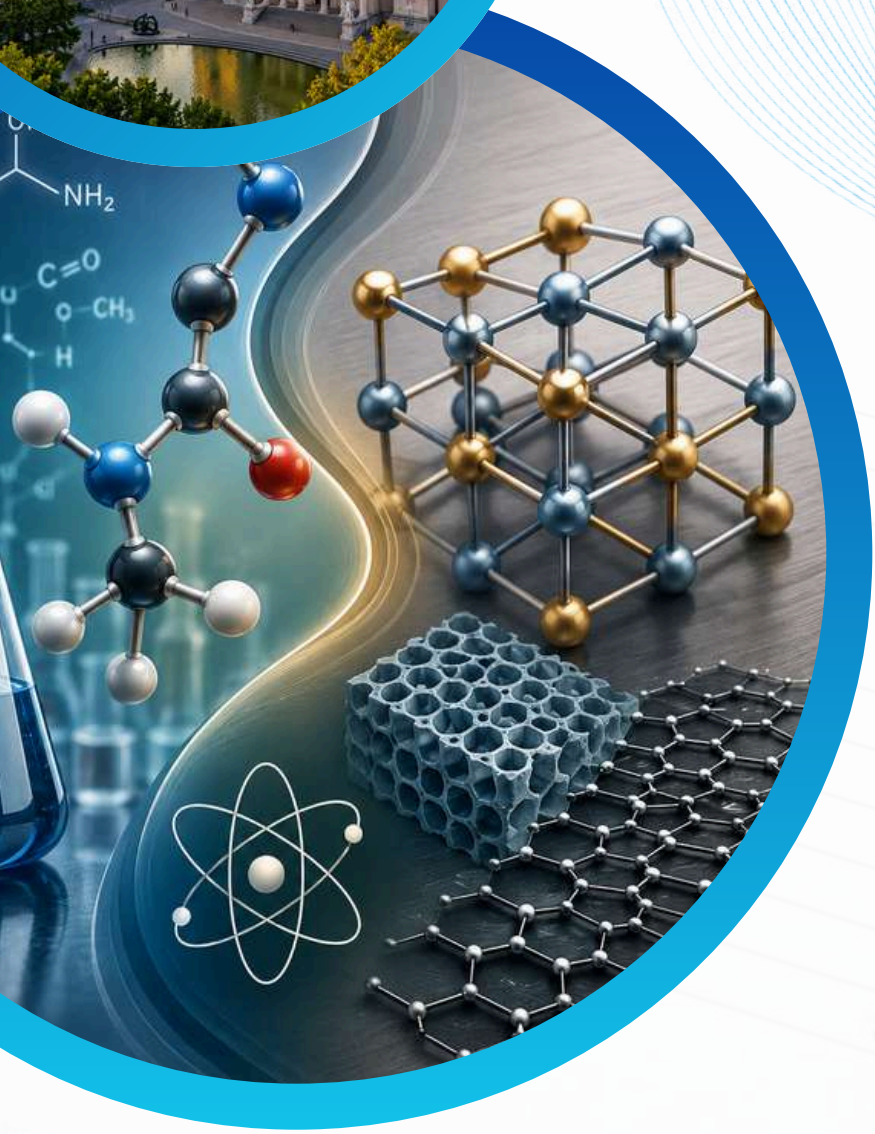
UNITED RESEARCH FORUM
(CONNECT WITH RESEARCH WORLD)

5th International Conference on

CHEMISTRY & CHEMICAL ENGINEERING



July 23–24, 2026

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VENUE

Rainer's Hotel Vienna
Gudrunstraße 184,
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Austria

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LETTER FROM THE CEO & DIRECTOR UNITED RESEARCH FORUM

On behalf of the United Research Forum, UK, we are delighted to announce the organization of the 5th International Conference on Chemistry and Chemical Engineering, which will be held at the Rainer's Hotel, Vienna, from July 23–24, 2026.

The conference aims to provide an international platform for researchers, scientists, academicians, industry professionals, and experts in the fields of chemistry and materials science to come together, exchange knowledge, discuss emerging trends, present innovative research findings, and explore recent advancements and applications across various disciplines.

We look forward to welcoming participants from around the world to Vienna for an inspiring and engaging scientific gathering. This conference will bring together distinguished researchers and professionals to share groundbreaking discoveries, foster collaborations, and highlight the latest developments in areas including chemical sciences, advanced materials, nanotechnology, sustainable materials, and related fields.

We hope you enjoy your visit to Vienna and take the opportunity to experience its rich cultural heritage, historic landmarks, and vibrant scientific environment.

Finally, I extend my best wishes for a successful and impactful conference and express my sincere appreciation to our partners, speakers, delegates, and the organizing team whose dedication and support make this event possible.

