen, carbon, nitrogen and oxygen atoms, including amino acids, nucleobases and Polycyclic Aromatic Hydrocarbons (PAH's), that can be formed under interstellar/circumstellar using the FTIR infrared absorption technique.

In addition, electrochemical energy storage systems such as super capacitors, solar cells and photo electrochemical studies such as hydrogen energy storage and CO2 reduction

BIODEGRADABLE THERMOPLASTIC FILMS FOR FLEXIBLE FOOD PACKAGING

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Innovation in Polymer Engineering (PIEP), Portugal

ABSTRACT

The barrier properties of food packaging are essential to ensure that food maintains its properties during its shelf-life. Typically, plastic packaging with superior barrier properties involves a multi-layer structure comprising different polymers, to combine different barrier properties, and adhesives, to promote compatibility between polymers and layers [1]. Despite the advantages associated with these structures, they are extremely difficult to recycle due to the use of adhesives and incompatible materials which makes the separation of these different polymers impossible using conventional recycling methods [2]. It is therefore necessary to promote a transition to more sustainable packaging focusing this study on the development of Polybutylene succinate (PBS), Polylactic acid (PLA) and Polybutylene adipate terephthalate (PBAT) based films, through compounding and film extrusion, to replace conventional multilayer packaging with biodegradable packaging with good barrier properties [3, 4]. In this study, PBS and PLA/PBAT-based composites with the incorporation of different additives were produced in a co-rotating twin-screw extruder, and their respective films by blown film extrusion. The materials and the monolayer films were subjected to characterization tests to analyse their morphology and barrier properties to oxygen, water vapour and light. The results showed that biodegradable films produced with relatively low thickness, with incorporation of additives and combination of materials have good barrier properties in comparison to the base polymers.

However, the films developed cannot yet compete with some commercial multilayer films with typical polymer structures such as low-density polyethylene (LDPE), for water vapour barrier, combined with Ethylene vinyl alcohol (EVOH), for oxygen barrier

Keywords: Biodegradable, food packaging, blown film, extrusion, permeability.

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The authors are grateful for the financial support granted by the Recovery and Resilience Plan (PRR) and by the Next Generation EU European Funds to PIEP, through the Green Agenda for Business Innovation “From Fossil to Forest – Sustainable packaging and products to replace fossil plastic” (Project no.8 with the application C644920945- 00000036).

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BIOGRAPHY

PhD in Polymer and Composite Science and Engineering from the University of Minho (July 2024).Currently, she is a Lead Technician in the Extrusion and Compounding team at PIEP, where she plans research activities related to the production of composites and the development of antimicrobial, antioxidant, and high-barrier and mechanical property films and filaments for the food and textile industries.
As a researcher at the University of Minho, she led several projects aimed at developing innovative recyclable flexible plastic packaging for the food sector. She has published eight scientific papers and one technical article in international journal. Previously, she completed a professional internship at a plastic injection industry, focusing on managing and optimizing maintenance plans for all factory assets, as well as production planning for injected parts and raw material needs.
Throughout her career, she has gained expertise in quality tools and standards, polymer processing techniques, materials, and polymer characterization techniques.

SYNTHESIS OF MULTI-METALLIC NANOPARTICLES USING A DENDRIMER REACTOR

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ABSTRACT

Dendrimers are highly branched organic macromolecules with successive layers or “generations” of branch units surrounding a central core. Organic inorganic hybrid versions have also been produced, by trapping metal ions or metal clusters within the voids of the dendrimers. Their unusual, tree-like topology endows these nanometer-sized macromolecules with a gradient in branch density from the interior to the exterior, which can be exploited to direct the transfer of charge and energy from the dendrimer periphery to its core.

We show that AuCl3, SnCl2, FeCl3, and so on complexes to the imines groups of a spherical polyphenyl-azomethine dendrimer in a stepwise fashion according to an electron gradient, with complexation in a more peripheral generation proceeding only after complexation in generations closer to the core has been completed. By attaching an electron-withdrawing group to the dendrimer core, we are able to change the complexation pattern, so that the core imines are complexed last. By further extending this strategy, it should be possible to control the number and location of metal ions incorporated into dendrimer structures, which might and uses as tailored catalysts, building blocks, or fine-controlled clusters for advanced materials.The metal-assembly in a discrete dendrimer molecule can be converted to a size-regulated metal particle with a size smaller than 1 nm as a molecular reactor. Due to the well-defined number of metal clusters in the subnanometer region, its property is much different from that of bulk or general metal nanoparticles. The chemistry of nanoparticles on the sub-nanometer scale is not yet well understood because precise multi-metallic nanoparticles are difficult to synthesize with control over size and composition. The template synthesis of multi-metallic sub-nanoparticles is achieved using a phenylazomethine dendrimer as a macromolecular template.

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BIOGRAPHY

Kimihisa Yamamoto received PhD degrees from Waseda University in Polymer Chemistry in 1990. He joined the Department of Chemistry at Keio University from 1997 as professor. Currently, he is a professor in Tokyo Institute of Technology since 2010. His present research €sl181€slmult0 interests are in developing supra-metallomolecules for nanosynthesizers involving nanoparticles, subnanoparticles and superatoms.

TRIBIOLOGICAL BEHAVIOR OF THREE LAYERED GALVANIZED MILD STEEL AND ALUMINUM UNDER DRY AND LUBRICATING CONDITION

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2 Department of Mechanical Engineering, DUET—Dhaka University of Engineering and Technology, Dhaka 1707, Bangladesh

ABSTRACT

Aluminum and mild steel are two important metals used in structures and machines. Due to friction, their life time reduces which causes billion-dollar loss every year to our property. Many researches are going around the world how friction and wear loss can be reduced. This research focuses the tribological study of coated aluminum and mild steel in different conditions. In the experiments, lubricant is used to find its efficiency. Both reciprocating motion of pin and simultaneous motion of pin and disc applied. Velocity of both pin and disc is also varied. Applied loads are changed in different experiments as well. Roughness analysis has also been done to observe the effect of lubricant, motion and applied load on the surface of the specimens. SEM, EDX, XRD and FTIR tests are also performed to check the morphology of the specimens. The experiments show that comparatively less friction and wear are in at lubricated, reciprocating and less velocity of pin and disc conditions.Less coefficient of friction is observed at higher applied load but less wear is produced at lower applied load.

