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2nd GLOBAL CONFERENCE ON
POLYMERS, PLASTICS AND COMPOSITES
&
5th WORLD
CHEMISTRY CONFERENCE AND EXHIBITION

Oct 04 - 05, 2022 at
London, United Kingdom

Venue:
St George's Hotel, Wembley LONDON, UK
London, United Kingdom

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WCCE-2022 & PPC-2022

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Scientific Program

Meeting Room- Wembley 2

08:00-08:40 — **Registrations**

08:40-09:00 — **Welcome Ceremony**

KEYNOTE TALKS

09:00-09:30 — **Recent Advances in Photocatalytic Chemical Conversion**

Jimmy C. Yu, *The Chinese University of Hong Kong, Hong Kong*

09:30-10:00 — **Quantum Light-Enhanced Two-Photon Imaging of Breast Cancer Cells**

Theodore Goodson III, *University of Michigan, United States*

10:00-10:30 — **Modelling and characterization of mixed-matrix membranes**

Jules Thibault, *University of Ottawa, Canada*

GROUP PHOTO

Refreshment Break 10:30- 10:50 @ Foyer

Technical Session-I

Session Chairs:

Ying Zhang, *University of Nottingham, UK*
Daniela Matias de Carvalho Bittencourt, *Embrapa Genetic Resources and Biotechnology, Brazil*

10:50-11:10 — **Polymeric materials as tools to study and direct immune function**

Christopher M. Jewell, *University of Maryland - College Park, USA*

11:10-11:30	**Surface-Immobilized Photoinitiators for Light Induced Polymerization and Coupling Reactions** ***Wolfgang Kern,*** *University of Leoben, Austria*
11:30-11:50	**Properties of polymer chains at interfaces revealed by quantum beam techniques** ***Hiroyuki Aoki,*** *Japan Atomic Energy Agency, High Energy Accelerator Research Organization, Japan*
11:50-12:10	**Development and characterisation of sustainable prepregs with improved fire behaviour based on furan resin and basalt fibre reinforcement** ***Patricia Ares Elejoste,*** *Gaiker Technology Centre, Spain*
12:10-12:30	**Understanding the Structural Organization of Synthetic Spider Silk for the Development of Novel Biomaterials** ***Daniela Matias de Carvalho Bittencourt,*** *Embrapa Genetic Resources and Biotechnology, Brazil*
12:30-12:50	**Sustainable act for construction chemicals by using recycled biopolymer in cementitious tile adhesive** ***Nevin Karamahmut Mermer,*** *Kalekim Construction Chemicals Co, Turkey*
12:50-13:10	**Predicting the lifetime of weathered polyolefins by relating mechanics to microstructure** ***Marta Chiapasco,*** *Imperial College, UK*

Lunch Break 13:10-14:10 @ Restaurant

Technical Session-II

Session Chairs:

Christopher M. Jewell, *University of Maryland - College Park, USA*
Tomas Sikola, *Brno University of Technology, Czech Republic*

14:10-14:30	**Something from Nothing: Bioplastic from one carbon feedstock** ***Ying Zhang,*** *University of Nottingham, UK*
14:30-14:50	**Temperature dependence of PSS diffusion in multilayers of entangled PDADMA: more than one diffusion constant** ***Annekatrin Sill,*** *University of Greifswald, Germany*
14:50-15:10	**The Microencapsulation of Tung Oil with Natural Hydrocolloid and Synthetic Emulsifiers for Extrinsic Self-Healing Applications** ***Abdullah Mustapha,*** *Technology Innovation Institute, UK*
15:10-15:30	**On-line ATR-MIR for real-time quantification of chemistry kinetics along the barrel in extrusion-based processes** ***Lucivan Pereira Barros Junior,*** *Case Western Reserve University, USA*
15:30-15:50	**Kinetics of Guided Growth of Horizontal Nanowires on Sapphire Surfaces** ***Tomas Sikola,*** *Brno University of Technology, Czech Republic*
15:50-16:10	**Preparation of Poly(ethylene glycol)@Polyurea Microcapsules Using Oil/Oil Emulsions and Their Application as Microreactors** ***Raed Abu-Reziq,*** *The Hebrew University of Jerusalem, Israel*

Refreshment Break 16:10-16:20 @ Foyer

16:20-16:40	**A synergistic multi material flame retardant formulation for reinforced PA6 on the basis of expandable graphite** ***Florian Tomiak,*** *Friedrich Alexander Universität Erlangen-Nürnberg, Germany*
16:40-17:00	**Greenhouse Gas Emission Reduction Potential of European Union's Circularity Related Targets for Plastics** ***Anna Tenhunen-Lunkka,*** *VTT Technical Research Centre of Finland Ltd, Finland*

Panel Discussion

Meeting Room - Wembley 2

Technical Sessions- III

Session Chairs:

Sourav Bhattacharjee, *University College Dublin (UCD), Ireland*
Konstantina Lambrinou, *University of Huddersfield, UK*

09.30-09.50 **Helical structure motifs made searchable for functional peptide design**

Lee Wei Yang, *National Tsing Hua University, Taiwan*

09.50-10.10 **Toward surface manipulation of engineered nanoparticles in drug delivery: The rise of in silico tools**

Sourav Bhattacharjee, *University College Dublin (UCD), Ireland*

10.10-10.30 **Environmental degradation of structural and fuel cladding stainless steels in liquid lead- and liquid lead-bismuth eutectic-cooled reactors**

Konstantina Lambrinou, *University of Huddersfield, UK*

10.30-10.50 **Cilostazol-imprinted polymer film-coated electrode as an electrochemical chemosensor for selective determination of cilostazol and its active primary metabolite**

Wlodzimierz Kutner, *Institute of Physical Chemistry, Polish Academy of Sciences and Cardinal Stefan Wyszynski University in Warsaw, Poland*

10.50-11.10 **Transition-metals perovskites electrocatalysts for boosting the electrochemical energy reactions**

Mohamed Ali Ghanem, *King Saud University, Saudi Arabia*

Refreshment Break 11:10-11:30 @ Foyer

Poster Session (11:30 – 12:30)

POSTER-1 — **Chemical Recycling of Real Complex Waste Streams**

Izotz Amundarain, *GAIKER, Spain*

POSTER-2 — **Origin of capacitance decay for a flower-like δ-MnO_2 aqueous supercapacitor electrode: The quantitative surface and electrochemical analysis**

Byung Chul Kim, *Suncheon National University, South Korea*

POSTER-3 — **The Synthesis of hyperbranched polymers based TADF materials for OLEDs applications**

Saif H D Althagafi, *University of Sheffield, UK*

POSTER-4 — **A highly efficient nanocomposite-containing coatings for the protection of Mg-alloy against corrosion in chloride containing electrolytes**

Mariam Abbi Abtidon, *Kuwait University, Kuwait*

POSTER-5 — **The Synthesis of TADF hyperbranched polymers based Oxadiazoles for OLEDs applications**

Fatemah Asiri, *University of Sheffield, UK*

POSTER-6 — **The formation mechanism of Choline Chloride and Glucose based Natural Deep Eutectic Solvents studied at the molecular level**

Zhassulan Sailau, *Al-Farabi Kazakh National University, Kazakhstan*

POSTER-7 — **The physico-chemical attributes that determine insulin agglomeration: Therapeutic implications**

Megren Fagihi, *University College Dublin, Ireland*

POSTER-8 — **The influence of different cross-linking methods of hydrogels based on PVA on self-healing performance and ionic conductivity**

Nujood Saeed Alshehhi, *Technology Innovation Institute, United Arab Emirates*

POSTER-9

Preparation and Characterization of Graphene-Enriched Tung oil-Urea Formaldehyde Microcapsules

Maitha Almheiri, *Technology Innovation Institute, United Arab Emirates*

Awards and Closing Ceremony

Lunch Break 12:30-13:30 @ Restaurant

Day
2
Wednesday

2nd GLOBAL CONFERENCE ON

POLYMERS, PLASTICS AND COMPOSITES

&

5th WORLD

CHEMISTRY CONFERENCE AND EXHIBITION

Oct 04 - 05, 2022 at London, UK

(Virtual Through ZOOM)
London Time (GMT+1) - 11:30- 17:20

11:30-12:00	**Plenary Talk: Environment-assisted degradation of fibres in FRP composites for advanced concrete structure**	***Raman Singh,*** *Monash University, Australia*
12:00-12:20	**High performance graphene-based devices with an affordable cost by using a wafer bonding**	***Hirokazu Fukidome,*** *Tohoku University, Japan*
12:20-12:40	**Vibro-impact response of FRP sandwich plates with a foam core reinforced by chopped fiber rods**	***Hui Li,*** *Northeastern University, China*
12:40-13:00	**Cost-efficient and recyclable epoxy vitrimer composite with low initial viscosity based on exchangeable disulfide crosslinks**	***Shaojian He,*** *North China Electric Power University, China*
13:00-13:20	**Asymmetry at ferromagnet/antiferromagnet interface: Route toward an advanced spin-orbit torque device**	***Chao-Yao Yang,*** *National Yang Ming Chiao Tung University, Taiwan*
13:20-13:40	**Palladium-catalyzed chemoselective direct α-arylation of carbonyl compounds with chloroaryl triflates at the C–Cl site**	***Chau Ming So,*** *The Hong Kong Polytechnic University, Hong Kong*
13:40-14:00	**Development of IrOx pH electrode modified by SP/SiOx/ImIL composite film with long stability and high anti-interference**	***Shen Yunwen,*** *Zhejiang University, China*

14:00-14:20 **Unraveling roles of lead ions in selective flotation of scheelite and fluorite from atomic force microscopy and first-principles calculations**

Wenjihao Hu, *Central South University, China*

14:20-14:40 **Mechanical and Electrical Performances of Polylactic Acid/Liquid Natural Rubber/Graphene Platelets Nanocomposites in the Light of Different Graphene Platelets Functionalization Routes**

Sahrim Ahmad, *Universiti Kebangsaan Malaysia, Malaysia*

14:40-15:00 **Electronic and steric effects on L-Lactide Ring-Opening polymerization with NSSN-type Zr(IV) Complexes**

Ida Ritacco, *University of Salerno, Italy*

15:00-15:20 **Mechanistic Insights on Ethylene Polymerization with Ni(II) Catalysts: the impact of the ligand on the polymer microstructure:**

Maria Voccia, *University of Salerno, Italy*

15:20-15:40 **Grid Cells in the Brain as a Synergetic Problem of Physical Chemistry and Neurophysiology**

Alexander Chalyi, *Bogomolets National Medical University, Ukraine*

15:40-16:00 **Effect of physical-mechanical treating of cellulose on the properties of elastomeric composites**

Ivan Labaj, *Alexander Dubcek University of Trencin, Slovakia*

16:00-16:20 **Manufacturing processes of bonded magnets for the automotive industry**

David Esteves, *CeNTI, Portugal*

16:20-16:40 **Electrical and mechanical investigation of silver-polyurethane composite film under applied pressure**

Saeid Mehvari, *Northumbria University Newcastle ,UK*

16:40-17:00 — **Parameter Screening and Optimization of a Polycaprolactone-Based Electrospun Membrane for Guided Tissue Regeneration Applications**

Yuanyuan Duan, *University of Mississippi Medical Center, USA*

17:00-17:20 — **Electrostatic sheathing of lipoprotein lipase is essential for its movement across capillary endothelial cells**

Wenxin Song, *UCLA, USA*

Closing Remarks

Keynote Talks

DAY-1

Recent Advances in Photocatalytic Chemical Conversion

Jimmy C. Yu

Department of Chemistry, The Chinese University of Hong Kong

Solar-driven photocatalysis is a sustainable alternative to the current energy-intensive chemical processes. It has the potential to convert earth-abundant starting materials to industrial chemicals (e.g. oxygen to hydrogen peroxide, nitrogen to ammonia, etc.). We found that a hydrothermal carbonaceous photocatalyst derived from biomass could reduce dissolved O2 to H2O2 at a rate of 1.16 mmol gcat-1 h-1 together with an apparent quantum yield of 18.2% (at 420 nm). Furthermore, to solve the limited solubility and slow diffusion of oxygen in the water-based photocatalysis, a gas-liquid-solid interface was formed by loading the photocatalyst onto a porous substrate. The hydrophobic and mesoporous properties of the photocatalyst lead to abundant triphase reaction sites with higher oxygen-transfer rate and higher interfacial oxygen concentration, thus, giving rise to a 10-times enhancement on H_2O_2 yield. Moreover, charge polarization effect was discovered in single crystal phosphorus microbelts, effectively driving the oriented migration of photo-generated electrons. The preferential accumulation of electrons on specific facets of catalyst contributed to a superior photocatalytic hydrogen evolution rate. Taking advantage of Br2 evolution in a photocatalytic BiOBr-Br- system, ethylene could be selectively converted to bromoethanol, a key building block for the synthesis of ethylene-derived commodity chemicals. This system exhibited both high selectivity (92%-100%) and long-term stability (>40 h). Finally, the challenging N2 fixation can also be realized by photocatalysis. Fe-doped BiOBr was found to be a powerful catalyst to reduce N2 to ammonia. The doped Fe could induce oxygen vacancies and donate electrons to effectively break the N≡N. These works highlight the great potential of photocatalysis, and would shed new light on the development of novel approaches for the conversion of chemicals.

Biography

Jimmy C. Yu is an emeritus professor at The Chinese University of Hong Kong. He received a B.S. degree from St. Martin's College and a Ph.D. degree from the University of Idaho. Professor Yu has been a highly cited researcher for many years. His major research interest is photocatalysis, and he holds several patents on the fabrication and application of photocatalytic nanomaterials. Dr. Yu has received numerous honors including a State Natural Science Award and Chang Jiang Scholar Chair Professorship.

Quantum Light-Enhanced Two-Photon Imaging of Breast Cancer Cells

T. Goodson III,

Department of Chemistry, University of Michigan, Ann Arbor, Michigan 48109

Correct biological interpretation from cell imaging can be achieved only if the observed phenomena proceed with negligible perturbation from the imaging system. Herein, we demonstrate microscopic images of breast cancer cells created by the fluorescence selectively excited in the process of entangled two-photon absorption in a scanning microscope at an excitation intensity orders of magnitude lower than that used for classical two-photon microscopy. Quantum enhanced entangled two-photon microscopy has shown cell imaging capabilities at an unprecedented low excitation intensity of ~3.6×10^7 photons/s, which is a million times lower than the excitation level for the classical two-photon fluorescence image obtained in the same microscope. The extremely low light probe intensity demonstrated in entangled two-photon microscopy is of critical importance to minimize photobleaching during repetitive imaging and damage to cells in live-cell applications. This technology opens new avenues in cell investigations with light microscopy, such as enhanced selectivity and time–frequency resolution.

Biography

Theodore Goodson III is the Richard Barry Bernstein Professor of Chemistry at the University of Michigan. Professor Goodson received his BA in liberal arts from Wabash College in 1991 and his Ph.D. from U of Nebraska-Lincoln in 1996. He was a postdoctoral assistant at the University of Chicago and Postdoctoral fellow at Oxford University. Dr. Goodson investigates ultra-fast, nonlinear and quantum optical properties in organic multi-chromophore and metal cluster systems for particular optical and electronic applications in the condensed phase. His research has been translated in to technology in the areas capacitors, two-photon remote and quantum light spectroscopy and microscopy. Presenting author details

Modelling and characterization of mixed-matrix membranes

Cao Z, Wu H, Kruczek B and **Thibault J***
Department of Chemical and Biological Engineering
University of Ottawa, Ottawa, Ontario, Canada K1N 6N5

Mixed matrix membranes (MMMs) combine the superior properties of fillers to modulate the membrane diffusivity and selectivity coefficients to achieve the membrane overall properties. One can use, for instance, porous crystalline aluminosilicates to enhance the selectivity of the MMM for the natural gas sweetening (CO_2-CH_4). Others could use montmorillonite nanoclay embedded in a polymeric membrane to develop a membrane with barrier properties. There are a large number of new applications appearing every day for gas separation with the ultimate objective to push the frontier of the the permeability/ selectivity tradeoff typically observed for polymeric membranes. Indeed, many studies have investigated the use of nanoparticles added in the polymeric membranes and have examined their impact on the permeation properties in addition to other properties such as hydrophilicity, fouling resistance, chemical stability, mechanical strength and antibacterial effect. There exists an increasing number of nanoparticles: quantum dots, metalloids and metal oxidebased nanoparticles, metallic organic frameworks (MOFs), carbon-based nanomaterials (activated carbon, fullerenes, carbon nanotubes and graphene oxides), montmorillonite nanoclay, etc.