BIOGRAPHY

Dedicated Mechanical Engineer with profuse enthusiasm about mechanical systems, design and their efficacious implementation in industrial and manufacturing process. More than 9 years of experience in professional engineering and extreme intrigue towards technical research propels to provide some international journals. Always being vigilant about modern technology comes in handy during their exertion in professional problem solving. As a voracious reader of research articles and diligent employee to astute any daunting problems can make a worthy candidate in the field of PhD programmes.

PERSONAL ACHIEVEMENTS

o Published a research article in Materials Research Express of IOP publishing on "Surface coatings analysis and their effects on reduction of tribological properties of coated aluminum under motion with ML approach". (2021)

o Published a research article in Materials of MDPI on "Effects of Self-Lubricant Coating and Motion on Reduction of Friction and Wear of Mild Steel and Data Analysis from Machine Learning Approach". (2021)

o Published a research article in International Journal of Engineering Research in Africa "Effects of Acetylene on deposition rate of stainless steels using thermal chemical vapor deposition". (2016)

Performed as President of English Language Club, DUET, Gazipur, Bangladesh, Session-2014-2015

CONFERENCES & COURSES

Conduct an online session to set-up new Air- conditioner assembly factory in Angola, Africa. (2022)

Training on AVIX software ‘’ How to analyse and visualize of resource method, Line Balancing & Ergonomic" (2022)

Training on Minitab software "How to study gauge R&R and & analytical data’’ (2021)

Visited and 7 days of training on "Production Manager's Benchmark" at AC, TV& washing machine factory in Turkey (2020)

Participated as a speaker "Seminar on Career Building for Industry 4.0" in University of IUBAT, Bangladesh (2020)

Participated as a keynote speaker "Seminar on Industrial behaviors & effective team management" in SIAC , Bangladesh (2017)

THE ROLE OF QUANTUM COMPUTING TO DEVELOP THE NEW TYPES OF POLYMERS (AN OVERVIEW)

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Islamic Azad University Tehran Science and Research, Iran

ABSTRACT

Today, the development of quantum technologies plays a very important role in the development of science and human knowledge. Quantum technologies include various aspects of quantum materials, modern quantum computers as well as quantum physics.
In the meantime, quantum computers with special capabilities such as high speed, unique processing performance and the ability to perform quantum computing have been considered.In this research, the latest achievements and findings regarding the importance of quantum computing and its development in the simulation of polymers are generally examined. The results have shown that the use of specific and solvable algorithms by quantum computers has a significant role in simulating more polymers and the growth of this science.

Keywords: Quantum science, Quantum computing, Polymer simulation, Material science.

BIOGRAPHY

I am Omid Ashakni. Ph.D. candidate of advanced materials and a full doctorate in business management (DBA from Tehran University). My general activities include the development of engineering materials and simulation. I specialize in the process of selective laser melting, the development of simulation of engineering materials and quantum materials, and I use all the necessary tools in the development of science and knowledge.

INTERFACIAL STABILITY OF POLYMER MATRIX COMPOSITES: A MOLECULAR DYNAMICS STUDY

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ABSTRACT

Recently, carbon fiber-reinforced thermoplastic polymer composites (CFRTPs) have attracted significant attentions for application as structural materials in automobiles. The performance of CFRTPs not only depends on the properties of reinforcing fibers and matrix polymers, but also on their interfacial properties. The force applied to the composite material is transmitted through the interface between the fiber reinforcement and polymers, and the composite material easily breaks when the interfacial adhesiveness is weak. To improve the interfacial stability,one approach is to modify the surface of the carbon fiber by functionalization via oxidation treatment or electroplating. In this study, we investigated the influence of carbon fiber functionalization on the interfacial stability at the atomistic scale using full atomistic molecular dynamics (MD) simulations.

MD simulation used in this study has certain advantages over the finite element method (FEM), which is usually used to investigate the mechanical properties of a composite. MD simulations calculate the thermodynamic properties based on atomic motion, whereas FEM requires the constitutive law of a material expressed as a continuum body. Therefore, MD simulations enable us to investigate the dependence of the interfacial strength on the material species at the atomistic scale. The purpose of this study was to determine the atomistic factors that aid in selecting an appropriate composite with excellent interfacial strength by using MD simulations. For this purpose, we selected polyethersulfone (PES) and polyetherimide (PEI) as matrix polymers and graphene sheets with and without functionalization as reinforcements. Furthermore, for the functionalized graphene, we selected -O-, -COOH, and -OH as functional groups bonded to the carbon atoms on the graphene sheet. The interfacial strength is strongly correlated to the interfacial stability; that is, the strength appears to be higher when the interfacial energy is lower. Therefore, a MD simulation was adopted to obtain the interfacial energies of eight species of the composite model, which constituted combinations of two types of matrix polymers and four types of graphene.

Based on the MD simulation results, the stability of the interface between PES

and functionalized graphene decreased in the order of -COOH, -OH, and -O. This contrasts with the interface stability with PEI, which decreased in the order of -O-, -OH, and -COOH. RDF analysis suggested that electrostatic interactions between atoms with a stronger charge bias around the interface play an important role in determining the order of the interfacial stability of PES. The interface between PES and graphene modified with -COOH was found to be the most stable among the various species investigated. This is attributed to the attractive forces between the atomic combinations of S and H atoms in PES and O atoms in FGR-COOH, which have positive and negative charge biases, respectively. Furthermore, our results also suggest that the functional groups of FGR prevent π-π stacking of aromatic rings between FGR and the polymer via excluded-volume effects. Therefore, the functional groups on graphene sheets play an important role in stabilizing and destabilizing the interface. Our findings may be beneficial for the selection of appropriate materials in the development of CFRTPs with superior thermomechanical properties.