This presentation will focus on the use of permeable and impermeable nanoparticles to modulate the permeability of a permeating gas across thin mixed-matrix membranes under ideal conditions. Modelling can be used synergistically with experiments to develop better membranes for a given application. Results, obtained by solving numerically the Fick's second law of diffusion, will discuss the impact of the permeability and the solubility of the nanoparticle fillers on the effective permeability of the MMM. The effective gas permeability, obtained under ideal conditions, can be used to diagnose the reasons for the departure from the expected trends frequently observed in the literature.

Biography

Since 2000, Jules Thibault is professor of chemical engineering at the University of Ottawa. His research interest are in process simulation and optimization applied to biotechnology and membrane processes.

Scientific Session DAY-1

Polymeric materials as tools to study and direct immune function

Christopher M. Jewell

University of Maryland – College Park, United States of America

Our research combines immunology and biomaterials to understand the interactions between polymeric materials and immune tissues, and to design more selective therapeutic vaccines for cancer and autoimmunity. This presentation will highlight our recent efforts combining materials science and bioengineering tools, cell culture, animal models, and samples from human patients. In one example I will discuss new degradable polymer depots that could improve the selectivity of therapies for autoimmune diseases such as multiple sclerosis and diabetes by locally reprogramming the function of lymph nodes – tissues that coordinate immunity. A second area will present the lab's efforts to self-assemble immune signals into modular nanostructures. This rational design approach allows activation of programmable combinations and levels of innate immune pathways. Modular control over these aspects of immune signaling could help improve the efficacy of vaccines for cancer and infectious disease, and enhance the efficiency of vaccine translation.

Biography

Christopher M. Jewell is the MPower Professor and the Minta Martin Professor of Engineering at the University of Maryland in the Fischell Department of Bioengineering. Dr. Jewell is a Fellow of the Biomedical Engineering Society (BMES), the American Institute for Medical and Biological Engineering (AIMBE), the Controlled Release Society (CRS), and the Alliance for Cancer Gene Therapy (ACGT). He has also been named a Miegunyah Distinguished Faculty Fellow in Australia. His work has been supported by over $23M, resulting in over 120 papers and patents, including in *ACS Nano, Nature, Nature Biotechnology, Nature Materials, PNAS,* and *Trends in Immunology*. Some of Dr. Jewell's awards include being honored by the White House as a recipient of the Presidential Early Career Award for Scientists and Engineers (PECASE), the United States's highest honor to scientist and engineers in the first half of their career. He has been selected as a Damon Runyon-Rachleff Innovator, appointed as an Associate Scientific Advisor for *Science Translational Medicine*, received the Outstanding Lectureship in Drug Delivery from the Materials Research Society and been selected as the University of Maryland's Graduate Faculty Mentor of the Year. Chris was also named the state of Maryland's Outstanding Young Engineer by the Maryland Academy of Science. Dr. Jewell graduated from Lehigh University with high honors, earning dual degrees in Chemical Engineering and Molecular Biology. He received his PhD from the University of Wisconsin – Madison, working with Professor David Lynn. Chris then joined the Boston Consulting Group in New York City, where he worked in R&D strategy with global pharmaceutical companies. Dr. Jewell carried out his postdoctoral training as a Ragon Fellow with Dr. Darrell Irvine at MIT and as a Visiting Scientist at Harvard with Dr. Dan Barouch.

Surface-Immobilized Photoinitiators for Light Induced Polymerization and Coupling Reactions

Wolfgang Kern*[1] Ch. Bandl[1], Matthias Müller[1], M. Haas, M. Drusgala

[1] *University of Leoben, Chair in Chemistry of Polymeric Materials, A-8700 Leoben, Austria*

[2] *Graz University of Technology, Institute of Inorganic Chemistry, A-8010 Graz, Austria*

The functionalization of inorganic surfaces by molecular layers, including self-assembled monolayer, is a widely applied and important technique for the fabrication of functionlized and nanostructured materials. By conferring photoreactivity to molecular layers at surfaces, various surface properties can be adjusted by UV illumination. It will be demonstrated how photosensitive units can be attached to inorganic surfaces utilizing thiol or trialkoxysilyl anchoring units. Surface photochemistry is transferred to inorganic particles by covalently attaching photoiniating groups onto silica nanoparticles. A series of tri(alkoxy)silyl functionalized acylphosphine oxides and other Norrish type I photoinitiators, among them Germanium based initiators, have been synthesized and coupled. The modified particles were then incorporated into acrylate resins and thiol-ene resins to study the photoinitiation efficiency of the covalently bound initiators. The concept of using immobilized photoinitiators follows a general strategy towards low-migration photoinitiators as required for UV curable printing inks.

Another approach is related to the immobilization of azidophenyl units onto the surface of inorganic particles. Using this approach, these particles (e.g., silica) can be attached to the surface of chemically inert polymer films and fibres such as polyethylene and poly(ethylene terephthalate) by a photoinduced clic reaction. This paves the way towards inorganic protective layers on polymer surfaces, and also towards the tuning of properties of particle composites via changing from weak to strong interfaces via radiation induced reactions.

Biography

W. Kern has studied Chemistry in Graz (Austria), and is Holder of the Chair in Chemistry of Polymeric Materials at the University of Leoben (Austria). He is also the Scientific Director (CSO) of the Polymer Competence Center Leoben (PCCL). The research interests of W.K. are special and functional polymers, polymer photochemistry, and chemistry at interfaces of inorganic / organic materials. He is author / co-author aof 170 journal articles, and inventor / co-inventor of 19 patents.

Properties of polymer chains at interfaces revealed by quantum beam techniques

Hiroyuki Aoki[1,2]

[1] Japan Atomic Energy Agency and [2] High Energy Accelerator Research Organization, Japan

The physical properties of the polymer materials in thin film states is modified from those in the bulk state. In order to understand the fundamental mechanism of the modification of the material properties, the behavior of the polymer chain should be discussed. Neutron and laser spectroscopy techniques has been used as powerful tools to study the structure and dynamics of the polymer chains in a bulk medium because they can extract the selective information only from the “labeled” polymer chain. In the current work, the dynamics of poly(methyl methacrylate) (PMMA) chains in spin-cast films prepared on a silicon substrate was investigated by neutron reflectometry (NR) and fluorescence microscopy using the acrylate polymer samples labeled by deuterium and fluorescent dye, respectively. The depth dependence of the diffusional motion of the polymer chain in thin films was examined by neutron reflection spectra. It was found that the polymer chain near the solid interface showed the lower mobility compared to that in a bulk medium. The detailed observation of the segmental motion of the polymer chain at the single molecule level was carried out by laser fluorescence microscopy. It revealed that the strong interaction between the polymer chain and the substrate interface hinders the rotational motion of the chain segment.

Biography

Dr. Hiroyuki Aoki is a Principal Scientist of J-PARC Center, Japan Atomic Energy Agency (JAEA) and a Professor of Institute of Materials Structure Science, High Energy Accelerator Research Organization (KEK). He obtained his PhD degree from Kyoto University in 2001. He became an Assistant Professor of Department of Polymer Chemistry, Kyoto University in 2001 and was promoted to an Associate Professor in 2006. He moved to JAEA as a Senior Scientist in 2016 and became a Principal Scientist of JAEA. He has been also a Professor of KEK since 2019. His research interests are focused on structure and dynamics of polymer materials at the single molecule scale. He was awarded with the Inoue Research Award for Young Scientist from Inoue Foundation for Science (2002), Young Scientist Lectureship Award (2008), SPSJ Award for the Outstanding Paper in Polymer Journal (2008), and Science Award from the Society of Polymer Chemistry, Japan (2016).

Development and characterisation of sustainable prepregs with improved fire behaviour based on furan resin and basalt fibre reinforcement

Patricia Ares Elejoste*, Alexandra Allue, Jesus Ballestero, Santiago Neira, José Luis Gómez-Alonso, KoldoGondra

GAIKER Technology Centre, Basque Research and Technology Alliance (BRTA) Parque Tecnológico de Bizkaia, Edificio 202, 48170 Zamudio, Spain

In recent years, the need to minimize environmental impact has led to the exploration of sustainable materials, avoiding those derived from petroleum. Considering, that these materials should proceed from nature, be harmless and durable. Therefore, throughout this work, the following raw materials were taken: furan resin, which comes from agricultural by-products and, basalt fibre, obtained by melting basaltic volcanic rock. Specifically, this work studies the development of a flame retarded furan prepreg manufactured by means of a continuous process combining a double belt lamination equipment with an impregnation system. Once the prepregs (flame and non-flame retarded) were obtained, they were subjected to various tests to analyze their fire behaviour, showing both an adequate performance. However, comparing both, concerning the toxicity index (CIT_G), the flame retarded prepreg generated fewer toxic gases during combustion than the non-flame retarded one, although the latter shows a lower smoke density. In short, the developed flame retarded material falls into R1HL3 (Requirement 1 and Hazard Level 3) classification demanded by products with large areas in railway vehicle interiors, which is the maximum safety level according to the risk index established in applicable regulations. Therefore, this material could be used in any railway vehicle for indoor applications.

Biography

Patricia works as a researcher in the department of Sustainable Composites and Functional Polymers. Graduated in Chemical Engineering at the University of the Basque Country (UPV/EHU) with a Master's degree in Biomedical Research (UPV/EHU) and currently pursuing a PhD in Materials Engineering and Sustainable Processes. Experience in the characterization of sustainable formulations for composites and in the development of composites. Participation in R&D projects.

Understanding the Structural Organization of Synthetic Spider Silk for the Development of Novel Biomaterials

Daniela M. de C. Bittencourt[1], Paula F. Oliveira[1,2], Betulia M. Souto[1], Sonia M. de Freitas[2], Luciano P. Silva[1], Andre M. Murad[1], Valquiria A. Michalczechen-Lacerda[1],Randolph V. Lewis[3], and Elibio L. Rech[1]

[1]*Embrapa Genetic Resources and Biotechnology, Brasília, DF, Brazil*

[2]*University of Brasília, Brasília, DF, Brazil*

[3]*Utah State University, Utah, USA*

Aiming for the possible use of the spider silks in the development of novel biomaterial we have designed and produced recombinant spider silks proteins based on spidroins from the Brazilian biodiversity. Besides their extraordinary mechanical properties, spider silks are also known for their biocompatible and biodegradable nature, pointing them as perfect biological macromolecules for improved drug delivery and various biomedical applications. However, in order to design a successful strategy for the production of innovative silk derived structural materials, it is crucial to comprehend the biochemical mechanisms responsible for fiber formation and mechanical properties. To investigate the relationship between flagelliform (Flag) silk structural organization and the mechanisms of fiber assembly, we produced the recombinant spidroin rNcFlag2222 in *Escherichia coli*. Among the silks produced by orb weaver spiders, Flag is extremely elastic and presents a very high hysteresis. In nature, it is used in the core of the web for prey-capturing. The rNcFlag2222 was based on key structural regions from *Nephylengys cruentata* spider's Flag spidroin, the glycine-rich structural motifs (GPGGX/GGX) and the spacer region. Using several approaches for nanomolecular analysis, including circular dichroism spectroscopy, atomic force and scanning electron microscopies, Raman spectromicroscopy and X-ray diffraction, we have compared structural data of rNcFlag2222, in its fibrillar and in its fully solvated states. Similar to natural spider silks, rNcFlag2222 behaved in solution like elongated semiflexible polymers with rigid sections, characterized mostly by the presence of helical structures, β-turn and β-sheet structural conformations. Our results add to the idea that the spacer region might be involved in 5-sheets formation, possibly serving as a linker for the flexible spirals adopted by the repeated glycine-rich sequence, conferring strength to the fiber. Therefore, our study of the structural conformational dynamics of Flag protein repetitive domains might be highly relevant for the development of novel biomaterials.

Biography

Daniela Bittencourt completed her D.Sc in Molecular Biology at the University of Brasília, Brazil, in 2007. In 2007, she also became a researcher at the Brazilian Agricultural Research Corporation (Embrapa). Since then she has collaborated with international institutions in the US and Europe, developing research focused on engineering oand the development of biomaterials based on spider silk proteins. Between 2019/2021, she was a Visiting Scientist at the J. Craig Venter Institute (JCVI, La Jolla/CA, USA) and currently remains as Associate Scientist collaborating with research for the study and development of synthetic cells. Currently, she is responsible for the Laboratory of Synthetic Biology at Embrapa and collaborator of the National Institute of Science and Technology in Synthetic Biology (Brazil).

Sustainable act for construction chemicals by using recycled biopolymer in cementitious tile adhesive

Nevin Karamahmut Mermer* **Mustafa Asim Ozkan, Dogan Genc, Ece Unlu Pinar**

Kalekim Construction Chemicals, Turkey

Starch-based recycled biopolymer as a consequence of the polymerization of starch, which is 44% in the structure of waste bread, with the bulk polymerization technology, was obtained from Plastic Move Company. The advantage of using biopolymer in the plastic industry is reducing the consumption of petroleum-based polymers by 30-40 %. In the current study, the use of starch-based recycled biopolymer instead of starch ether in C2TE S1 class high performance cementitious flexible adhesive with extended open time and reduced slip for ceramic tiles was evaluated. Utilizing sustainable strategy, the use of starch-based recycled biopolymer, which has not been reported before in the construction chemicals market, leads an alternative field of use to starchbased recycled biopolymer. The characterization of the biopolymer was performed using FTIR and STA instruments and analysis results were compared with commercially used starch ether.

Characterized biopolymer was added to the C2TE S1 class adhesive samples at the determined rates and was subjected to the mandatory tests. Both fresh mortar tests and performance tests (according to EN 12004-1/2 standard) of the C2TE S1 class cementitious adhesive were carried out. In addition to using the biopolymer instead of starch ether, it has been tested whether it will be effective in reducing the rate of raw materials used as a rheology modifier. According to the test results, using that biopolymer as a main rheology modifier in cementitious tile adhesives is not suitable for current situation. As a result of the study, starch-based recycled biopolymer can be used instead of starch ether in cementitious materials. For further investigation this sustainable act leads novel approach to cementitious and polymeric coatings.

Biography

Dr. Nevin Karamahmut Mermer completed her graduation project at Brno University of Technology, Czech Republic in 2010. She obtained her BSc, MSc and PhD degrees in Chemical Engineering Faculty at Yildiz Technical University, Turkey. During her PhD studies, she worked as a Research Engineer in Seranit Porcelain Company for 1.5 years. She has been working for Kalekim Construction Chemicals as R&D Senior Engineer since 2019. She has 20 presentations shared in national/international congresses and 12 articles published in national/international refereed journals.

Predicting the lifetime of weathered polyolefins by relating mechanics to microstructure

Marta Chiapasco

Department of Materials, Imperial College London, UK

Designing polymers with a specific microstructure can affect how the polymer degrades once released in the environment. Not only the amount but also the distribution of different phases determines a polymers' degradability. The following research investigates the use of a combination of spectroscopy analysis and thermal analysis to study changes of polymers' amorphous and crystalline phases during degradation, comparing different microstructures of polypropylene and polyethylene (1). The materials are subsequently studied with mechanical tests to understand when the structure fails. The use of nanoindentation helps studying how degradation proceeds across a material by looking at changes in phases while bulk tensile test shows when the material fails (2). This research allows to design materials that degrade faster when released in the environment and hence exposed to UV, thermal difference and microorganisms. The goal is to create materials that degrade at faster rates without releasing microplastics in the environment (3).

References:

(1) Blakey I, George GA. Raman spectral mapping of photo-oxidised polypropylene. *Polymer Degradation and Stability*. 2000; 70 (2): 269-275.

(2) T. Pertin, G. Minatchy, M. Adoue, A. Flory, L. Romana. Investigation of nanoindentation as a fast characterization tool for polymer degradation *study, Polymer Testing*. 2020; 81; https://doi.org/10.1016/j.polymertesting.2019.106194.

(3) (46) Gaillard T, George M, Gastaldi E, Nallet F, Fabre P. An experimental and theoretical study of the erosion of semi-crystalline polymers and the subsequent generation of microparticles. *Soft matter*. 2019; 15 (41): 8302-8312.

Biography

I am in my third year of PhD at Imperial College London. I have been focusing my research on plastic pollution since the beginning of my studies. During my bachelor thesis I have worked at Northwestern University studying ways to filter microplastics pollutants in wastewater systems. During my master at Imperial College I focused on the degradation of polystyrene simulation rivers shores. I have a personal interest in reducing humans' impact on the environment and I have always applied my knowledge in personal projects and working experiences around this field.