BIOGRAPHY

I am Yutaka Oya, an Assistant Professor at the Faculty of Advanced Engineering, Tokyo University of Science. I obtained my Ph.D. from the Department of Physics at Tohoku University in 2014. My research primarily focuses on numerical simulations of polymer materials, including the analysis of phase-separated polymer structures using density functional theory and the mechanical properties of thermosetting polymers for composite materials through all-atom molecular dynamics simulations. Additionally, I am interested in integrating numerical simulation with machine learning to achieve multidisciplinary optimum design of polymeric materials.

POSTER PRESENTATION ABSTRACTS

USE OF POSIDONIA OCEANICA AS AN ENVIRONMENTAL WASTE AND ESTER OF CINNAMIC ACID TO IMPROVE THE DUCTILITY OF POLY(LACTIDE)

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ABSTRACT

In this work, new composite materials have been developed with poly(lactide) fibers (PLA) and a residue called Posidonia oceanica (PO) (Figure 1) through reactive extrusion in the presence of dicumyl peroxide (DCP) and subsequent injection molding. The main objective of this work is to study the effect of different amounts of the plasticizer derived from cinnamic acid (methyl transcinnamate, MTC) on the mechanical properties, highlighting the ductile properties of PLA-based composites reinforced with PO fibers. The main role of DCP is to improve the interaction between fibers, plasticizers and matrix during the extrusion process. Reactive extrusion is expected to help improve the interactions between the base polymer and the lignocellulosic filler [1] and the presence of a carbon-carbon double bond in the cinnamate could play a key role in anchoring the plasticizer to provide greater toughness. to the developed composites.

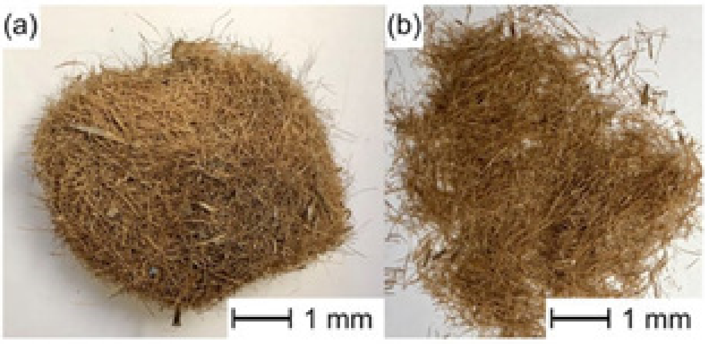

Figure 1. Images of (a) as-received fibrous ball of Posidonia oceanica and (b) Posidonia oceanica fibers (PO) after the cleaning process. Images with a marker scale of 10 μm.

Keywords:Poly(lactide);Posidonia oceanica;reactive extrusion;plasticizer;ductility.

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BIOGRAPHY

I have a degree in Chemistry from the University of Castilla-La Mancha. I completed a master's degree in research there and then completed my PhD. My doctoral thesis was based on the development and validation of analytical methods incorporating nanoparticles for the control of residues in food samples.My entire career is based on the determination of compounds. Now,I work in Valencia, where I am carrying out research related to polymers, as well as their determination in different matrices.

3D-PRINTED BACTERIAL CELLULOSE/ALGINATE/ CHONDROITIN SULPHATE/SI-BIOCERAMICS SCAFFOLDS FOR BONE TISSUE ENGINEERING

Dr. Elena Iulia Oprita, Elena Uțoiu, Vasile-Sorin Manoiu, Rodica Tatia, Teodora-Cristina Ciucan, Viorica Coroiu, Oana Craciunescu
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ABSTRACT

3D printing is an emerging technology that provides personalized scaffolds for bone regenerative medicine at a high reproducible, rapid and customizable level. The aim of this study was to develop novel 3D-printed composite scaffolds for better solving of bone tissue engineering issues. Methods: Bacterial nanocellulose (BNC) membranes were prepared by black tea broth fermentation in the presence of SCOBY consortium. After purification, they were homogenized and lyophilized. Hydrogels were prepared by homogenization of bacterial nanocellulose, chondroitin sulphate and Si-hydroxyapatite (Hap-Si), in weight ratios of 2:1:1 and 2:1:0.5, in 8% alginate solution, for use as bioinks. Similar hydrogel variants were prepared using methylcellulose. Scaffolds with variable porosity were fabricated layer-by-layer with high precision using Bio X 3D-printer (Cellink, UK). Physico-chemical analyses were conducted to evaluate the porosity, density, stability and biodegradability under physiological and inflamed conditions using gravimetric methods and a 5 decimal analytical balance (Sartorius, Spain). SEM observations (Hitachi, Japan) were carried out to evaluate the morphological and structural parameters of the printed scaffolds. In vitro cytocompatibility testing of the scaffolds cultivated in direct contact with L929 cell culture was performed according to ISO 10993-5 for medical devices by MTT assay and cell culture observations using an inversed microscope (Carl-Zeiss, Germany).

Results: The results showed that the 3D-printed composite scaffolds were porous, stable and not cytotoxic (cell viability higher than 80%). Additionally, 3D-printed scaffolds enriched with Si supported cell adhesion and metabolism. The variants containing bacterial cellulose produced the best results in terms of texture and bioactivity, compared to those with methylcellulose, being the selected formulations for biomedical applications. Conclusions: All these data recommended novel biodegradable and biocompatible composites with 3D porous patterned structure as promising candidates for bone tissue engineering. Future work will improve these composites to facilitate interaction with stem cells and the synthesis of new extracellular matrix within bone defects.

Keywords: composites, bacterial cellulose, 3D printing, bone scaffold.

Acknowledgments:
We thank .... for kindly providing the Si-enriched bioceramics. This work was supported by the Ministry of Research, Innovation and Digitization, program Nucleu, project no. 23020201 and UEFISCDI, project no. PN-IV-P8-8.1-PRE-HE-ORG-2024-0190 within PNCDI IV.

THE EFFECT OF HYDROPHILIC MONOMER RATIO ON THE ISOTHERMAL CRYSTALLIZATION KINETICS OF PET COPOLYMERS

Ms. Halenur Karakaya
Boğaziçi University, Turkey

ABSTRACT

Polyethylene terephthalate (PET) is a well-known polyester with its superior mechanical properties, physical and chemical stability, making it a commonly industrialized polymeric material in a wide range of applications. The structure of PET facilitates itsuse in packaging, textiles, films and coatings. However, due to the lack of hydrophilic groups in the main chain, PET falls short of hydrophilicity which makes it a non-privileged polymer in some applications. Hydrophilic nature can be introduced to PET by copolymerization with monomers having hydrophilic groups or polymers having hydrophilic fragments.However, such modifications changes the thermomechanical properties of PET. In this study the isothermal crystallization kinetics of PET copolymers with various ionic hydrophilic monomersis investigated. The differential scanning calorimetry (DSC) analyses of samples was used in the deduction of alteration in the equilibrium melting temperature (T0m) and glass transition temperature (Tg). The Avramikinetic parameters, half time of crystallization (t0.5), overall kinetic constant (k), and Avrami exponent (n) of isothermal crystallization were calculated by using DSC.

BIOGRAPHY

Halenur Karakaya earned her PhD in Chemistry from Boğaziçi University in 2024, focusing on dynamic covalent chemistry and microstructure analysis for tailored properties in powder coating resins. She previously obtained her MS and BS in Chemistry from the same institution in 2015 and 2013, respectively.

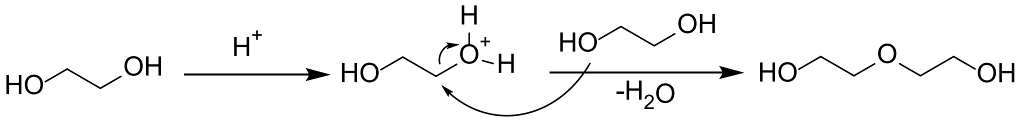
Halenur served as a Teaching Assistant at Boğaziçi University from 2014 to 2022, instructing various chemistry courses. Since 2022, she has been a researcher at SASA Polyester Sanayi A.Ş. in Istanbul, where she develops PET derivatives for various applications.

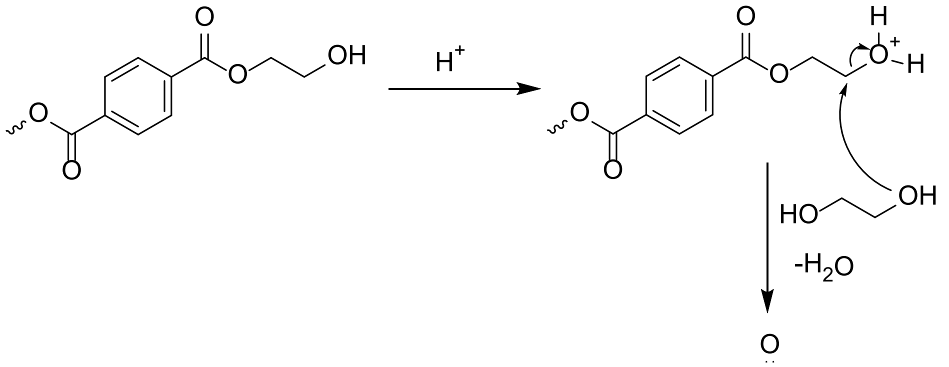
THE EFFECT OF DEG CONTENT IN PET ON THE ISOTHERMAL CRYSTALLIZATION

Mr. Hüseyin Bozkurt
Boğaziçi University, Turkey

ABSTRACT

Polyethylene terephthalate (PET) is one of the widely used polyesters which is synthesized from the terephthalic acid (or dimethyl terephthalate) and ethylene glycol monomers. PET has diverse industrial applications especially in packaging and textiles, it can be either amorphous or semi-crystalline depending on the processing conditions and thermal history. In the industrial synthesis of polyethylene terephthalate (PET) unavoidable side reactions produce diethylene glycol (DEG) from hydroxyethyl terephthalate or ethylene glycol itself with the following mechanisms:





As a result, most commercial PET's contain diethylene glycol terephthalate units in their backbone,1-4 mol-%. DEG content may vary depending on the reaction conditions, monomer ratio, type and the amount of catalyst, influencing the mechanical and physical properties as well as the thermal behavior of the polymer. In this report the effect of DEG content,on the isothermal crystallization kinetics of PET is presented. Differential scanning calorimetry (DSC) analyses were used to investigate the variation of the equilibrium melting temperature (T0m) and glass transition temperature (Tg) at different DEG levels.

Using the thermograms, the kinetic parameters of isothermal crystallization, such as half-time of crystallization (t0.5) and crystallization ratewere calculated.

BIOGRAPHY

Hüseyin Bozkurt is a first year MSc student at Boğaziçi University, specializing in the polymer chemistry field. He is mainly developing knowledge on organic monomer or polymer synthesis and their applications. His current focus is on the synthesis and modification of polyesters of special properties and their implementation to various practical areas.