Something from Nothing: Bioplastic from one carbon feedstock

Ying Zhang

BBSRC/EPSRC Synthetic Biology Research Centre (SBRC), School of Life Sciences, University of Nottingham, Nottingham, NG7 2RD, UK

Traditional plastics' production and recalcitrance in nature have negative effects on the environment, which leads an urgent need for alternative materials to replace traditional plastics. Polyhydroxyalkanoates (PHAs) comprise a group of natural polymers that are biologically synthesized by microorganisms, which are potential alternatives to plastic on account of their availability from renewable sources, plastic-like properties and biodegradability. Bacteria such as Methylocystis parvus can accumulate PHB(Poly-3-hydroxybutyrate) utilizing methane and/or methanol; Cupriadavidus necator is capable of using CO2 as a carbon source to produce PHB at high yield. All of those one carbon feedstocks can be obtained from industrial waste gases and renewable sources.

Furthermore, through synthetic biology approaches, those one carbon fixing bacteria can be genetic engineered to produce co-polymers with desired mechanical properties (much greater elasticity and lower melting temperatures) such as poly(3-hydroxybutyrate-co-3-hydroxypropionate and poly(3-hydroxybutyrate-co-3-hydroxyhexanoate). The ratio of the two monomers can be modulated via fine-tuning of the engineered pathway at molecular level. In this manner it is possible to produce a range of polymers with different properties by varying the amount of one monomer present in the copolymer.

Biography

YZ is an ECR (PhD University of Nottingham, 2007) with strong interests in applied microbial engineering and synthetic biology. YZ's group routinely handle and genetic modify “difficult” bacteria including expertise in the genetics and genomics of one-carbon fixing bacteria.

Temperature dependence of PSS diffusion in multilayers of entangle PDADMA: more than one diffusion constant

Annekatrin Sill*, Peter Nestler, Peter Thran, Christiane A. Helm

University of Greifswald, D-17489 Greifswald, Germany

Assemblies of oppositely charged macromolecules (proteins, DNA, polyelectrolytes) are often used for surface modification and functionalization. Yet the mobility of the different composites within the surface coating is unknown. As model system, polyelectrolyte multilayers are used. They were prepared by sequential adsorption of oppositely charged polyelectrolytes, the polyanion PSS, and the polycation PDADMA. We study the vertical diffusion constant of PSS using neutron reflectivity. The diffusion constant DPSS could be varied by five orders of magnitude by varying (i) the molecular weight of the polycation PDADMA and (ii) the salt concentration of the preparation solution. The dependence of DPSS on the molecular weight of PDADMA can be described by different power laws. Below the entanglement limit, the exponents are consistent with the predictions of the sticky reptation model. The PSS diffusion constant of films built from 100 mM NaCl drops three orders of magnitude when exceeding the entanglement limit. To figure out if an immobile PSS fraction exists in a film built from 72 kDa PDADMA (beyond the entanglement limit), the film was annealed at 1 M NaCl solution at different temperatures. The observed diffusion could not be described by a simple diffusion model. Instead, two different PSS fractions (one mobile and one almost immobile, i.e. different diffusion constants) are the simplest model to describe the time dependence of the scattering length density profiles. Increasing the annealing temperatures (20 – 50 °C) increases the diffusion constant of both the fast and slow PSS fraction. Additionally, the fraction of fast PSS molecules is increased. We suggest that an immobile or nearly immobile fraction of polyelectrolytes is always present when the polymer length is beyond the entanglement limit and the sticky reptation model fails.

Biography

Dr. Annekatrin Sill trained as a chemical laboratory assistant, then studied biochemistry at the University of Greifswald and completed her Ph.D. in 2022 on the topic of “Vertical diffusion of polyelectrolytes in polyelectrolyte multilayers during film preparation and post preparation treatment” at the Institute of Physics at the University of Greifswald. Currently, she is a Postdoc at the Soft Matter and Biophysics group headed by Prof. Christiane A. Helm and continues her research on the diffusion of polyelectrolytes in multilayers. She is an associate member of the collaborative research centre “Electrically Conductive Multilayers for Surfaces of Implants” (CRC 1270/2 – ELAINE).

The Microencapsulation of Tung Oil with Natural Hydrocolloid and Synthetic Emulsifiers for Extrinsic Self-Healing Applications

Abdullah Naseer Mustapha*, Maitha AlMheiri

Technology Innovation Institute, Masdar City, Abu Dhabi

In this work, self-healing microcapsules were prepared with a urea-formaldehyde shell, via a one-step in situ polymerization process. The chosen core material was tung oil, a drying oil often used for corrosion resistance applications. For the onestep in situ polymerization process, the emulsifier of choice is of vital importance, and synthetic polymers were compared to more environmentally friendly hydrocolloid alternatives. The conventionally used poly(ethylene-alt-maleic-anhydride) (PEMA) polymer is compared with poly(vinyl-alcohol) (PVA), poly (ethylene-glycol) (PEG), as well as Gelatin (GEL) and Xanthan Gum (XG), and Gum Arabic (GA). The hydrocolloid GEL emulsifier produced the highest payload microcapsules (96.5 %), yield (28.9 %) and encapsulation efficiency (53.6 %) respectively, much higher than that of the synthetic emulsifiers. The GEL microcapsules also conveyed the highest self-healing efficiency of 91 %, compared to PEMA's 63 %, PVA's 52 %, PEG's 12 %, XG's 72 % and GA's 68 %. Focussed ion beam (FIB) measurements also confirmed the containment of the tung oil in the microcapsules, in an innovative and novel characterization procedure. Additionally, the corrosion resistance also conveyed the GEL conveyed the highest corrosion resistance visually, proving it to be the most viable emulsifier in this process.

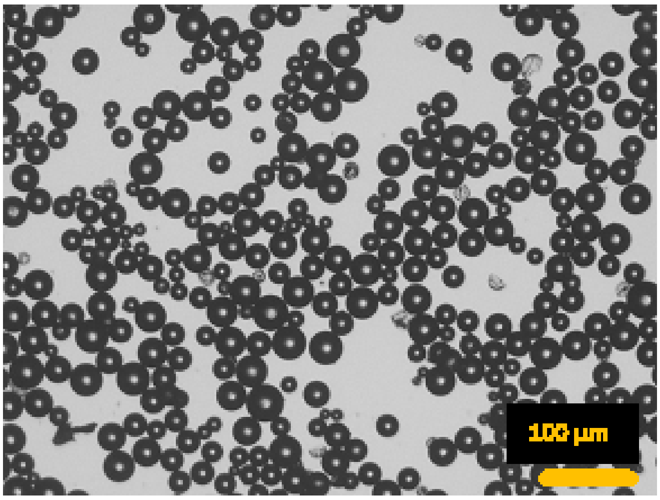

Figure1: OM images of the GEL microapsules

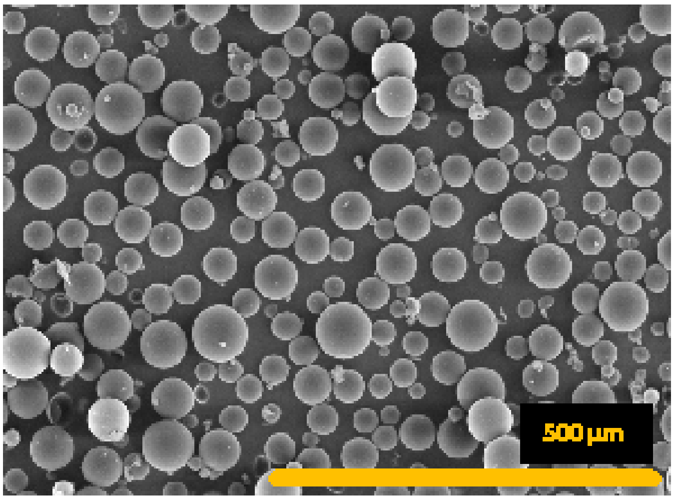

Figure2: SEM micrographs of the GEL microcapsules

On-line ATR-MIR for real-time quantification of chemistry kinetics along the barrel in extrusion-based processes

Lucivan P Barros Jr, Sebastiao Canevarolo a , Joao Maia b

[a] Department of Materials Engineering, DEMa, Federal University of São Carlos, São Carlos, SP, 13565-905, Brazil

[b]Department of Macromolecular Science and Engineering of Case Western Reserve University, USA

This work deals with the development and validation of an on-line infrared spectroscopic set-up for the real time quantification of the melt extrudate during reactive extrusion based processes. The arrangement consists of an infrared spectrophotometer operating in attenuated total reflectance ATR-FTIR, fitted on-line, along the extruder barrel. The setting helps understand the effects of extrusion process parameters and the reaction conversion during development of polymer blends and compound in-processing. The ATR-FTIR spectroscopic probe has been coupled along with an extruder to analyze/understand the process during operation in the MID region of the infrared spectrum. The ATR-FTIR prototype probe was calibrated and validated using off-line measurements. The probe is interfaced to the extruder through to a probe holder unit (PHU), also described herein. The on-line ATR-FTIR measurements were conducted at various locations (L/D) along the length of the extruder. Polymer blends of PP/PA6 in various compositions were investigated and reactive blend of PP-g-AA/PA6 were used to validate the on-line measurements compared to the standard off-line ATR-FTIR analysis.

Biography

Lucivan holds a bachelor's degree in Metallurgical and Materials Engineering and a master's degree in Materials Science and Engineering from the Universidade Estadual do Norte Fluminense – UENF – (Campos, RJ, Brazil). He earned two doctorates. The first in Polymer Engineering at Case Western Reserve University – CWRU - (Cleveland, Ohio, USA), the second in Materials Science and Engineering at the Federal University of São Carlos – UFSCar - (São Carlos, SP, Brazil). He is a research associate at the CWRU. His research includes extrusion process, infrared spectroscopy, polymer blends and in-process monitoring. His work currently focuses on high-performance polyurethane systems, with an emphasis on thermoplastic polyurethane and its carbon-based filler nanocomposites.

Kinetics of Guided Growth of Horizontal Nanowires on Sapphire Surfaces

Tomas Sikola

Brno University of Technology, Institute of Physical Engineering & CEITEC, 612 00 Brno, CzechRepublic

Surface-guided growth of planar nanowires has been shown to enable their assembly and alignment on substrates during growth, thus eliminating the need for additional post-growth processes. However, accurate control and understanding of the growth of the planar nanowires were achieved only recently, and only for ZnSe, ZnS and GaN nanowires [1], [2]. In the talk, the results obtained in the papers on the growth kinetics of these surface-guided planar nanowires on flat and faceted sapphire surfaces, based on a growth model will be presented. The data resulting from this model confirm the presence of two limiting regimes-either the Gibbs-Thomson effect controlling the growth of the thinner nanowires or surface diffusion controlling the growth of thicker ones. The qualitative comparisson of surface-guided planar nanowires consisting of different semiconductor materials indicates the generality of the growth mechanism. This general model enables us better control of the nanowire dimensions and thus more reliable fabrication of nanowires.

References:

[1] Rothman, A.; Dubrovskii, V. G.; Joselevich, E., Kinetics and mechanism of planar nanowire growth. Proc. Natl. Acad. Sci. U.S.A. 2020, 117 (1), 152.

[2] Rothman A; Maniš J,; Dubrovskii V.G.; Šikola T.; Mach J.; Joslevich E.; Kinetics of Guided Growth of Horizontal GaN Nanowires on Flat and Faceted Sapphire Surfaces. Nanomaterials 2021, 11, 624.

Biography

Tomas Sikola is a full Professor of Applied Physics, director of the Institute of Physical Engineering at Brno University of Technology (BUT), and leader of the “Fabrication and Characterization of Nanostructures” research group of the Central European Institute of Technology (CEITEC) in Brno. He also acts as a coordinator of the Advanced Nano and Microtechnology Research Programme of CEITEC. His present research interests are in surface science; thin film physics; nanoscale science and technology; fabrication of nanostructures and investigation of their functional properties for plasmonics, micromagnetism, and spintronics; and development of analytical and measurement methods and instruments.

Preparation of Poly(ethylene glycol)@Polyurea Microcapsules Using Oil/Oil Emulsions and Their Application as Microreactors

Raed Abu-Reziq

Institute of Chemistry, Casali Center of Applied Chemistry and Center for Nanoscience and Nanotechnology, The Hebrew University of Jerusalem, Israel

Microencapsulation processes, in which core-shell particles can be produced by interfacial polymerization, have been investigated intensively. These processes are utilized usually for the controlled release of bioactive substances or for the protection of functional materials. In addition, microencapsulation has been reported as a promising method for the catalyst immobilization. The size of these catalytic microcapsules is several tens of microns, and this could facilitate their separation using conventional filtration techniques. In most cases, the microcapsules prepared for catalytic applications are formed using oil-in-water (o/w) emulsions, and because of that moisture sensitive catalysts cannot be immobilized by this method. In order to circumvent such limitation, we focus on developing a method for the preparation of polyurea microcapsules using oil-in-oil (o/o) emulsions. Oil-in-oil emulsion systems consist of a polar organic phase dispersed in a non-polar organic solvent containing a proper surfactant. In our study, polyethylene glycol (PEG) was chosen as the polar organic phase. The process of preparation the polyurea microcapsules is based on emulsification of PEG in non-polar solvent such as heptanes or toluene and then the polymeric shell around the PEG droplets is created by interfacial polymerization of isocyanate and amine monomers. In our presentation we will describe the preparation method of these capsules, their characterizations and applications as catalytic microreactors.

Biography

Prof. Abu-Reziq completed his doctorate at the Hebrew University in catalysis and sol-gel chemistry. After receiving his Ph.D. degree in 2004, he moved to Ottawa University, Canada, to do his postdoctoral research in the field of nanocatalysis. In 2006, he joined the company Sol-Gel Technologies as Senior Researcher and spent two years in developing micro and nano-encapsulation systems based on sol-gel process as drug delivery systems. In 2008, He was appointed as Senior Lecturer at Casali Center for Applied Chemistry and Institute of Chemistry and on 2015 he was promoted to Associate Professor. His research focuses on nanocatalysis, magnetic materials, green chemistry and developing micro and nanoencapsulation methods.

A synergistic multi material flame retardant formulation for reinforced PA6 on the basis of expandable graphite

Forian Tomiak

Friedrich Alexander Universität Erlangen-Nürnberg, Erlangen 91058, Germany

This presentation reports the development of a multi-material flame retardant system based on expandable graphite for glasfiber reinforced polyamide 6 (PA6). The multi material system is based on Expandable Graphit (EG) combined with a variety of synergistis Aluminum Diethylphosphinat (AlPi), Melamine Polyphosphat and Montmorillonite (MMT). 20 wt.% additivation has been found to be sufficient in glasfiber reinforced PA6 to achieve a V0 classification. Due to the enormous expansion of EG, providing a thermally stable, thick isolation layer on the polymer surface, excellent fire behavior has been identified particullarly in cone calorimeter tests. A very low heat response parameter (HRP) indicates good reaction to fire properties and a low burning rate provides a minimal smoke production level. The presentation provides results regarding the fire behavior/ characteristics measured in cone calorimeter and UL-94 V fire tests. Flame retarding properties are extensively discussed. Additional information about mechanical properties will be provided.

Biography

The autor studied industrial engieering at the Friedrich Alexander Universitat Erlangen-Nurnberg (FAU) and is currently working as scientific assistant at the Institute of Polymer Technology (FAU). His main topic is the investigation of the flame behavior of polymeric material systems.

Greenhouse Gas Emission Reduction Potential of European Union’s Circularity Related Targets for Plastics

Anna Tenhunen-Lunkka, Tom Rommens, Ive Vanderreydt & Lars Mortensen

VTT Technical Research Centre of Finland Ltd, Finland

Current rising concerns about environmental and climate impacts in production, consumption and end-of-life of plastics have led to efforts to switch from linear to circular economy of plastics in Europe. Greenhouse gas emissions are likely to decrease with a transition to a circular system; however, a systematic and integrated perspective on plastics and the carbon cycle is currently missing in the debate on plastics.

In this study, a model to estimate greenhouse gas emissions of the current mostly linear plastics value chain of the EU in 2018 and a future scenario, 2025 model, were created. By 2025 if current policy targets are reached, the plastic packaging recycling rate should be 50%, PET-based drinking bottles should include 25% recycled content, 77% collection target for plastic bottles, 10 Mt recyclates should enter the markets, uptake of bio-based plastics is estimated by European bioplastics to increase from current 1 to 1.32% and landfilling will continue to decrease according to the current trend at 3.85%.

Total greenhouse gas emissions caused by the current plastics value chain in Europe are estimated at 208 million tonnes of CO2-eq. The 2025 model estimates that total plastics value chain emissions will be 182 Mt of CO2-eq. Reduction potential is approximately 26 Mt of CO2-eq or 13%.

The oral presentation will present the work done and the results based on ‘Greenhouse Gas Emission Reduction Potential of European Union’s Circularity Related Targets for Plastics’ publication (Tenhunen-Lunkka, A., Rommens, T., Vanderreydt, I. et al. Greenhouse Gas Emission

Reduction Potential of European Union’s Circularity Related Targets for Plastics. Circular Economy and Sustainability (2022). https://doi.org/10.1007/s43615-022-00192-8)

Biography

Anna Tenhunen-Lunkka M.Sc.(Tech) works as Senior Scientist and Project Manager at VTT Technical Research Centre of Finland in the Material Processing and Circular Solutions research team. She is the coordinator of SusChem Finland National Platform, which is part of the European Technology Platform for Sustainable Chemistry. Her research is focused on sustainable circular economy and material and product circulation (especially plastics) as well as management and strategic research. Currently she coordinates Horizon Europe projects TREASoURcE and PRIMUS (20M€), and has managed H2020 and BBI JU projects (NONTOX, BIOSWITCH, WoodCircus). She has also managed several privately and nationally funded plastic recycling and recyclate upgrading and reuse related RDI projects. Previously, she has led and internationally awarded biobased packaging material development project (Ellen MacArthur Foundation, EcoPack Challenge 2018, Sustainability Awards 2018).

Scientific Session

DAY-2

Helical structure motifs made searchable for functional peptide design

Cheng-Yu Tsai, Emmanuel Oluwatobi Salawu, Hongchun Li, Guan-Yu Lin, Ting-Yu Kuo, Liyin Voon, Adarsh Sharma, Kai-Di Hu, Yi-Yun Cheng, Sobha Sahoo, Lutimba Stuart, Chih-Wei Chen, Yuan-Yu Chang, Yu-Lin Lu, Simai Ke, Christopher Llynard D. Ortiz, Bai-Shan Fang, Chen-Chi Wu, Chung-Yu Lan, Hua-Wen Fu, Lee Wei Yang*

National Tsing Hua University, Hsinchu 300040, Taiwan

To ensure a desired sequence motif to adapt the helical structure, we extract 1.7 million helices from the PDB and compile them into a database, Therapeutic Peptide Design dataBase (TP-DB) that allows queries of compounded patterns to facilitate a data-driven design of therapeutic peptides. By our pattern-based search engine but not PHI-BLAST, we identify a motif DYKYLE recognized by the anti-FLAG M2 antibody and repurpose a known purification-tag-specific antibody into a molecular diagnostic tool for H. pylori. Also, with TP-DB, we can design a new antimicrobial peptide (AMP) that contain the MD-elucidated membrane-insertion pattern WXXWXXW. The AMP has a better minimal inhibitory concentration and a much lower cytotoxicity against Candida albicans (fungus) than its template homologs. We also demonstrate how TP-DB can suggest point mutations on helical structures to enhance (or abolish in other cases) the peptide-peptide interaction in the development of tumor suppressors. Other strategies on therapeutic peptide design, including using PCA-based hydrophobic moments and partition free energy, will be mentioned when time allows. TP-DB is made accessible at http://dyn.life.nthu.edu.tw/design/. A full reference can be found at Nat Commun. 13: 102 (2022); https://www.nature.com/articles/s41467-021-27655-0

Biography

Prof Lee-Wei Yang is currently a Full Professor and the Director in the Institute of Bioinformatics and Structural Biology as well as Director of the PhD program in Biomedical Artificial Intelligence at National Tsing Hua University (NTHU), Taiwan. Trained as a chemical engineer throughout his B.S. and M.S. from National Taiwan University and NTHU, respectively, he joined School of Medicine, University of Pittsburgh to research in protein dynamics and structural bioinformatics under the supervision of Prof Ivet Bahar, a NAS member. After obtaining his PhD at age 29, he went through postdoctoral trainings in University of Tokyo (with Profs Nobuhiro Go and Akio Kitao) and Harvard University (with Prof Eugene Shaknovich) before taking the faculty position at NTHU in 2011. Prof Yang currently has an H-index of 23 with ~3500 citations from 40 SCI publications. He is also currently an honorary Professor in Mathematical Sciences, University of Liverpool, UK (via Dual PhD Degree Program), a visiting Professor in IPR, University of Osaka (2018) and in DCSB, University of Pittsburgh (2022).

Toward surface manipulation of engineered nanoparticles in drug delivery: The rise of in silico tools

Sourav Bhattacharjee

School of Veterinary Medicine, University College Dublin (UCD), Belfield, Dublin 4, Ireland

It is established now that the surface chemistry of a nanoparticle decides the range of interactions it undergoes within a biological milieu. The culmination of such events influences how nanoparticles behave in a nano-bio interface, including their cytotoxicity, cellular internalization, ability to permeate through a biological medium and release in case of encapsulated nanoformulations kinetics. Functionalization of nanoparticulate surfaces with ligands of pre-defined properties provides an opportunity for designing tailor-made nanoformulations that can negotiate with physiological barriers, such as the mucus barrier and the blood-brain-barrier with subsequent release of the encapsulated cargo of biomacromolecules. For example, polyethylene glycol—a hydrophilic polymer—when bioconjugated to nanoparticles, is known to enhance mucopermeation that remains a challenge, especially in the field of nanomedicine given nanoparticles adhere to the gut mucus layer, and after that gets wasted with the mucus recycled inside human body every 3–4 hours. Therefore, having an initial idea of the chemistry of surface ligands before grafting them on nanoparticles is crucial to designing nano-drug delivery systems (nano-DDSs) that can negotiate with the physiological barriers at a desired time, site, and kinetics. Various in silico tools can provide interesting insights into understanding the surface ligands, especially while dealing with a large library of molecules. Many of these tools, such as SwissADME and ChemDes, are freely available, run on web-based platforms without extensive computer power, and provide an interactive, user-friendly interface. The analyses provide a wealth of information on the surface ligands as molecular descriptors. The data can often be extrapolated as numerical read-outs while used for quantitative and comparative analyses. This talk will showcase the utility of such emerging in silico tools and make a case for broader utilization in nanomedicine.

Biography

Sourav Bhattacharjee was born in Kolkata (India), where he also received his schooling. He joined the Medical College and Hospital, Kolkata (India), in 1997 and graduated with an M.B.B.S. (Bachelor of Medicine and Surgery) in 2004. After a brief period of resident training in Orthopedic Surgery, he joined M.Sc. in Biomolecular Sciences/Cell Biology at the Vrije Universiteit Amsterdam (2006). In the meanwhile, he moved to Edinburgh (UK), where he conducted research on the toxicity of nanoparticles under the supervision of Prof. Vicki Stone (Napier University Edinburgh). He began his Ph.D. at Wageningen University (Netherlands) in 2008, which he successfully defended in 2012 with a very good thesis grade and quite a few research papers. Following that, he worked for a year as a postdoc at the MESA+ Institute for Nanotechnology (University of Twente, Netherlands). In March 2014, he joined Prof. David Brayden's group at University College Dublin (Ireland) as a postdoc working on the EU FP7-funded TRANS-INT consortium trying to develop nanoparticulate drug delivery platforms for oral insulin delivery. In February 2016, Bhattacharjee joined the UCD School of Veterinary Medicine as an Assistant Professor of anatomy. His current research interests include developing advanced theranostic platforms using biophotonic and in silico tools.

Environmental degradation of structural and fuel cladding stainless steels in liquid lead- and liquid lead-bismuth eutectic-cooled reactors

Konstantina LAMBRINOU

School of Computing & Engineering, University of Huddersfield, HD1 3DH, UK

A principal challenge in the deployment of Gen-IV lead-cooled fast reactors is the inherent corrosiveness of the primary heavy liquid metal (HLM) coolant for many structural and fuel cladding steels. Lead (Pb) and lead-bismuth eutectic (LBE) are used as primary coolants and spallation targets in accelerator-driven nuclear systems (ADS), such as the LBE-cooled ADS system MYRRHA under development at SCK CEN, Belgium. The candidate MYRRHA stainless steels are the 316L for structural components and the DIN 1.4970 for fuel cladding tubes. Understanding the liquid metal corrosion (LMC) behaviour of the MYRRHA candidate steels is key for the design and safe operation of this system, as the severity of LMC effects is determined by the operation conditions, i.e., temperature (T), time, LBE oxygen concentration (C_O), and LBE flow velocity (v). During nominal operation, the anticipated LMC mechanisms are oxidation (favourable, if controlled), and dissolution corrosion (undesirable). Dissolution corrosion becomes severe at high temperatures (T > 450 C) and low LBE oxygen concentrations (C_O < 10-8 mass%), i.e., in conditions suppressing the formation of protective oxide scales on the steel surface. Dissolution 'pitting', in particular, might jeopardize the structural integrity of thin-walled components (e.g., fuel cladding & heat exchanger tubes) within a short time span. This work focuses mainly on the dissolution corrosion behaviour of the 316L steel grade, which was studied by exposing different steel heats to oxygen-poor (C_O < 10-8 mass%), static liquid LBE, in the 350-550 C range, for up to 12,500 h. This work highlights the importance of the steel microstructure and thermomechanical state, demonstrating that the ingress of liquid LBE into the steel is facilitated by specific microstructural features, such as grain boundaries, annealing and deformation twin boundaries, secondary steel precipitates, etc. Various analytical techniques were used to characterize the corroded 316L steels, i.e., LOM, SEM/EDS, EBSD, FIB/TEM/STEM, etc.

Biography

Konstantina LAMBRINOU is Professor in Advanced Materials at the University of Huddersfield. Prior to her academic appointment, she worked for 10 years at SCK CEN, Belgium, investigating LMC effects in stainless steels for HLM-cooled reactors and developing LMC mitigation approaches. She is the principal investigator (PI) of the H2020 IL TROVATORE project on accident-tolerant fuel (ATF) claddings & the HORIZON SCORPION project on the radical performance optimization of SiC/SiC composite ATF claddings, and the European lead of the I-NERI (US/EURATOM) PERSEUS project on the post-irradiation examination (PIE) of ATF claddings irradiated in the BR2 test reactor within H2020 IL TROVATORE.

Cilostazol-imprinted polymer film-coated electrode as an electrochemical chemosensor for selective determination of cilostazol and its active primary metabolite

Jyoti,[a] Renata Rybakiewicz-Sekit[a,b,c] Teresa Z˙ołek,[d] Dorota Maciejewska,[d] Edyta Gilant,[e] Katarzyna Buś-Kwaśnik,[e] Andrzej Kutner,[f] Krzysztof R. Noworyta,[*,a] and Wlodzimierz Kutner

[a]Institute of Physical Chemistry, Polish Academy of Sciences, Kasprzaka 44/52, 01-224 Warsaw, Poland

[b]Faculty of Mathematics and Natural Sciences, School of Sciences, Institute of Chemical Sciences, Cardinal Stefan Wyszynski University in Warsaw, Wóycickiego 1/3, 01-815 Warsaw, Poland

[c] Laboratory of Organic Electronics, Linköping University, Bredgatan 33, 602 21 Norrköping, Sweden

[d] Department of Organic Chemistry, Faculty of Pharmacy, Medical University of Warsaw, Banacha 1, 02-097, Warsaw, Poland

[e] Łukasiewicz Research Network – Industrial Chemistry Institute, Rydygiera 8, 01-793, Warsaw, Poland

[f] Department of Bioanalysis and Drug Analysis, Faculty of Pharmacy, Medical University of Warsaw, Banacha 1, 02-097 Warsaw, Poland

An electrochemical chemosensor for cilostazol (CIL) selective determination was devised, engineered, and tested. Toward that, a unique conducting film of the functionalized thiophene-appended carbazole-based polymer, molecularly imprinted with cilostazol (MIP-CIL), was potentiodynamically deposited on a Pt disk electrode by oxidative electropolymerization. Due to electro-oxidation potentials of carbazole monomers lower than that of CIL, these monomers outperformed pyrrole, thiophene, and phenol monomers, in this electropolymerization. The pre-polymerization complexes' quantum-chemical and molecular dynamics structure optimization enabled the selection of the most appropriate monomer from the three thiophene-appended Figure 1. Computer optimized structure of the MIP molecular cavity with the CIL molecule entrapped.

carbazoles examined. Then, the electrode was applied as a selective CIL chemosensor in the linear dynamic concentration range of 50 to 924 nM CIL with a high apparent imprinting factor, IF = 10.6. The MIP-CIL responded similarly to CIL and CIL's pharmacologically active primary metabolite, 3,4-dehydrocilostazol (dhCIL), thus proving suitable for their determination together. Simulated models of the MIP cavities binding of the CIL, dhCIL, and interferences' molecules allowed for predicting chemosensor selectivity. The MIP film sorption of CIL and dhCIL was examined by DPV peaks fitting with the Langmuir (L), Freundlich (F), and Langmuir-Freundlich (LF) isotherms. The LF isotherm best described this sorption with the sorption equilibrium constant (KLF) for CIL and dhCIL of 12.75 × 10-6 and 0.23 × 10-6 M, respectively. Moreover, the chemosensor selectivity to common interferences, including cholesterol and dehydroaripiprazole, was 1.52 and 8.0, respectively. The chemosensor proved helpful in determining CIL and dhCIL in spiked human plasma with the appreciable recovery of 99.3 to 134.1% and the limit of detection, LOD = 15 nM.

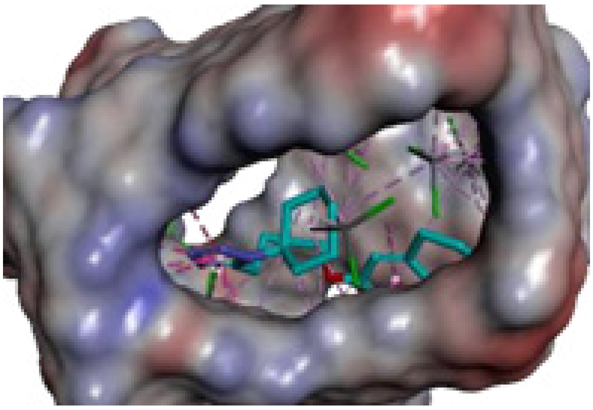

Figure 1. Computer optimized structure of the MIP molecular cavity with the CIL molecule entrapped

References

1. Jyoti et al. J. Mater. Chem. B 2021 advance article.

Biography

At 27, Wlodzimierz Kutner received his Ph.D. Degree from the Chemistry Department, Warsaw University (Warsaw, Poland); at 47, the D.Sc. Degree (habilitation) from the Institute of Physical Chemistry, Polish Academy of Sciences, IPC PAS (Warsaw, Poland), and at 54, the Professor title. Employed in IPC PAS and Cardinal Stefan Wyszynski University (Warsaw, Poland), he published over 190 papers, cited more than 6300 times (H-index 42, Web of Science), in high-impact factor journals, patented over 35 innovations, and promoted 14 Ph.D. students. His current research interest involves supramolecular chemistry of inclusion and molecularly imprinted polymers, electrochemistry and spectroscopy of electrode-solution interfaces, the Langmuir and Langmuir-Blodgett films for devices of energy conversion and storage, and functionalized conducting polymers modified electrodes for chemo- and biosensing.

Transition-metals perovskites electrocatalysts for boosting the electrochemical energy reactions

Mohamed A. Ghanem, Abdullah M. Al-Mayouf,[a] Prabhakarn Arunachalam,[a] Mabrook Amer,[a] Mark T. Weller[b]

[a]Electrochemical Sciences Research Chair (ESRC), Chemistry Department, King Saud University, Riyadh 11451, Saudi Arabia

[b]Chemistry Department, Cardiff University, Cardiff, CF10 3AT, UK.