THE INCREASE IN DIETHYLENE GLYCOL CONTENT IN PTA-BASED POLYESTER: A COMPARATIVE STUDY AGAINST DMT-BASED PET PRODUCTION

Mr. Mustafa Faik Tümer
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ABSTRACT

The production of polyethyleneterephthalate (PET) is primarily carried out using two main rawmaterials; purified terephthalic acid (PTA) and dimethyl terephthalate (DMT). While both routes lead to the formation of PET, differences in the side reactions and by-products are not able. This study investigates the increase in diethyleneglycol (DEG) content when PET production is conducted using PTA instead of DMT. Diethyleneglycol, a commonby-product in polyester synthesis, affects the quality and physical properties of the polymer. Experimental results indicate that PTA-based processes lead to significantly higher DEG levels than DMT-based processes due to the different mechanisms involved in the esterification and transesterification. In PTA-basedproduction, the esterification reaction between ethyleneglycol and terephthalic acid is more prone to side reactions that produce DEG. Understanding these differences is crucial for optimizing the process conditions, such as temperature, catalyst concentration and reaction time, to control DEG levels. This report provides insights into the influence of raw material selection on DEG formation and highlights potential strategies to mitigate its impact in thepolyester manufacturing.

BIOGRAPHY

Mustafa Faik Tümer works as an R&D and operation engineer in SASA Polyester San. A.Ş., Adana, Turkey. As a cost improvement projecto rganizer at SASA, he led various projects. These projects include increasing PBT production capacity, optimization of chemical washing times of reactors, transition of polyester production from DMT-basedto PTA-based synthesis. Priorto SASA, he conducted his Master's studies on organo catalytic asymmetric synthesis at Middle East Technical University, Ankara-Turkeywhere he received as well his BSdegree. He currently is carrying out research on the production of various PET based materials.

INVITRO MODELS FOR PREDICTING BIOADHESION FRACTURE STRENGTHIN EXVIVO ANIMAL BUCCAL TISSUE

Ms. Valeria Rahamim
Ariel University, Israel

ABSTRACT

The motivation and rationale of current research are based on requirements to provide a framework for avoiding or replacing the use of animal tissues in drug delivery studies. The commitment to the principles of 3Rs (Replacement, Reduction, and Refinement) led us to perform the standardization and validation of the novel developed method to measure in vitro the bio adhesion of mammalian soft tissues. Additionally, we have focused on advancing the comparison between the bio adhesion capacity of commonly used tissues from theoral cavity: buccal and esophageal tissues. The in vitro models were developed using human buccal epithelial cells (i.e.,TR146). Full confluencyTR146 cells grown on SYLGARG surface were defined as ‘Model I,’and Model II—TR146 cells grown on SYLGARG and covered with a mucous layer. Standard hydro gels were used to determine the behavior trends and to measure the absolute bio adhesion values of ex vivo porcine buccal and porcine esophageal tissues and in vitro models. Two tested exvivo tissue showed an upward trend in the effect of contact time/applied force/tested materials of bio adhesion fracture strength when the tested parameters increased. It allowed us to create a clear and representative baseline for further comparisons to the developed in vitro models. Additionally, comparing the bio adhesion capacity of both ex vivo tissues resulted in higher bio adhesion values for porcine esophageal tissue. Analysis of invitro models displayed similar behavior trends of developed models to those obtained by ex vivo tissues. Furthermore, Model I exhibited comparable absolute bio adhesion values to those of porcine buccal tissue. Our designed invitro Model I can predict the effect of materials/duration time/applied force as all these parameters are similar to ex vivo porcine buccal tissue. Our designed in vitro method was also validated and standardized to evaluate the interaction between two soft or semi-liquid materials using a texture analyzer.

BIOGRAPHY

Valeria Rahamim is a PhD student at the Chemical Engineering Department in Ariel University. She received a Bachelor's (2014) and Master's (2019) degrees in Chemical Engineering and Biotechnology from Ariel University. Thesis subject specialized in alternative energies and biofuels. Experienced in development of continuous and environmentally friendly bioreactor for bioethanol production. Her current research focuses on developing novel noninvasive biomimetic and bioinspired drug delivery systems based on epithelial carcinoma cells".

YOUNG
RESEARCH FORUMS

ECO-FRIENDLY, BIOCOMPATIBLE CONDUCTIVE COMPOSITES FOR SUSTAINABLE ELECTRONIC APPLICATION

Ms. Aleksandra Kadziela, Sandra Lepak-Kuc
Warsaw University of Technology, Poland

ABSTRACT

Sustainable electronics is one of the major trends in today's world. Non-toxic chemical materials and recyclable parts open up pathways not only to environmental saving issues but also to novel solutions. Innovative conductive components may find applicability among others in biomedical applications. One such solution, in which we have undertaken research, could be modern electrocardiographic electrodes, which are not only disposable, but their production will be sustainable and, once used, they will be thermally recyclable by incineration without leaving a harmful trace. Here we present extensive research into modern sustainable electrically conductive composite materials dedicated to such an application. We have investigated the applicability of new matrices for electrically conductive composites in technologies like screen printing and flexography. We have investigated both established biopolymers and also other materials that have not yet been used in electronics. A functional printing composite has to provide the relevant physical parameters. We have studied key properties of printing composites such as viscosity, printability, substrate compatibility and electrical parameters. In addition, due to biomedical applications, cytotoxicity was studied, and due to environmental friendliness, degradation issues under climatic loads.

Keywords: printing composites; printed electronics; sustainability; recyclable ECG sensors.

BIOGRAPHY

Aleksandra Kądziela is a PhD student at Warsaw University of Technology (Poland) specializing in the development of biomedical sensors manufactured using industrial printing techniques like screen-printing. Her main research area is the study of biodegradable conductive printing composites for screen printing, based on carbon nanostructures. Her research is leading to the advancement of environmentally friendly disposable medical devices, such as ECG electrodes. She has co-authored several publications and is involved in numerous R&D projects focusing on potential applications in the field of printed electronics.

EXTENSIONAL VISCOSITY MEASUREMENTS OF COLLAGEN: A NEW EXPERIMENTAL METHODOLOGY WITH NOVEL MATHEMATICAL MODELS

Mr. Fadi Alzarzouri, Jan Štípek, Jaromír Štancl, Jan Skočilas
Dept. of Process Engineering, Czech Technical University in Prague, Faculty of Mechanical Engineering, Technická 166 07 Prague

ABSTRACT

Extensional (i.e., elongational) flows are of great importance in polymer processing operations such as fiber-spinning, blow molding and film blowing. Hence, knowledge about extensional flows is essential for designing of flow channels and optimizing processing conditions to produce and develop final products with the desired properties. One of the well-known methods in literature for the determination of extensional viscosity of liquids is the method performed by Cogswell.Cogswell method considers as one of the early experiments for extensional viscosity measurements from converging flows. On the other hand, numerous techniques and devices have been developed for measuring the extensional viscosity of polymers in recent decades. The rheometer witha modified hyperbolic contraction has been developed and used by many researchers recently for shear viscosity measurement in two slit sections and extensional viscosity measurement. Despite that both Cogswell and modified hyperbolic contraction rheometer approaches are well established in literature, these methods are used basically for axisymmetric geometries, and there is lack of information regarding the determination of extensional viscosity for converging flows in asymmetric geometries where novel experimental methods and mathematical models are required. In this study, new experimental methodology with new mathematical models have been developed to measure extensional viscosity of collagen where there is little published information regarding its extensional viscosity. The test solutions consisted of natural bovine collagen (type I) and water. The mass fraction of the collagen was 3.0%. The experimental apparatus is an extrusion capillary rheometer equipped with a slit die and five pressure transducers. The slit die consists of capillary with different shapes. The capillary rheometer was constructed at the Czech Technical University in Prague, and it consists of a capillary, a sample storage cylinder and a piston with a hydraulic unit. There were two different capillaries used for the measurements. The first one isan asymmetric convergent-divergent capillary of constant width

and the second is X-die which has constant width and consists of two straight capillaries linked by a defined contraction wedge. The chosen cross-section for all capillaries is rectangular. Two mathematical correlations have been derived for calculating the value of extensional viscosity of collagen for the used capillaries. Experimental results revealed that extensional viscosity of collagen for both capillaries decreases with increasing elongation rate showing extension thinning behaviour. The values of extensional viscosity of collagen were between 45 and 226 Pa.s in the extensional rate ranged between 298 and 1867 s-1. The new mathematical developed models have been able to calculate the shear pressure with deviation of 0.018% and 0.030%. Shear pressure was the key to calculate extensional pressure and subsequently extensional viscosity calculation. This method can be used as well for studying the rheological properties of polymer melts in extrusion process for single and twin-screw extruder.

BIOGRAPHY

Fadi Alzarzouri is a second-year PhD student at the Department of Process Engineering of the Czech Technical University in Prague. His current research focuses on studying the rheological behavior of collagen matter using an extrusion rheometer. He is an experienced polymer engineer and researcher specializing in polymers processing and characterization. Fadi is proficient in a wide range of polymers characterization techniques, including spectroscopy, thermal analysis, mechanical analysis, rheology, and microscopy, with a particular focus on polymer rheology (flow behavior of polymers, temperature, and pressure effects, etc.). He has published four papers on the topic of polymer rheology and plans to continue his research in this field

EFFECT OF NON-HALOGENATED FLAME RETARDANTS ON POST-CONSUMER LOW DENSITY POLYETHYLENE

Mr. Gustavo Kampa, Luis F. S. Silva, Catarina S. Dias, João Ribeiro, Marisa Branco, Renato Reis, Sónia R. A. Machado and Catarina Basto -Silva
a. PIEP-Innovation Center in Polymer Engineering
b. Sirplaste – Industrial Society of Recovered Plastics

ABSTRACT

Polymers, in general, are insulating materials due to the absence of free electrons or ions and can therefore be used in a variety of applications, such as electrical piping [1], [2]. However, polymers have limitations when it comes to fire resistance, because when exposed to heat sources in the presence of oxygen (O2), hydrocarbon bonds break into smaller units, which can lead to intense heat release, flame propagation, the release of non-flammable gases (H2O and CO2) and smoke/toxic gases (essentially CO) that can compromise human health and the environment [3]. To mitigate these risks, it is necessary to incorporate flame retardants into the polymers [4]. The aim of this work is to develop materials (polymeric compounds) with a view to obtaining electrical pipes that meet current international flammability standards, by incorporating non-halogenated flame retardants (HFFR) into post-consumer low-density polyethylene (PCR- LDPE). The flame retardants selected are compounds that can promote an intumescent effect and/or act synergistically in flame retardancy, namely expandable graphite, polyphosphates (integrated into an intumescent system) and lanthanum compounds [4],[5],[6]. Thecompositions were made in a co-rotating twin-screw extruder. The flame tests were carried out in accordance with the international UL-94 vertical standard, and the results obtained were compared to a reference composition. This reference composition is a commercially available flame retardant. Overall, the compositions with expandable graphite performed better. As this work is part of a project, further optimization of these formulations is still planned, but so far some of the compositions look promising for the final application and, likewise, for society.

Acknowledgments:

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BIOGRAPHY

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

PREDICTING TENSILE MODULUS OF POLYMERIC MATERIALS USING DEEP LEARNING AND PROPOSING NEW MATERIALS

Mr. Masaharu Katabira, Yutaka Oya and Jun koyanagi
Department of Materials Science and Technology, Graduate School of Advanced Engineering, Tokyo University of Science

ABSTRACT

Carbon Fiber Reinforced Plastics (CFRP) are composite materials made by combining a resin matrix with carbon fibers. They have garnered significant attention in industries such as aerospace due to their exceptional mechanical properties and formability. Traditionally, thermosetting resins, particularly epoxy resins, have been used as the matrix in CFRP for applications such as aircraft. However, in recent years, the use of thermoplastic resins in CFRP has been increasing, owing to their advantages such as impact resistance, recyclability, and shorter molding cycles. This shift has greatly expanded the options available for matrix resin selection. Given the complexity of this selection process, digital technologies such as machine learning can be useful for identifying the most suitable material for a specific application. In this study, we aim to develop a machine learning model to predict the tensile modulus of polymer materials, using molecular force field data as applied in molecular dynamics simulations. Traditionally, chemical structures have been input into machine learning models as linear notations known as SMILES. However, this method has shown limitations in handling polymers with complex structures, such as block copolymers. As an alternative, potential energy, which directly determines the molecular structure, is a possible candidate. If validated, this approach could become a powerful tool for the exploration of optimal materials without the need for experimental verification. For our machine learning model, we collected density and tensile modulus data from PolyInfo, a polymer database maintained by the National Institute for Materials Science (NIMS). The potential energy of each polymer was calculated using the following methodology. First, the chemical structures of the polymers were generated using Marvin Sketch and Open Babel, and the force field parameters and atomic charges were assigned using Polypergen. In this study, we utilized the OPLS-AA force field, and charges were assigned using density functional theory (DFT) calculations at the B3LYP/6-31G level of theory. Energy minimization was performed on the generated molecular models to derive the respective potential energies.