Transition metals perovskites are of interest for a variety of applications for developing renewable and clean energy sources. This work presents the synthesis and electrochemical characterizations of new transition metal oxides and oxyhalides with improved electrocatalytic properties for water splitting, and fuel-cell reactions. A range of cobalt and iron oxide doped with different halides ions having the chemical formula of A2BO4-xHx (where A = Sr or Pb, B = Co or Fe and H = F, Cl and Br; x = 0, 1 and 2) (Fig. 1) were prepared via solid-phase synthesis approach and evaluated as bifunctional electrocatalysts of oxygen evolution (OE) and oxygen reduction (OR) reactions [1,2]. The electrochemical performance towards oxygen evolution and reduction reactions as examined by cyclic voltammetry, chronoamperometry, RRDE, and impedance techniques have shown that the introduction of F, Cl, or Br into the cobalt oxide framework increases the catalytic activity towards both oxygen evolution and oxygen reduction reactions in comparison to pristine cobalt oxide. The electrochemical activity and the reaction kinetics, however, are the greatest with halide ratio (x = 1 and decreased when x = 2) and the oxyfluoride being the superior bifunctional catalyst. This work demonstrates that the perovskites of transition metals oxyhalides are a new class of high-performance electrocatalysts for oxygen evolution (OE) and oxygen reduction (OR) reactions in alkaline media.

Acknowledgements:

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References:

[1] M.A. Ghanem, P. Arunachalam, A.M. Almayouf, M.T. Weller, J. Electrochem. Soc. (2016) 163 (6) H450-H458

[2] M.A. Ghanem, M.S. Amer, A.M. Al-Mayouf, P. Arunachalam, M.T. Weller, Catalysts (2021) 11 (11) 1408 .

Biography

Professor Mohamed A. Ghanem obtained his PhD in Chemistry in 2002 from the University of Southampton (UK) in the field of synthesis, characterizations, and applications of nanostructured materials. He works as postdoctoral researcher at Southampton and Bath University (2003-2008). He joins King Saud University in 2010 as associate Professor of physical chemistry and promoted to full professor in 2017. His research interests focus on nanomaterials, fabrication, characterization, and applications for energy production and storage. He acts as editor for the Journal of Saudi chemical society and awarded the IAAM Medal in 2018 for notable and outstanding research in the field of New Age Energy Materials & Technology. He published about 120 papers, five patents and his i10-index is 70 with 3800 citations. He has been included among the top 2% Scientist according to Stanford university study in 2021.

Posters Presentations

DAY-2

Chemical Recycling of Real Complex Waste Streams

A. Asueta, J. Leivar, I. Amundarain*, L. Fulgencio, R. Miguel, S. Arnaiz, A. Barredo, I. Nekoiza

Gaiker Technology Centre, Basque Research and Technology Alliance (BRTA), Parque Tecnológico de Bizkaia, edificio 202 E-48170 Zamudio (Spain).

Nowadays, the huge growing of plastic production has resulted in a massive generation of this kind of waste. Despite not being considered a hazardous waste, plastic waste causes cumulative and long-term environmental impacts due to its high lifetime [1,2]. In order to reduce adverse effects presented by plastic waste, recent European Directive 2018/851 has been renewed to promote the recovery of plastic waste for recycling, avoiding the deposition in landfill [3]. Nevertheless, the amount of waste that ends up in landfill is still very high. According to a recently published report, in Spain, landfill is the most recurrent measure to get rid of post-consume plastic waste (46%) [4]. Increasing the recycling rate and reducing the landfill disposal only through conventional mechanical recycling routes is sometimes complicated and not an economically viable alternative, since there are a lot of plastic waste streams that are composed by a wide and intermingled variety of materials, especially those that came from industrial recovery processes [5,6]. Therefore, new recycling alternatives are required, and chemical recycling, seems to be a promising option [7,8]. Chemical recycling is based on the decomposition of polymers by means of heat, chemical agents and catalysts to obtain a variety of products from the starting monomers to mixtures of compounds, mainly hydrocarbons, with applications as a source of chemicals or fuels.

In this work different chemical recycling processes have been studied for the treatment of real and complex waste streams. On the one hand, catalytic solvolysis processes applied to PET wastes have been studied for the recovery of the chemical monomers bis(2-hydroxyethyl)terephthalate (BHET) and terephthalic acid (PTA), from glycolysis and alkaline hydrolysis processes, respectively. Likewise, the catalytic glycolysis process of rigid PU wastes for the recovery of green polyols has been studied. And finally, the pyrolysis process applied to reject fractions with a high plastic content, generated in 1) light packaging waste sorting plants, 2) paper recycling industry, and 3) waste treatment plants of electrical and electronic equipment (WEEE), has been studied. The results obtained allow evaluating the suitability of the different real and complex waste to be treated by means of the proposed chemical recycling processes. Thus, the most suitable operating conditions are defined to carry out the chemical reactions, and the post-treatment processes necessary to achieve the necessary specifications for the chemical monomers and the pyrolysis oils, for their inclusion in the synthesis of new plastics (Plastic2Plastic concept). Specifically, the suitability of the chemical monomers (BHET and PTA) from the catalytic solvolysis of PET for the synthesis of new chemically recycled PET and for the manufacture of polyester resins (PET2PET concept), the validation of the inclusion of the recovered polyols, in the processes of catalytic solvolysis of rigid PU foams, for the manufacture of new rigid PU foams (PU2PU Concept), and finally the analysis of the pyrolysis oil to be used as a feedstock for polymer production in, for example, a steam cracker (replacing naphtha).

Origin of capacitance decay for a flower-like δ-MnO2 aqueous supercapacitor electrode: The quantitative surface and electrochemical analysis

C. Justin Raja, Won-Je Choc, Byung Chul Kimb*

[a] Associate Professor Physics Division, School of Advanced Sciences,Vellore Institute of Technology (VIT University), Chennai Campus Chennai-600127, Tamil Nadu, India

[b] Department of Advanced Components and Materials Engineering, Sunchon National University, 255, Jungang-ro, Suncheon-si, Jellanamdo 57922, Republic of Korea

[c] Accelerator Application Research Division, Korea Atomic Energy Research Institute, Gyeongju, Gyeongbuk 38180, Republic of Korea

Herein, we report the electrochemical energy storage performance of δ-MnO2 (K-birnessite MnO2) as supercapacitor electrode material in Na2SO4 aqueous electrolyte. The electrode exhibited considerable electrochemical performances due to the fast intercalation/deintercalation reactions of Na+ on the pseudocapacitive MnO2 surface. However, a long-term cyclic stability test of the electrode at a low specific current (1 A g–1) demonstrated a decline in its initial capacitance value to the tune of ~ 21%. To quantify the above discrepancy, the electrochemical intercalation of Na+ ions on the electrode surface was quantitatively studied employing electrochemical impedance spectroscopy, EDAX analysis and X-ray photoelectron spectroscopy. Further, the surface of the electrode was analyzed by performing complete charge and charge/discharge measurements at a low specific current of 0.1 A g–1. These results disclosed that, besides the surface intercalation/deintercalation reactions, some Na+ ions have permanently substituted into the bulk (layer) of δ-MnO2 by replacing the host K ions from the layered nanostructure. Thus, this finding suggests that Na+ ions replaced in the site of K in δMnO2 considerably affect the electrochemical properties of the supercapacitor electrode.

The Synthesis of hyperbranched polymers based TADF materials for OLEDs applications.

Saif Hussain D Althagafi

Sheffield University, Faculty of Scince, Chemistry Department, UK

Organic light emitting diodes (OLEDs) technology has been applied and used widely; contributing to improve various fields such as electronic devices, industrial control, transportation and medical field; making them affordable, lightweight, easier, more solution processable with great conductivity and efficiency. To achieve these, OLEDs require to have a new class of organic thermally activated delayed fluorescence (TADF) molecules; enabling the internal efficiency to be 100%, utilising high exciton ration, narrow ΔEST and simplifying the conversion between ΔEST via the reverse intersystem crossing (RISC). Carbazole derivatives based hyperbranched polymers have been selected to be the target for this study due to the unique features they owned. Carbazole has an excellent hole transporting performance, easy to be functionalised and delocalise electron density, have a great conjugated system, thermally and photochemically stable.

Biography

Saif has gained his MSc degree from the University of Sheffield on 2018 in Polymers for Advanced Technologies. Currently, he is a PhD researcher at the University of Sheffield, trying to enhance the OLEDs technonlogy using a new class of TADF hyperbranched polymers.

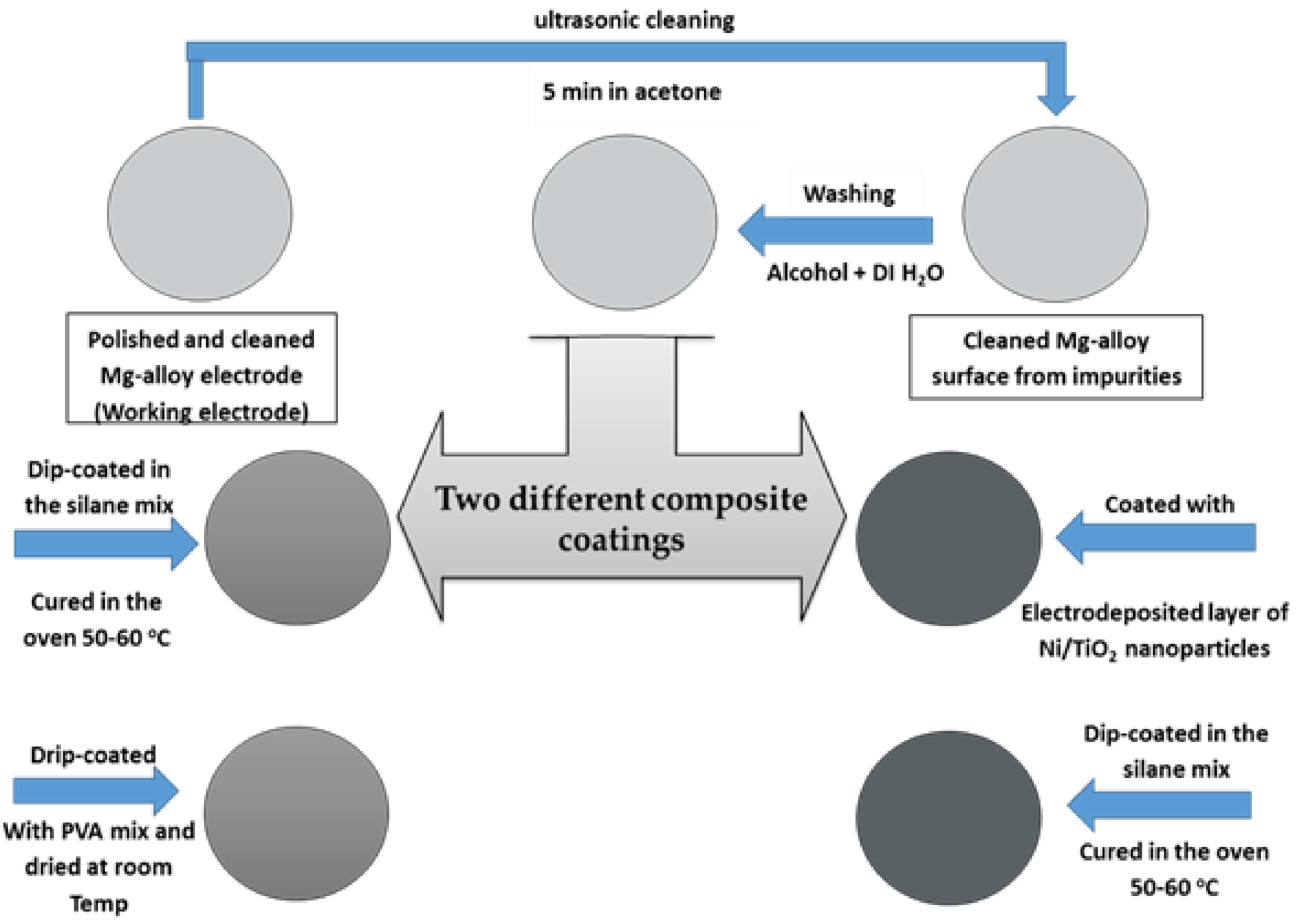
A highly efficient nanocomposite-containing coatings for the protection of Mg-alloy against corrosion in chloride containing electrolytes.

Mariam ABTIDON*, Mohammad BINSABT, Ahmed GALAL, Faizah ALKHARAFI

Cairo University, Egypt

Chemistry Department, Faculty of Science, Kuwait University, P.O. Box 5969, Safat 13060, Kuwait.

The electrochemical behavior of magnesium-aluminum-zinc alloy with composition Mg(93)Zn(1)Al(6) alloy is studied in a corrosive media solution containing 3.5% NaCl aqueous electrolytes. Electrochemical techniques including D.C polarization and electrochemical impedance (EIS) measurements are used to characterize the behavior of the alloy in these electrolytes. The data indicated the direct dissolution of the alloy as evidenced from ICP measurements and surface examination after exposure to the corrosive media.



The alloy was treated with a silane-polymer coating that proved effective in protecting the surface against corrosion. To improve its corrosion protection ability and film quality, another approach to coat the magnesium-based alloy was examined. For example, the electro - deposition of another metal layer on top of the surface of the magnesium-based alloy. This includes utilizing a protective layer administered from nickel and TiO2 nanoparticles containing electrolyte and followed by a protective silane film. The protecting film is composed of 1,2- bis(triethoxysilyl)ethanepoly(vinyl alcohol) hybrid (TESEPVA). The hybrid film was applied to the alloy surface either by sequential spin-coating or layer-by-layer spin-coating. Surface examination of the alloy or film-coated alloy was performed before and after exposure to the corroding electrolyte. The techniques used are field-emission scanning electron microscopy (FE-SEM) with energy dispersive X-ray analysis (EDX) and X-ray photoelectron spectroscopy (XPS).

The Mg-alloy coated with the hybrid films has been tested for prolonged exposure to the chloride solution and both coatings have proven effective in protecting the Mg alloy.

Biography

Mariam Abbi Mohamud Abtidon Highly skilled in chemistry techniques, terminology and equipment and supplies in depth knowledge of laboratory tests used in chemistry work Proficient in methods and practices of chemical analysis Demonstrated ability to prepare technical reports and research papers.

The Synthesis of TADF hyperbranched polymers based Oxadiazoles for OLEDs applications.

Fatemah Asiri

Sheffield University, Faculty of Scince, Chemistry Department, UK

Organic light-emitting diodes (OLEDs) have been broadly considered for application in displays and lighting; making them low cost, simple deposition, high production efficiency, and high commercial value. The 3rd generation of OLED; Thermally activated delayed Fluorescence (TADF) is a promising alternative to phosphorescence (2nd generation), which based on heavy, unaffordable and non-friendly environmentally materials. TADF emitters can realize highly-efficient OLEDs, permitting 100 % of the internal quantum efficiency, depending on the high ratio of exciton, narrow ΔEST and ease the conversion between ΔEST via the reverse intersystem crossing (RISC).

TADF macromolecules based Oxadiazole moieties have been targeted for this project because of the great features they possessed. 1, 3, 4-oxadiazole derivatives considered as an efficient thermal stability, luminescence, excellent transporting materials. They can be used as a holes blocker which are key factors in the structuring of efficient optoelectronic devices.

Biography

Fatemah has gained his MSc degree from King Abdul Aziz University in 2015 in Organic Chemistry (Natural Products). Currently, She is a PhD researcher at the University of Sheffield, attempting to develope the OLEDs technonlogy utilising a new class of TADF hyperbranched polymers.