Molecular dynamics (MD) simulations were carried out using the LAMMPS software. The prediction accuracy of the tensile modulus using a neural network model was approximately 96% for the training data and 81% for the test data. The results indicate that the tensile modulus increases with bond energy, dihedral angular energy, and density, while it decreases with charge bias and angular energy.

BIOGRAPHY

My name is Masaharu Katabira, and I am currently a first-year master's student at Tokyo University of Science. I specialize in materials engineering, particularly focusing on composite materials and polymers. My current research involves “development of new materials using machine learning”.

My goal is to create a learning model to predict tensile modulus from molecular structure information obtained by MD simulation, and to develop polymer materials with higher modulus

MOLECULAR DYNAMICS SIMULATION FOR CUMULATIVE FATIGUE DAMAGE OF A THERMOSETTING CROSS LINKED POLYMER

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Department of Physics, Graduate School of Science, Tohoku University

ABSTRACT

CFRP (Carbon Fiber Reinforced Plastics) has a complex structure composed of carbon fibers and thermosetting resin. Under mechanical loading, it exhibits various forms of damage and failure, such as fiber breakage, transverse cracks, and matrix cracks. These damage phenomena often initiate and propagate from the thermosetting resin portion. The thermosetting resin forms a three-dimensional crosslinked structure through covalent bonds, which fracture under mechanical loading, leading to macroscopic material failure. Thus, identifying nanoscale damage modes under stress loading is crucial for understanding the failure mechanisms of CFRP. This study investigates the nanoscale damage mechanism of thermosetting crosslinked resins using molecular dynamics (MD) simulations. MD simulations allow for the modeling of thermodynamic properties, including mechanical behavior, based on atomic motion, providing much higher spatial resolution than standard experiments, which often struggle to capture nanoscale details. In this study, we focus on microscopic damage under cyclic loading conditions. Quantitatively evaluating damage in thermosetting resins under cyclic loading is closely correlated with estimating remaining service life and ensuring the reliability of structural materials. To quantitatively assess microscopic damage, we focus on the degradation of mechanical properties, entropy generation, and void content within the system. Entropy is expected to serve as a physical quantity for measuring material degradation, including bond dissociation and void formation—both difficult to measure experimentally. Therefore, verifying the correlation between entropy, bond dissociation, and void content is highly significant for assessing the remaining life of CFRP. The crosslinked thermosetting resins were modeled using DGEBA ($C_{21}H_{24}O_4$) and 4,4'-DDS ($C_{12}H_{12}O_2N_2S$). Each molecular model was constructed using Marvin Sketch and PolyParGen. In our simulation, we employed the all-atom optimized potentials for liquid simulation (OPLS-AA) force field to reproduce

the molecular structure. The particle mesh Ewald (PME) method was used to calculate Coulomb interactions, with cutoff distances for both Lennard-Jones (LJ) and Coulomb interactions set at 1.0 nm. The electrostatic potential charges were obtained through density functional theory (DFT) calculations using the B3LYP/6-31G (Hamiltonian/basis set) method for each atom to reproduce the electrostatic field around each molecule. The crosslinking reaction between DGEBA and 4,4'-DDS was performed to create crosslinked thermosetting resins. Subsequently, long relaxation calculations were performedto obtain the equilibrium structure of the crosslinked resin. Finally, cyclic loading calculations were performed on the equilibrium structure, considering bond dissociation based on bond length.All MD simulationswere carried outusing LAMMPS software. Under cyclic loading, both entropy and void volume increased, resulting in non-elastic behavior in the thermosetting resin. The accumulated entropy and void volume showed a strong positive correlation with the number of dissociated bonds. Our findings suggest the following microscopic degradation process in the crosslinked resin: Initially, under cyclic loading, the covalent bonds align in the direction of the applied load. Subsequently, bonds under tension begin to break. The covalent bonds surrounding the dissociated bond then fracture in succession, leading to the formation of significant voids. As a result, the stress-strain curves exhibit non-linear and inelastic behavior. In conclusion, covalent bond dissociation is crucial for properly assessing damage in thermosetting resins through MD simulations.

BIOGRAPHY

My name is Naoki Yamada, and I am currently a second-year Master's student at Tokyo University of Science. I specialize in materials engineering, particularly focusing on composite materials and polymers. My current research involves "Molecular Dynamics Simulation Considering Covalent Bond Breaking in Thermosetting Resins."

I have submitted one paper on this research topic and plan to submit another one in the near future.

MOLECULAR DYNAMICS INVESTIGATION OF MICROSCOPIC MECHANISMS IN THE SELF-HEALING BEHAVIOR OF A VITRIMER WITH DISULFIDE BONDS

Mr. Tomoya Uyama, Yutaka Oya, Naoki Kishimoto and Jun koyanagi
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ABSTRACT

Vitrimer, a new polymeric material that imparts self-healing functionality to conventional thermosetting resins, is attracting attention. The material properties are restored on a macroscopic scale as the cross-linked structure destroyed by external stress loading is repaired. By controlling these properties, it is believed that in addition to the high strength and rigidity derived from thermosetting resins, improved durability and reduced environmental impact will be possible, and the material is expected to be a potential substitute for existing thermosetting resins. However, the current vitrified resin has low mechanical properties such as strength, and its application as a structural material has not yet expanded. To improve this situation and develop superior vitrimer resins, it is important to elucidate the mechanisms of self-healing and mechanical property through numerical calculations. In this study, quantum chemical (QM) and molecular dynamics (MD) calculations were coupled to investigate the self-healing mechanism of vitrimers at the molecular scale. Vitrimers are multiscale materials in which quantum chemical phenomena such as covalent bond recombination affect the macroscopic thermo-mechanical properties of the condensed system, and therefore, approaches that focus solely on QM and MD cannot provide a fundamental understanding of the phenomena. By incorporating the information on reaction pathways obtained by QM into MD calculations, accurate self-healing of crosslinked structures by condensed systems can be expected to be reproduced. In this study, we focused on "epoxy vitrimers with disulfide bonds", which are expected to be applied to structural materials. This material is a crosslinked structure obtained by chemical reaction between an amine hardener (4-aminophenyl disulfide, AFD) with disulfide bonds and an epoxy main agent (Bisphenol A diglycidyl ether, DGEBA) with epoxy groups. Although it is expected that the thermo-mechanical properties are restored on a macroscopic scale by the breaking and re-bonding of disulfide bonds, to the best of our knowledge, no specific reaction pathway has yet been reported. Using QM calculations aided by the Global Reaction Route Mapping

(GRRM) algorithm, we will explore the reaction pathway for the recombination of dissociated disulfide bonds.Then, the mechanism of stress recovery is discussed using MD calculations that incorporate information on the reaction path. QM calculation finds out the following two types of stable bonds before recombination of the disulfide bond.In these bonding patterns, a sulfur atom is bonded to carbon atoms at the ortho and para positions of a benzene ring. The disulfide bond, ortho substitution, and para-substitution are more stable in that order, and there are activation barriers of about 60 kJ/mol and 70 kJ/mol, respectively, between each stable structure. These activation barriers are sufficiently lower than the that with disulfide bond exchange (about 150 kj/mol), which is often considered in conventional MD calculations, and can be judged to occur predominantly. Subsequentially, the uniaxial tensile simulation is performed by MD simulations with and without considering obtained reaction pathways. In the results, tensile simulation with considering reaction pathways exhibit the superior mechanical properties to those without the reaction pathways. These results indicate that the reaction pathways discovered in the QM calculations promote the recovery of the disulfide bonds and also the macroscale mechanical properties.

BIOGRAPHY

My name is Tomoya Uyama, and I am currently a first-year Master's student at Tokyo University of Science. I specialize in materials engineering, particularly focusing on composite materials and vitrimers. My current research involves "self-healing properties of vitrimers using molecular dynamics." Using MD simulation methods, we are exploring how disulfide bonds within vitrimers enable reversible bond exchange reactions that trigger self-healing.

SYNERGISTIC BIOINTERFACES: ENGINEERING DOUBLE NETWORK HYDROGELS FROM PEGDA AND ECM-MA FOR 3DBIOPRINTING

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ABSTRACT

Background: Biointerfaces play a critical role in various medical and biotechnology applications including medical devices and tissue engineering related technologies.

Research goal and scope: To develop a fast and reliable 3D bioprinting method that can seamlessly integrate an engineered tissue with other synthetic components. This study explores the development of a biosynthetic interface based on the concept of an interpenetrating polymeric network (IPN) that can reduce shear-induced delamination and increase the biointerface strength of adhesion.

Methods: The IPN is constructed by co-assembling poly (ethylene glycol) diacrylate (PEGDA), a synthetic polymer, and methacrylate-functionalized extracellular matrix (ECM-Ma), a natural biopolymer that can confer tissue-specific bioactivity. This unique double network (DN) architecture was created by preparing two types of hydrogels, PEGDA 8% and ECM-Ma 15% (W/W) in PBS and mixing them in a 1:1 ratio. We utilized digital light processing (DLP) 3D bioprinting technology, a precise method that allowed us to control the interface architecture. Several characterizations were then conducted to understand the DN biointerface, including swelling and mechanical (compression) tests for the printed hydrogels. Viability tests for stromal-type cells were performed by bioprinting the cells with the bio-ink and using the AlamarblueTM assay. This was followed by a detailed histological analysis and high-resolution scanning electron microscopy (SEM) to examine cell distribution and morphology under static culture conditions.

Results: We successfully printed models from the combination of the two hydrogels, and the DN demonstrated significant support for cell growth over time, surpassing the performance of PEGDA alone. A histological analysis confirmed the formation of DN between the hydrogels, with the presence of collagen fibers indicated by blue

areas. The SEM analysis further highlighted the distinct surface differences between each hydrogel and the combination, highlighting the success of our approach.

Conclusion:

This research underscores the synergistic benefits of combining synthetic PEGDA and natural ECM-Ma within a biomimetic IPN biointerface that is advantageous in mechanical stability while conferring tissue-specific biological functionality. The resulting improved mechanical integrity, coupled with enhanced bioactivity, holds immense promise for applications in tissue engineering and regenerative medicine.

BIOGRAPHY

Shachar Sofer is an MSc student in the Department of Chemical Engineering at Ariel University. His current research focuses on developing and characterizing synthetic bio-supportive ink for 3D bioprinting (3DBP). The goal of his research is to develop platforms that combine 3DBP with microfluidics mimicking barrier tissue function. An example from the engineering of endometrial tissue biochip will be presented focusing on unique challenges and potential solutions that allow instantly interfacing 3DBP biological tissues with microfluidic support systems. This enables rapidly achieving physiological-like cell densities soon after bio-chip fabrication. The interfacing biomaterial technology presented is expected to provide an excellent platform for studying basic barrier tissue science and numerous related biomedical applications in the fields of disease modeling and drug screening.

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