The formation mechanism of Choline Chloride and Glucose based Natural Deep Eutectic Solvents studied at the molecular level

Zhassulan Sailau[1*], Nurlan Almassov[2], Kainaubek Toshtay[1], Anuar Aldongarov[3]

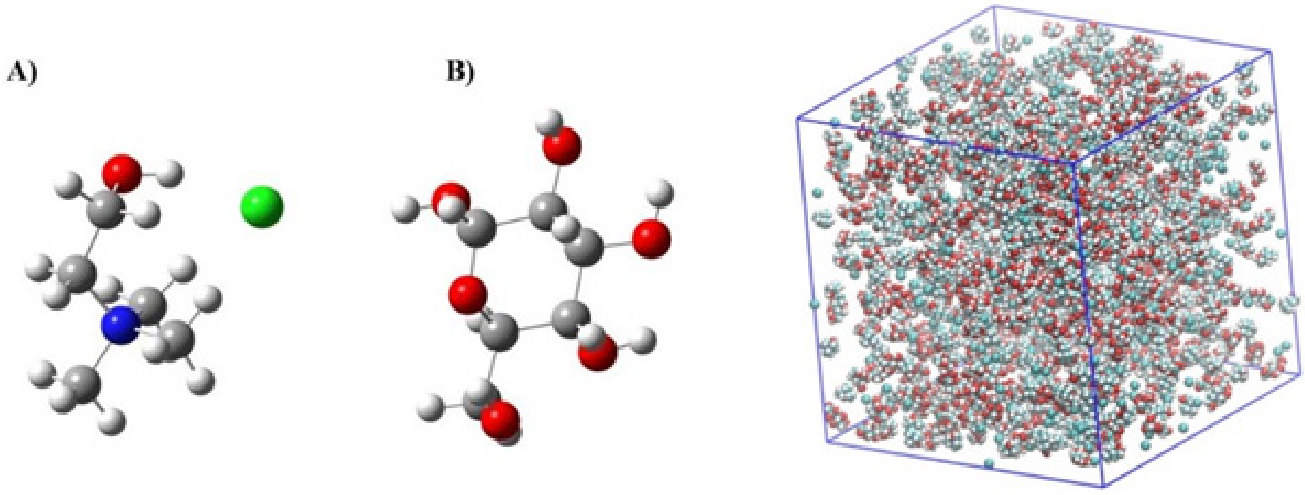
[1]Department of Chemistry and Chemical Technology, Al-Farabi Kazakh National University, Almaty 050000, Kazakhstan

[2]Office of the Provost, Nazarbayev University, Nur-Sultan 010000, Kazakhstan

[3]Department of Technical Physics, L.N. Gumilyov Eurasian National University, Nur-Sultan 010000, Kazakhstan

The liquid waste is the main component of waste, and that is commonly obtained from labs of industry and academy during the synthesis, purification, separation, extraction, separation, and pretreatment processes. These chemical and biological processes require a greater number of solvents. Herein, there is a need to develop more environmentally friendly, cheaper, non-toxic solvents that are harmless to humans and the environment. In this regard, deep eutectic solvents (DES) and their derivatives so called natural deep eutectic solvents (NADES) are a new field in the search for green alternative solvents.

In our work, the formation of choline chloride based NADESs using Density Functional Theory (DFT) calculations, and classical all-atom Molecular Dynamics (MD) simulations was studied in detail using Gaussian09 and Gromacs software's.



I) DFT structures ***II) MD simulation box***

Figure 1: I) Structure of A) ChCl, and B) glucose, II) MD simulation box [1].

The electronic state DFT optimizations were simulated using DFT B3LYP 6-31+G(d) level of theory. In addition, all-atom MD modeling and simulations were used via Gromacs force field. After the all-atom classical MD modeling and simulations, the results of DFT work revealed the molecular interaction of NADESs via formation (creation) of binding between chlorine and choline, and chlorine and glucose. Moreover, the outcomes of all-atom MD modeling and simulations, stated that the N atom of choline ion, and chloride ion have higher intermolecular interactions, while glucose have also higher intermolecular interaction with chloride ion during NADES formation. After mixing with glucose and water, it was noted that the increasing number hydrogen bonds are higher for chlorine and glucose, choline and glucose, chlorine ion and water. The results of radial distribution function stated that there is strong bonding between chlorine/water, and chlorine/glucose components.

References:

[1] Sailau, Z., Almassov, N., Toshtay, K., Aldongarov, A. (2022). Molecular Modeling and Simulation of the formation mechanism of Choline Chloride and Glucose based Natural Deep Eutectic Solvents. Journal of Molecular Modeling.

Biography

Zhassulan Sailau is a second-year PhD student in oil-chemistry at Al-Farabi Kazakh National University. He received a master's degree in oil-gas business from Al-Farabi Kazakh National University in Almaty, Kazakhstan. He is interested in computational chemistry and physical chemistry.

The physico-chemical attributes that determine insulin agglomeration: Therapeutic implications

Megren Hassain A Fagihi[1-2]

[1] *School of Veterinary Medicine, University College Dublin (UCD), Belfield, Dublin 4, Ireland*

[2] *Clinical Laboratory Sciences Department, College of Applied Medical Sciences, Najran University, Najran, Kingdom of Saudi Arabia*

With diabetes now widespread in every age group, including the adolescents and young adults, insulin has emerged to be a drug of importance. While celebrating the centenary year of insulin discovery, it is important to be aware of the challenges in insulin-based therapeutics. One of the many such challenges is the unavailability of oral formulations of insulin as a highly acidic gastric juice denatures its intrinsic molecular structure. As a result, insulin continues to be administered via parenteral routes in injectable forms that, unfortunately, comes with certain disadvantages, including poor patient compliance. To address such issues, encapsulation of insulin within a cloak of protective biomaterials, such as pHresponsive silica or polymers, have emerged as viable options that shall protect the encapsulated insulin core in an acidic milieu but will gradually dissolve in a higher pH, such as in small intestine, which in turn will release the insulin payload. However, insulin is known to be vulnerable toward subtle changes in its biochemical environment (e.g., pH, ionic strength, temperature, and close contact with hydrophilic surfaces) and undergoes amyloid fibril formation that not only makes encapsulation difficult to achieve but also renders its therapeutic impact unpredictable.

In this project, we are investigating the effect of such physico-chemical attributes on insulin agglomeration, and how it influences its physiological effect. To begin with, we have thoroughly characterized human insulin, including its photochemistry, to understand the molecule in detail. The insulin agglomerates were characterized by techniques like dynamic light scattering and zeta potential while imaged with transmission electron microscopy with elemental analysis coupled to energy dispersive X-ray spectroscopy. It is noticed that an acidic pH certainly triggers amyloid degeneration in insulin although it will be interesting to see if such biochemical changes alter its physiological effects.

Biography

Megren Hassain A Fagihi was born and raised in the Kingdom of Saudi Arabia. He joined the College of Applied Medical Sciences at Najran University (Saudi Arabia) in 2007 and graduated with a Bachelor of Medical Laboratory Sciences in 2012. After finishing his internship, he got admitted to the University of Manchester (UK) in 2015 and earned his M.Sc. in Clinical Biochemistry in 2016. Followed to that, he spent four years working as a lecturer in the Department of Biochemistry at Najran University. He started his Ph.D. at the University College Dublin (Ireland) in January 2022 under the supervision of Prof. Sourav Bhattacharjee. In his Ph.D. program, Megren investigates the biochemical features of insulin agglomerates that influence the current drug delivery systems in diabetes patients. In his free time, Megren loves to travel, read books, and spend time with his family.

The influence of different cross-linking methods of hydrogels based on PVA on selfhealing performance and ionic conductivity

Nujood. Alshehhi, Maitha Almheiri, Nataša Z. Tomić

Technology Innovation Institute, Advanced Materials Research Center, Masdar City, Abu Dhabi, United Arab Emirates

Nowadays, conductive nanocomposite hydrogels having self-healing capability with excellent stretchability are showing high potential for application in biomedical devices. Furthermore, conductive hydrogels have attracted extensive attention in wearable/flexible electronic devices (EC). However, designing and preparing such a multifunctional material remains a challenge. In this work, ionically conductive hydrogels based on polyvinyl alcohol (PVA) and xanthan gum (XG) with different cross-linking techniques were developed. Three different methods used for crosslinking were: (a) using the sodium tetraborate hexahydrate (borax), (b) the freeze-thaw method (varying the number of cycles), and (c) using citric acid during the freezing step. The self-healing properties of synthesized hydrogels were analyzed and compared using time-dependent measurements in a shear strain mode by RSO Rheometer. The mechanical stability and flexibility of obtained samples were studied by Dynamic Mechanical Analysis (DMA). Microstructural properties of polymer networks obtained by different cross-linking methods were analyzed by optical microscopy. The difference in ionic conductivity of synthesized hydrogels was examined by Electrochemical Impedance Spectroscopy (EIS). Furthermore, using xanthan gum opens up new possibilities for developing high-performance hydrogels with applications in wearable electrical sensors and healthcare monitoring.

Keywords: conductive hydrogel; xanthan gum; PVA; freeze; citric acid; sensors.

Biography

Nujood Al Shehhi Senior Engineer in Advanced Materials Research Center AMRC, She has a MSc in Material Science and Engineering. Since joining TII, AlShehhi is receiving trainings for various techniques related with sample preparation and sample characterization for metallography and selfhealing materials. AMRC is part of the Technology Innovation Institute (TII), a UAE-based research center that aims to lead global advances in artificial intelligence, autonomous robotics, quantum computing, cryptography and quantum communications, directed energy, secure communication, smart devices, advanced materials, and propulsion and space technologies. We belong to the Abu Dhabi Government's Advanced Technology Research Council (ATRC), which oversees technology research in the emirate.

Preparation and Characterization of Graphene-Enriched Tung oil-Urea Formaldehyde Microcapsules

Maitha Almheiri, Abdullah Naseer Mustapha* (AM), Nujood Alshehhi (NA), Natasa Tomic (NT)

Technology Innovation Institute, Masdar City, Abu Dhabi, UAE

In this study, a series of novel tung oil (TO) microcapsules (MCs) were synthesized via one-step in situ polymerization, with the addition of graphene. The addition of graphene conveyed a series of advantageous properties to the MCs, including the enhanced curing behaviour of the tung oil, reduction in size distribution, reduced foaming during the formulation process and a reduction in the contact angle with the addition of graphene. The experimental results from the X-ray diffraction (XRD) analysis show that the graphene had excellent dispersion in the TO, due to the corresponding comparative diffraction patterns. Furthermore, the X-ray photoelectron spectroscopy (XPS) results expresses the confirmation of tung oil adsorption on the surface of the graphene. Moreover, the Raman spectra shows the reduction in the intensity of the Raman intensity peaks over a duration of 4 days, during the curing process, associated with the degradation of the C=C double bonds. After the formulation of the MCs, the SEM images displayed enhanced shell roughness for the TO-GNP MCs in comparison to the pure TO MCs. Lastly, high resolution TEM images confirm the presence of graphene on the outer layer of the MCs.

Biography

Maitha Al Mheiri obtained her Bachelor's degree in Chemical Engineering from United Arab Emirates University in 2020. After joining TII Maitha is acquiring experience of a variety of fabrication and characterization techniques for creation of advanced materials with self-healing capabilities.

Virtual talks

DAY-2

Environment-assisted degradation of fibres in FRP composites for advanced concrete structure

Raman Singh

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

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. (Up to 300 words)

Biography

Professor Raman Singh's expertise includes: Alloy Nano/Microstructure-Corrosion Relationship, Stress Corrosion Cracking (SCC), Corrosion/SCC of Biomaterials, Corrosion Mitigation by Novel Material (e.g., Graphene), Advanced and Environmentally Friendly Coatings, High Temperature Corrosion. He has supervised 50 PhD students. He has published over 255 peer-reviewed international journal publications and 15 books/book chapters. His professional responsibilities include editor-in-chief of two journals, Fellow ASM International and Engineers Australia, nearly 50 keynote/plenary talks at international conferences (besides numerous invited talks), leadership (as chairperson) of a few international conferences. (Up to 100 words)

High performance graphene-based devices with an affordable cost by using a wafer bonding

Hirokazu Fukidome

Tohoku University Research Institute of Information Communication, Sendai 9808577, JAPAN

Graphene is promising for next-generation devices, such as those for Beyond 5G owing to excellent properies for electronic and photonic applications. One of the primary challenges in realizing these devices is the scalable growth of high-quality few-layer graphene (FLG) on devicetype wafer. It is difficult to do so while balancing both quality and affordability. High-quality graphene is grown on expensive SiC bulk crystals, while graphene on SiC thin films grown on Si substrates (GOS) exhibits a quality to be improved but affordable cost, which we have developed for applications of devices to fuse with Si-based electronics. We propose a new method for the growth of high-quality FLG on a new template named "hybrid SiC" [2]. The hybrid SiC is produced by bonding a SiC bulk crystal with an affordable device-type wafer and subsequently peeling off the SiC bulk crystal to obtain a single-crystalline SiC thin film on the wafer. The quality of FLG on this hybrid SiC is comparable to that of FLG on SiC bulk crystals and much higher than of GOS. FLG on the hybrid SiC exhibited high carrier mobilities, comparable to those on SiC bulk crystals, as anticipated from the linear band dispersions. Field-effect transistors using FLG on the hybrid SiC showed the potential to operate in terahertz frequencies. The proposed method is suited for growing high-quality FLG on desired substrates with the aim of realizing graphene-based high-speed devices for Beyond 5G. Part of this work has been supported by KAKEHI, ShinEtsu Chemicals, and the funding for Beyond 5G researches and developments from NICT.

Biography

Fukidome has completed his PhD from Osaka University and postdoctoral studies from Bell laboratories. He is an associate professor of Tohoku University. He has published more than 100 papers in reputed journals and 28 patents, and has been serving as an editorial board member of Scientific Reports and an associate editor of e-Journal of Surface Science and Nanotechnology.

Vibro-impact response of FRP sandwich plates with a foam core reinforced by chopped fiber rods

Hui Li

Northeastern University, China

In the present study, both the impact and vibration response characteristics of fiber reinforced polymer (FRP) sandwich plates (FRPSPs) with a foam core (FC) reinforced by chopped fiber rods (CFRs) are investigated. Initially, a dynamic model is proposed to predict the vibro-impact characteristics of the FC-CFRs-FRPSP structures. Here, by considering the influence of the dispersion pattern of chopped fiber rods, the equivalent material parameters of this complex core are redefined. Also, by employing the modified mid-plane displacement equation based on the principle of virtual work at the impact point, together with the progressive quasi-static approach and Reddy's high-order shear deformation principle, the key parameters such as impact contact force and displacement related to each failure event are obtained. In addition, with consideration of the impact damage, the natural frequencies and vibration responses are solved by using the energy principle, the proportional damping method, and the Duhamel integral technique. Finally, a number of the FC-FRPSP specimens with and without reinforcement of CFRs are fabricated and tested under different impact energies for verifying the present model. Also, the influences of critical geometric and material parameters on the vibro-impact response of the FC-CFRs-FRPSP structures are discussed. It has been found that the FC-CFRs-FRPSP specimens have a smaller vibro-impact response compared to the specimens without CFRs. For example, when impact energy of 10 J is applied, the impact peak force increases by 19.1 %, the impact displacement reduces by 26.6 %, and the maximum time-domain vibration response reduces by 5.8 %. To reduce the vibro-impact response of such structures, it is recommended to adopt a large thickness ratio of the CFR reinforced foam core to the overall sandwich plate as well as volume fraction of CFRs to the foam core with a uniform dispersion pattern.

Biography

Hui Li is an associate professor in Northeastern University, China. He has published more than 30 top-level SCI papers , 40 EI papers and 60 invention patents. He once was a vibration engineer in SMTCL, a postdoctoral fellow at Shenyang Engine Research Institute, and a visiting scholar in Liverpool University. His research interest includes: nonlinear vibration , vibration and impact modeling, dynamic thermal evaluation of porous, hybrid and multifunctional composite materials and structures.

Cost-efficient and recyclable epoxy vitrimer composite with low initial viscosity based on exchangeable disulfide crosslinks

Shaojian He

North China Electric Power University, China

Epoxy (EP) vitrimer with excellent processing and recyclability is of great potential for industrial application. In this study, we prepared an EP vitrimer based on the low viscosity homogenous mixture of diglycidyl ether of bisphenol A (DGEBA) and a liquid hardener dimethyl 3,3'-dithiodipropionate (DTDP) catalyzed by 2,4,6-tris (dimethylaminomethyl) phenol (DMP30). The optimal curing condition was determined to be 110 oC×12 h for the original EP vitrimer. Owing to the exchangeable disulfide crosslinks, rapid stress relaxation was found for the vitrimer with a relaxation time of 1.9 s at 160 oC. Moreover, the prepared EP vitrimer possessed excellent self-healing ability and recyclability, with recovery ratio of at least 94.1% during 3 times recycling. The self-healing ability, recyclability and processing performance remain excellent for the vitrimer even after incorporating 30 wt% boron nitride (BN), which can be recycled using DMF as a solvent.

Biography

Shaojian He is an associate professor at North China Electric Power University in China. He works at high performance rubber composites/insulating polymer composites, where he is recognized nationally and internationally for his research contributions and achievements in materials science.Dr. Shaojian He is currently an associate professor at North China Electric Power University, China. His current research is focused on high-performance rubber nanocomposites and high voltage insulation material. He has undertaken several research projects including two research funds from the National Natural Science Foundation of China (NSFC) and published more than 60 papers. He is a recipient of Alan Glanvill Award by the Institute of Materials.

Asymmetry at ferromagnet/antiferromagnet interface: Route toward an advanced spin-orbit torque device

Chao-Yao Yang

Department of Materials Science and Engineering National Yang Ming Chiao Tung University
Hsinchu 300, Taiwan

The antiferromagnet (AFM) and ferromagnet (FM) interface is a unique branch of magnetics of broad scientific interest. AFMs play an important role in spin-orbit torque (SOT) devices based on their ability to generate spin-polarized current and exchange bias when combined with FMs. Since the exchange bias of the AFM/FM bilayer appeared to be tailorable by SOT, it opens a great opportunity for AFM-based spintronics technology that the SOT can modify the spin texture of AFM and FM can serve for detection. In this talk, several AFM/FM systems will be demonstrated for studying the interfacial dynamics of AFM spins. An interesting spin-orbit torque (SOT) ratchet involving the exchange spring effect in an IrMn/CoFeB bilayer device with perpendicular anisotropy and exchange bias is developed. The combined use of electrical and spectroscopic analysis reveals that the exchange spring in IrMn/CoFeB bilayer yields unidirectional anisotropy, resulting in a collinear/orthogonal AFM/FM spin configuration at the interface upon switching CoFeB magnetization upward/downward. The ratcheting characteristics resulting from unidirectional anisotropy manifest in SOT switching. In this process, magnetization against the exchange spring features digital-like switching with a sharp transition, whereas the reverse function is characteristic of analog switching with a gradual transition tail. The dual digital-analog characteristics of the IrMn/CoFeB bilayer may be of benefit in neuromorphic and memory applications.

Biography

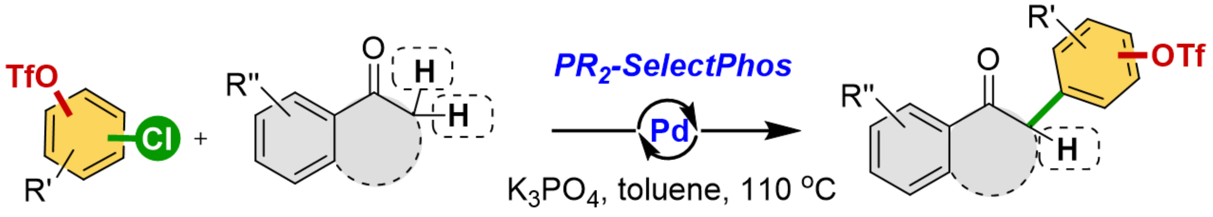
Dr. Chao-Yao Yang completed his doctor degree of material science and engineering at National Chiao Tung University. During his Ph. D., he focused on the studies of crystalline/electronic structure of materials and the related physical properties. After he graduated, he re-orientated his research topic to the valleytronics of two-dimensional materials and spin-orbit torque (SOT)-related device. His current focus is strongly associated with antiferromagnet (AFM), which is conventionally a passive role in the magnetic society but currently appears to be more active and promising for the advanced MRAM applications.

Palladium-catalyzed chemoselective direct α-arylation of carbonyl compounds with chloroaryl triflates at the C–Cl site

Chau Ming So, Zicong Chen, Changxue Gu, and On Ying Yuen

State Key Laboratory of Chemical Biology and Drug Discovery and Department of Applied Biology and Chemical Technology, The Hong Kong Polytechnic University, Kowloon, Hong Kong

The control of chemoselectivity for arenes bearing multiple electrophilic sites in cross-coupling processes remains a challenge. As ligands are indispensable factors in cross-coupling reactions, developing the appropriate ligands that can directly manipulate the reactivity sequence (i.e., –Cl > –OTf) is a desirable strategy and significantly broadens the choice of synthetic routes in actual applications. In this study, we described palladium-catalyzed chemoselective direct α-arylation of carbonyl compounds with the chloroaryl triflates in the Ar–Cl bond. The Pd/SelectPhos system showed excellent chemoselectivity toward the Ar–Cl bond in the presence of the Ar–OTf bond with a broad substrate scope and excellent product yields. The electronic and steric hindrance offered by the –PR2 group of the ligand with the C2-alkyl group was found to be the key factor affecting the reactivity and chemoselectivity of the α-arylation reaction. The chemodivergent approach was also successfully employed in the synthesis of flurbiprofen and its derivatives (e.g., –OMe and –F).



- ***Oxindoles / Ketone derivatives***
- ***Chemoselectivity: Ar-Cl > Ar-OTf***
- ***32 examples (ALL new compounds)***
- ***Flurbiprofen and its derivatives synthesis***

Reference

1. Chen, Z.; Gu, C.; Yuen, O. Y.; So, C. M.* Chem. Sci., 2022,13, 4762-4769.

Biography

Chau Ming So is currently an Assistant Professor in the Department of Applied Biology and Chemical Technology at The Hong Kong Polytechnic University. He received his B.Sc. (1st class honor) from PolyU in 2006. He pursued his postgraduate study at the same university and obtained his Ph.D. degree in 2010. In 2012-2013, he moved to Institute of Materials Research and Engineering (IMRE) as postdoctoral fellow in Prof. Tamio Hayashi's research group. So's research interests focus on the development of ligands and their application in transition metal-catalyzed chemo-/regio-/enantioselective reactions. He has published 62 papers in well-recognized journals.

Development of IrOx pH electrode modified by SP/SiOx/ImIL composite film with long stability and high anti-interference

Yiwen Pan, Yunwen Shen, Zhentao Sun,

Zhejiang University Ocean college, zhoushan 31600, China

pH is a fundamental parameter in understanding the chemical processes in many fields. Metal-oxide pH electrodes have advantages in fabrication, maintenance, cost, as well as their optimum performance in pH response, which could also be utilized in elevated temperature and pressure systems. However, redox substances in the solution may cause severe electrode potential drift, resulting in the inaccuracy of in situ measurements. This paper reports the development and optimization of an improved iridium oxide electrode which is fabricated by adding sodium peroxide (Na2O2) powder into a Li2CO3 melt in a semi-closed/closed reactor at a high temperature to increase the regional peroxide(O22-) ion concentration in the iridium-melt interface. The iridium oxide film (IROF) of prepared electrodes has a dense and uniform surface with small and cone-shaped particles. The XRD pattern and XPS results suggested the newly produced material Hy-xLix[LiIr2]O6 was a mixture of H5-xLix[LiIr2]O6 and H3-xLix[LiIr2]O6 with a HCrO2 structure. Approximately 95% of Li+ was replaced by H+ after acid treatment. The pH sensing process was found to be an irreversible redox reaction between the tetravalent and trivalent iridium oxides according to the CV and XPS results. The presence of lithium ion in the lattice combined with well-crystallized small crystals corresponded to the fast response during the pH sensing process. The open-circuit tests show that electrodes exhibit a near-Nernstian pH response with good linearity, fast response, high stability (as light periodic fluctuation of potential change with standard deviation < 0.65mV in 48h and < 2.30 mV over 139 h), good reversibility in the pH range of 2.00–10.00, and anti-interference to low concentration of oxidants.

Nonetheless, the IrOx electrode cannot tolerate high concentrations of redox substances in the solution, which still constrain its application in field. We then developed SPEEK (SP) with silica-stabilized imidazole-type ionic liquid (ImIL) to fabricate a composite film (SP/SiOx/ImIL) to achieve a high anti-interference ability for metal electrodes. The composite film was especially designed to address the interference mainly in sulfide anions and other small-sized anions (i.e., I-, F- and ascorbic acid). The results suggested that the potential of the SP/SiOx/ImIL modified IrOx electrode fluctuated within 0.3 mV in 30 min continuous test at a concentration of 10-3 M Na2S, indicating good stability in moderately high sulfide solution. It also exhibited fast response and good reversibility. In addition, no potential drift was measured under other anions interferences.

Biography

Yiwen Pan received her B.S. in Biomedical Engineering, Zhejiang University, her M.S. in Geology and Geophysics, University of Minnesota, and a PhD in Zhejiang University. She joined Zhejiang University and became an associate professor in 2016. Dr. Pan is now a deputy director of the Institution of Marine Chemistry and Environment, Zhejiang University. Her research interests mainly focus on marine carbon cycling and electrochemical sensor development, especially on monitoring the key parameters to reveal the carbon cycling response to the artificial system such as artificial upwelling.

Unraveling roles of lead ions in selective flotation of scheelite and fluorite from atomic force microscopy and first-principles calculations

JianyongHe, WeiSun, HongboZeng, RuihuaFan, WenjihaoHu*, ZhiyongGao*

School of metallurgy and environment, Central South University, China

Metal ions are widely used to achieve selective hydrophobization of different mineral particles. However, the atomic understanding of the roles of metal ions is insufficient due to the limitation of experimental techniques. Herein, the in-situ atomic force microscopy (AFM) force curves and first-principles calculations were combined with the conventional experiments [i.e., batch flotation, zeta potential tests, and X-ray photoelectron spectroscopy (XPS)] to investigate the roles of lead ions (Pb2+) in flotation separation of scheelite and fluorite. The conventional experiments showed that Pb2+ could enhance the flotation recovery of scheelite but suppress fluorite. AFM force curves showed that, due to the presence of Pb2+, the interaction force between benzohydroxamic acid (BHA) and the scheelite surface was a stronger adhesion than the adhesion between BHA and fluorite without lead ions. First-principles calculations revealed that the strong electrostatic attraction resulted in the adsorption of BHA on fluorite surfaces. However, BHA could hardly bond with the scheelite surface with negative charges and hydroxylated Ca sites. The reaction between BHA and Pb2+ was the most favorable. The formed BHA-Pb complexes demonstrated repulsive interactions on fluorite surfaces but attractions on scheelite surfaces. Lead ions played as an inhibitor for fluorite flotation and an on-off switch for scheelite flotation. AFM and first-principles calculations have shown great potential in the analysis of the complicated interface interactions.

Biography

Wenjihao Hu, male, born in Changsha, Hunan, professor, School of metallurgy and environment, Central South University. He received a double bachelor's degree from Central South University and Monash University (with honors) in Australia (Majored in Chemical Engineering), and Ph.D degree from the University of Alberta in Canada. It is mainly engaged in the research of mineral stripping, assembly, modification, mineral surface properties and intermolecular forces, including a variety of intermolecular interactions and interface phenomena in engineering systems such as mineral processing and Petroleum Engineering. (mineral flotation, oil-water separation, design and application of mineral materials, etc.)

Mechanical and Electrical Performances of Polylactic Acid/ Liquid Natural Rubber/Graphene Platelets Nanocomposites in the Light of Different Graphene Platelets Functionalization Routes

Sahrim Ahmad and Ruey Shan Chen

School of Applied Physics, Faculty of Science and Technology, Universiti Kebangsaan Malaysia,

43650 UKM Bangi Selangor, Malaysia

This research is aims to investigate the effect of functionalization of graphene platelets (GNPs) and its low loadings of 0.25, 0.50, 0.75, and 1.00 wt% on the chemical, mechanical, and electrical properties of polylactic acid/liquid natural rubber (PLA/LNR) blend prepared by melt blending method. GNPs are treated with amino dodecanoic acid via covalent interaction and Triton X-100 (TX100) via non-covalent interaction to produce ADA-functionalized GNPs (GNP-A) and TX100functionalized GNPs (GNP-T), respectively. At 0.75 wt% GNPs, the PLA/LNR nanocomposites exhibit the highest tensile strength of 24.38, 35.70, 45.47 MPa for untreated GNPs (GNP-u), GNPT, and GNP-A, respectively. Variable pressure scanning electron microscopy proves better interaction of treated-GNPs with the matrix, while transmission electron microscopy micrographs have shown that PLA/LNR/GNP-A has the best filler dispersion with minimal stacking and agglomeration found. A remarkable improvement of electrical properties is obtained for treatedGNPs nanocomposite with lower percolation threshold value of 0.3 wt% as compared to that of GNP-untreated nanocomposite (0.4 wt%).

Biography

Professor Dr Sahrim Ahmad obtained his PhD from University of Loughborough, United Kingdom in 1988. He is an expert in the field of magnetic, nanocomposites and advanced materials. He has completed more than 50 research projects and consultancy work as a leader and co-researcher. His work on novel radar absorbing materials (RAM) subjected to transverse electromagnetic (TEM) has been successfully developed. His team managed to produce products that offered proper characteristics for handling, flexibility and lightweight, meeting requirement for various applications. He has published more than 250 papers in various journals related to polymer, composites, materials and supervised more than 60 PhD students. Dr Sahrim was former Dean of Faculty Science of Technology and Editor In Chief of Journal Sains Malaysiana (ISI/WOS). Currently he is the Fellow Academy of Science Malaysia. Fellow Academy Profeesor Malaysia and Fellow of Malaysia Solid Science Society.

Electronic and steric effects on L-Lactide Ring-Opening polymerization with NSSN-type Zr(IV) Complexes

Ida Ritacco

DCB, Department of Chemistry, University of Salerno, Via Giovanni Paolo II, 84084-Fisciano (SA), Italy

The mechanism of lactide polymerization promoted by NSSN zirconium complexes was investigated through DFT methods. It was observed that the rate determining step is the step that corresponds to the opening of the lactide ring and the steric and electronic parameters of the ligand have a direct consequence on the reaction path. In particular, it was observed that the increase of the steric hindrance or the increase of the electron-withdrawing properties of the ligand causes an increase of the energy barrier related to the rate determining step. Our calculations foresee that, in order to have an active catalyst, the ligand must bear on the nitrogen atom, a small and electron-releasing substituent, such as the methyl group.

Biography

Ida Ritacco has completed his PhD at the age of 28 years from University of Calabria (Cosenza, Italy) and postdoctoral studies from CNR-IOM-Democritos National Simulation Center and International School for Advanced Studies (SISSA), Trieste (Italy) and University of Salerno (Salerno, Italy). She has published more than 20 papers in international journals.

Mechanistic Insights on Ethylene Polymerization with Ni(II) Catalysts: the impact of the ligand on the polymer microstructure

Maria Voccia

Department of Chemistry and Biology (DCB), University of Salerno, Street Papa Paolo Giovanni II, 84084 Fisciano (Italy)

Cyclophane structures can control steric pressure in the otherwise open spaces of square-planar d8-metal catalysts, providing new highly active catalysts with improved thermal stability for ethylene polymerization. This elegant concept was so far limited to symmetrical coordinated metals.[1]

We have recently report how a cyclophane architecture can be generated in ligands that chelate via two different donors.[2]

An ancillary second imine in the versatile κ^2-N,O-salicylaldiminato catalyst type enables ring closure via olefin metathesis and selective double bond hydrogenation to yield a 30- membered ring efficiently. Experimental and theoretical analyses had shown the ancillary imine is directed away from the active site and inert for catalysis. In ethylene polymerization the cyclophane catalyst is more active and temperature stable *vs*. an open structure reference, notably also in polar solvents.

Increased molecular weights and decreased degrees of branching can be traced to an increased energy of sterically demanding transition states by the encircling cyclophane while linear chain propagation remains highly efficient.

Reference

[1] D. H. Camacho, E. V. Salo, J. W. Ziller, Z. Guan, Angew. Chem. Int. Ed. 2004, 43, 1821-1825.

[2] E. Schiebel, M. Voccia, L. Falivene, I. Gçttker-Schnetmann, L. Caporaso, S. Mecking, Angew. Chem. Int. Ed. 2021, 60, 18472–18477.

Biography

Maria Voccia is pursing her title of Ph.D. at University of Salerno (DCB) and she has a professionalizing research grant on EU Project Under Horizon 2020 “ECO2FUEL” at Council National of Research “Nicola Giordano” (CNR-ITAE). She is author of about 10 papers in internation journals.

Grid cells in the brain as a synergetic problem of physical chemistry and neurophysiology

Alexander Chalyi, Kyrylo Chalyy[1], Luydmila Chernenko[2]

[1]Department of Medical and Biological Physics and Informatics, BogomoletsNational Medical University, Kyiv, Ukraine

[2]Chuiko Institute of Surface Chemistry, National Academy of Sciences of Ukraine, Kyiv, Ukraine

The presentation is devoted to explaining the hexagonal grid cells in the brain discovered by the Norwegian neurophysiologists May-Britt Moser and Edward Moser in 2005 and receiving the 2014 Nobel Prize in Physiology and Medicine "…for their discovery of cells that constitute a positioning system in the brain", together with the American and British neurophysiologist John O'Keefe discovered place cells in 1971. Both place and grid cells create a coordinate system in the brain for determining the space position, angular orientation and velocity of movement of humans and animals. To explain the emergence of hexagonal grid cells in the brain, Edward Moser who also has a scientific degree in mathematics, statistics and programming, proposed in the Nobel lecture (1) to apply the similarity between grid cells and vortex structures resulting from fluctuating phase transitions in superconductors of the 2nd type in magnetic fields, discovered by Alexei Abrikosov, 2003 Nobel laureate in physics.

Here, we will propose another theoretical explanation for the emergence of grid cells in the brain using a synergetic approach (2), which allows us to transfer the quantitative results of one science like physical chemistry to another more complex and at the same time rather qualitative than quantitative science like neurophysiology. For a consistent explanation of the process of the appearance of hexagonal grid cells, a theoretical model based on the fluctuation part of the Gibbs free energy for a biochemically reacting system is considered. The order parameter of such a system is the reaction coordinate, and the conjugated field (in the thermodynamic sense) is the affinity depending on the chemical potentials of reaction's components. One of our important findings is the establishment of the fact that the system of grid cells in the brain near the bifurcation point of formation of coherent ordered structures belongs to the same universality class as the real liquid-vapor system near to the critical point, and also the 3-dimensional Ising model in an external magnetic field (3,4). To prove this statement, such main results of the fluctuation theory of phase transitions and synergetics as the Ginzburg-Landau Hamiltonian, the hypotheses of scaling and conformal invariance, as well as Haken's approach to Benard cells were used.

References:

1. O'Keefe J, Moser MB, Moser EI (2014) Nobel Prize in Physiology or Medicine.

Nobel Prize org Nobel Media AB 2020.

2. Haken H (1978) Synergetics, An Introduction. Nonequilibrium Phase Transitionsand Self-Organization in Physics, Chemistry and Biology. Springer-Verlag: Berlin, Heidelberg, New York.

3. Chalyi AV (2021) Synergetic dialogue “physics-medicine”: Hexagons in living andinanimate nature. J Mol Liquids 329: 114238.

4. Chalyi AV, Bulavin LA, Chekhun VF, Chalyy KA, Chernenko LM, et al. (2013) Universality classes and critical phenomena in confined liquid systems. Condensed Matter Physics 16(2): 23008.

Biography

Professor Alexander Chaly - Head of the Department of Medical and Biological Physics and Informatics of the National Medical University named after A.A. Bogomolets, Doctor of Physical and Mathematical Sciences, Corresponding Member of the National Academy of Pedagogical Sciences of Ukraine, Honored Worker of Science and Technology of Ukraine. Scientific interests of Prof. Chaly A.V. devoted to the problems of synergetics, theoretical and molecular physics, pedagogical aspects of higher education. He is the author of about 500 scientific publications (monographs, textbooks, articles) in well-known scientific journals and publishing houses. Prof. Chaly A.V. worked as a visiting professor at the Pierre and Marie Curie University (Paris, France) and a Fulbrighter professor at the University of Wisconsin-Madison (USA), made presentations at many international scientific conferences and symposiums.

Effect of physical-mechanical treating of cellulose on the properties of elastomeric composites

I. Labaj, P. Skalková, J. Vršková, L. Genšorová

Faculty of Industrial Technologies in Púchov, Alexander Dubček University of Trenčín, I. Krasku 491/30, 020 01 Púchov, Slovakia,

This study deals with the treating of cellulose (CEL) as a filler by using physical and mechanical methods. The influence of filler treating on the properties of elastomeric composites of natural rubber (NR) with cellulose was studied. The mechanical treating of the filler consists of pressing of cellulose at various time intervals from 2 to 6 minutes and temperature at 110 ° C. A plasma discharge with power of 350 W at 4 min exposure and 0.25 mm distance between cellulose and electrode surface was used to physical treat of the cellulose. The treated cellulose was used in amount of 45 phr to prepare of elastomeric composites with NR matrix. Rheological, physical-mechanical properties and cure characteristics were studied on the prepared NR/CEL composites with the evaluation of the influence of filler treating on these parameters. The result of this study is the identification of the most suitable combination of physical-mechanical treating parameters of cellulose using as a majority filler for elastomeric composites in comparison with the composite filled with the untreated cellulose. This research work has been supported by the Operational Program Integrated Infrastructure, co-financed by the European Regional Development Fund by the project: Advancement and support of R&D for “Center for diagnostics and quality testing of materials” in the domains of the RIS3 SK specialization, Acronym: CEDITEK II., ITMS2014 + code 313011W442.

Biography

Ivan Labaj works as a researcher on the CEDITEK II project at the Faculty of Industrial Technology in Púchov, Alexander Dubček University in Trenčín. It focuses on the preparation, development and research of elastomeric composites for use in industrial applications. He has collaborated with several companies on the development of elastomeric composites with specific properties according to industry requirements.

Manufacturing processes of bonded magnets for the automotive industry

David Esteves, José Silvaa*, J. Fonsecaa, J. Camarinhaa, D. Diasa, P. Costab, M. Silvab

[a]*CeNTI – Centre for Nanotechnology and Smart Materials, V. N. Famalicão, Portugal*

[b]*GLN, Leiria, Portugal*

Nowadays, nearly 1/3 of automotive parts are made of plastics or polymer composites, from structural parts of consoles and dashboards to parts of complex mechanical systems. The different parts have different requirements, and over time, to meet ever-evolving consumer expectations, the plastic and polymer composite industries have faced numerous challenges, discovered new materials and invented new manufacturing processes.

The present work will focus on the automotive industry's manufacturing processes of bonded magnets, particularly in a specific case study: manufacturing magnetic gear wheels of hard-ferrite-based composites to be used in steering wheel angle sensors. The developed composite gear wheels were mainly composed of hard-ferrite and PA12 and were magnetised during the injection process, minimising production steps. In this process, permanent magnets are incorporated into the injection mould, creating a magnetic field in the cavity that ensures the composite material's complete magnetisation while the polymeric composite mixture is injected.

The design of the mould was assisted by numerical simulation studies focused on the influence of magnets' position, the geometry of the magnets and the geometry of the cavity field. In addition, the impact of mould materials on magnetic field distribution was also thoroughly evaluated by numerical simulation.

The Magnetized Gears project consortium is constituted by GLN Molds, the promoting company, and GLN Plast, CeNTI, PIEP and the University of Minho as co-promoters. The project is co-financed by Portugal 2020, under the Operational Programme for Competitiveness and Internationalization (COMPETE 2020), from European Regional Development Fund (ERDF).

Biography

José Silva holds a degree in Chemistry from the Faculty of Sciences of the University of Porto, and since 2008 has worked as a researcher at CeNTI where he has developed R&D activities. Throughout his career, he has acquired skills in research, development and integration, through participation in different R&D projects (national and European) and conferences, accumulating experience and the necessary skills in the areas of processing, integration and characterisation of conventional electronics in various structures, processing technologies and characterisation of conventional printed and electronic systems/sensors using different types of substrates.

Electrical and mechanical investigation of silver-polyurethane composite film under applied pressure

Saeid Mehvari, Ben Goodhew, Sergio González, Khalid Lafdi, Yolanda Sanchez-Vicente

Department of Mechanical & Construction Engineering, Faculty of Engineering & Environment, Northumbria University Newcastle, Newcastle upon Tyne, NE1 8ST, United Kingdom.

Today, there is a growing demand for flexible, lightweight, inexpensive conductive materials in the electronic industry. Many scientific studies have focused on conductive polymer composites because they are ideal materials for electronic applications such as wearable sensors, smart fabrics, flip-chips and switching devices. This research investigates the electrical and mechanical properties of micro silver polyurethane (Ag-PU) composite films with and without segregated structures. AgPU composite films were prepared by adding micro silver particles (<3.5 m) into thermoplastic polyurethane (PU) matrix using solution mixing method followed by spin-coating or casting techniques. This method led to the formation of conductive network of silver microparticles with concentrations from ranging from 0 to 10 vol.%. To achieve a uniform dispersion of filler into polymer matrix, the silver solution was shear mixed in ultra-sonic bath then PU solution was added. All composites were characterized using an optical microscope and SEM. The electrical conductivity of the composites was measured using a developed set-up with a digital multimeter. Both composites, with or without the silver network, showed an electrical conductivity only through thickness when compressed under vertical pressures. Spin-coated samples showed a significant change in electrical conductivity at percolation threshold of 1.2 vol.% silver, whereas the casted counterparts showed this increment at higher concentrations, at around 6.6 %.vol of filler. The maximum conductivity value for these composites was about 4×10-3 S/m. The percolation threshold and conductivity values of the composite film with uniform distribution of silver were lower than those of the casted composite. Mechanical properties were also measured using a tensile test based on the D882 standard. Generally, tensile strength and elongation at break decreased as filler concentration increased for both composites. The electrical performance of fabricated composites was numerically simulated using finite element method based on the representative volume element model (FE-RVE, MSC-Digimat software). This method enabled to simulate the electrical behaviour under applied pressure for the agglomerated and uniform dispersed microstructure of Ag-PU composite.

Keywords: electrical conductivity, micro silver, percolation threshold, simulation, RVE

Parameter Screening and Optimization of a Polycaprolactone-Based Electrospun Membrane for Guided Tissue Regeneration Applications

Yuanyuan Duan

University of Mississippi Medical Center, MS 39216, USA

This presentation reports the development and optimization of a novel, biomimetic guided tissue regeneraton (GTR) membrane using Taguchi design and electrospinning technique. Mechanical properties and morphology of GTR membranes play an essential role in their success. Therefore, tensile strength (TS), elastic modulus (EM), and mean fiber diameter (MFD) were the response variables optimized in this study. Polycaprolactone (PCL) wt%, chicken eggshell membrane (ESM) wt%, nano-hydroxyapatite concentration (nano-HAp) wt%, applied voltage (AV), flow rate (FR), and spinneret-collector distance (SCD) were the independent variables investigated. Electrospun membrane specimens were prepared with varying concentrations of PCL, ESM, nano-HAp, and altered electrospinning parameters as generated by DOE++ software, and their MFD and mechanical properties were determined. Taguchi orthogonal array L8 design was used to screen significant factors affecting the response variables. ANOVA outlined ESM wt%, nano-HAp wt%, AV, FR, SCD, and an interactive effect between PCL wt% and AV to be the significant factors affecting modulus values of an electrospun PCL/ESM membrane ($p < 0.05$). Also, concentrations of PCL and ESM were the significant factors affecting MFD ($p < 0.05$). There were no significant factors observed affecting the TS. Furthermore, optimization using DOE++ software predicted that the maximal TS of 3.125 MPa, modulus of 278.168 MPa, and MFD of 882.75 nm could be achieved.

Biography

Dr. Duan received her DDS and PhD degrees from Air Force Medical University, China, and completed her postdoctoral training at the University of Mississippi Medical Center, USA. She is currently an associate professor with tenure at the University of Mississippi Medical Center School of Dentistry. She has published more than 55 peer-reviewed journal articles/book chapters, and made more than 80 presentations at scientific conferences worldwide.

Electrostatic sheathing of lipoprotein lipase is essential for its movement across capillary endothelial cells

Wenxin Song

University of California, Los Angeles, School of Medicine, CA 90024, USA

GPIHBP1, an endothelial cell (EC) protein, captures lipoprotein lipase (LPL) within the interstitial spaces (where it is secreted by myocytes and adipocytes) and transports it across ECs to its site of action in the capillary lumen. GPIHBP1's three-fingered LU domain is required for LPL binding, but the function of its acidic domain (AD) has remained unclear. We created mutant mice lacking the AD and found severe hypertriglyceridemia. As expected, the mutant GPIHBP1 retained the capacity to bind LPL. Unexpectedly, however, most of the GPIHBP1 and LPL in the mutant mice was located on the abluminal surface of ECs (explaining the hypertriglyceridemia). The GPIHBP1-bound LPL was trapped on the abluminal surface of ECs by electrostatic interactions between the large basic patch on the surface of LPL and negatively charged heparan sulfate proteoglycans (HSPGs) on the surface of ECs. GPIHBP1 trafficking across ECs in the mutant mice was normalized by disrupting LPL-HSPG electrostatic interactions with either heparin or an AD peptide. Thus, GPIHBP1's AD plays a crucial

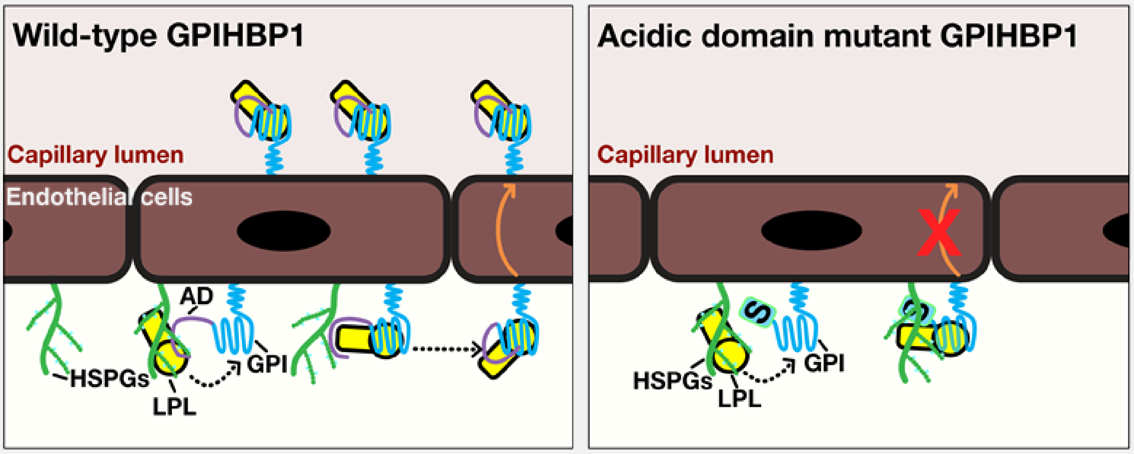


Fig. 1. GPIHBP1's AD is required for trafficking of LPL–GPIHBP1 complexes to the capillary lumen. In wild-type mice (left), GPIHBP1's AD (purple) disrupts electrostatic interactions between LPL's basic patch and abluminal HSPGs, freeing LPL–GPIHBP1 complexes to move across ECs. In the mutant mice (right), the absence of GPIHBP1's AD permits persistent abluminal LPL–HSPG interactions, trapping GPIHBP1–LPL complexes on the abluminal surface of ECs.

function in plasma triglyceride metabolism; it sheathes LPL's basic patch on the abluminal surface of ECs, thereby preventing LPL-HSPG interactions and freeing GPIHBP1-LPL complexes to move across ECs to the capillary lumen.

Biography

Wenxin Song has completed his PhD at the age of 27 years from Tsinghua Univerisity, China and postdoctoral studies from University of California, Los Angeles, School of Medicine. She has published more than 15 papers in reputed journals and has been serving as an editorial reviewer of repute for 12 jounals including Science Advances and PLOS Biology.

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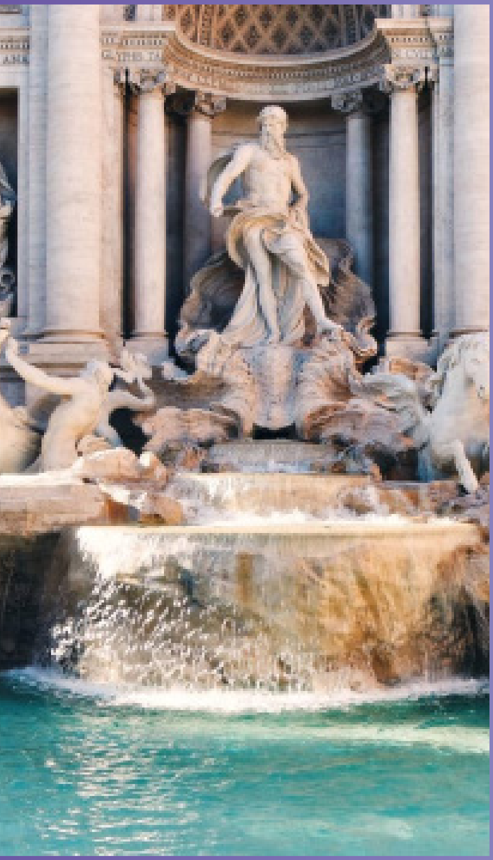

Innovinc International
5201 Great America Pkwy #320, Santa Clara, CA 95054,
United States
Ph: +1-408-352-1010

Innovinc International
301, Sri Venkateswara Residency, Balaji Nagar, Nizampet, Hyderabad,
TS, India. 500072
Ph: +918374242127