Sincerely,
Dr. Vanga
CEO, Director | United Research Forum
United Kingdom

IN-PERSON

Day 01

July 23, Thursday

REGISTRATIONS AND OPENINGS

08:00 – 09:00

PLENARY SESSION

Cutting-edge Research and Global Perspectives

09:00 - 09:30

Prof. Abul Kasem Fazlur Rahman,
Oklahoma School of Science and Mathematics, USA

Metal catalyzed water oxidation is a key step in artificial photosynthesis

09:30 - 10:00

Prof. Maria Holuszko, University of British Columbia, Canada

Critical metals extraction from secondary sources; Valorization of Critical Elements recovery from post-industrial waste

10:00 – 10:30 Networking Break + Group Photo

KEYNOTE SESSION

10:30 - 11:00

Prof. Abul Kasem Fazlur Rahman,
Oklahoma School of Science and Mathematics, USA

Synthesis of a Cobalt Cube: A Potential Catalyst for Water Oxidation

11:00 - 11:30

Prof. Mu-Hua Huang, Beijing Institute of Technology, China

Flexible Porous Organic Polymers with Well-Defined Structures via Bottom-up Strategy for Precious Metal Recovery and Gases Separations

TECHNICAL SESSION – I

11:30 - 11:55

Prof. Ulrika Nilsson, Stockholm University, Sweden

Automated thermal desorption-gas chromatography/mass spectrometry for rapid screening of hazardous chemicals in clothing and other textiles

IN-PERSON

11:55 - 12:20

Mr. Julien Göthel, Rouge H2 Engineering AG, Austria

Advanced Oxygen Carrier Materials for Clean H_2 Production and CO_2 Separation in Chemical Looping Processes

12:20 - 12:45

Prof. Ivan Chodak, Polymer Institute SAS, Slovakia

Correlation between electrical conductivity and deformation of polymeric composites

12:45 - 13:10

Dr. Visnja Vrdoljak, University of Zagreb, Croatia

Engineering Nuclearity in Vanadium Assemblies:
From metallosupramolecular isomerism to Tunable Oxidation Catalysis

13:10 – 14:00 Lunch @ Restaurant

14:00 - 14:25

Dr. Katarzyna Zielińska,
Institute of Heavy Organic Synthesis, Blachownia, Poland

Non-halogenated flame retardants for various applications in advanced materials

14:25 - 14:50

Dr. Mohammad Hassan Mazaherifar,
Transilvania University of Brașov, Romania

Performance of Carbon Fiber-Reinforced Date Palm Midrib Composites

14:50 - 15:15

Dr. Harry Z. Ha, Fluor Canada Ltd, Canada

Molecular Representation and Modeling of Renewable Diesel Processing with Canola Oil

15:15 - 15:40

Dr. Tim Åström, Stockholm University, Sweden

Towards a safe and environmentally sustainable valorisation of post-consumer garments made of cotton and cotton blends

IN-PERSON

15:40 – 16:10 Refreshment Break & Poster Presentations

POSTER - 1

Mr. Leonardo Andres Vergara, UTFSM, Chile

Structural and morphological tuning of CuO thin films for enhanced ethanol gas sensing

POSTER - 2

Mr. Fernando Alvarez Asencio, UTFSM, Chile

Spintronic potential of Co/Cr_2O_3 interfaces: oxidation and exchange bias effects

POSTER - 3

Prof. Maria Clara Goncalves, Instituto Superior Técnico, Portugal

Nanoparticle-Assisted Sustainable Regeneration of Spent Dialysate

POSTER - 4

Dr. Magdalena Strzebońska, AGH University of Krakow, Poland

Development of Titanium Dioxide-Free Drotaverine 80 mg Film-Coated Tablets and Validation of HPLC Methods forAssay and Impurity Determination

POSTER - 5

Prof. Nabil Al-Zaqri, King Saud University, Saudi Arabia

Highly efficient nanosized Sn0.96Y0.02M0.02O2 (M = Mo, Zr) photocatalysts for mineralization of methyl green and chlorpyrifos waste

SESSION CONTINUES

16:10 - 16:35

Dr. Fahimeh Zare, Instituto Superior Técnico, Portugal

Enhancing Spent Dialysate Regeneration: The Role of Magnetic Nanoplatforms and Advanced Membranes

IN-PERSON

16:35 - 17:00

Prof. Norman H. L. Chiu, University of North Carolina Greensboro, USA

Towards Standard-free Quantitative Profiling of RNA Modifications Using Mass Spectrometry

17:00 - 17:25

Mr. Ernest Ewert, Adam Mickiewicz University, Poland

Comparison of the interactions of 18-membered lanthanide macrocycles with G-quadruplexes

17:25 - 17:50

Prof. Alexander A. Kamnev,
Saratov Federal Scientific Centre of the Russian Academy of Sciences, Russian Federation

Invited talk: Microbial reduction of selenite with the formation of Se(0) nano-structures

End of Day 1

Day 02: July 24, Friday

09:00 – 09:30 KEYNOTE SESSION

09:00 - 09:30

Prof. Ernst Wagner, Ludwig-Maximilians-Universität, Germany

Chamaeleon Nanocarriers for RNA Delivery and Genome Editing

09:30 - 10:00

Prof. Bin Fei, Hong Kong Polytechnic University, Hong Kong

Environmental Photonic Energy Manipulation with Fire Safety Coatings

10:00 – 10:30 Networking Break

TECHNICAL SESSION – II

IN-PERSON

10:30 - 10:55

Prof. Nezihe Ayas, Eskisehir Technical University, Turkey

Biomass as Both Feedstock and Functional Material for Hydrogen Production: A Dual Role in Sustainable Energy

10:55 - 11:20

Dr. Pedro Silva, Lumar Metals, Austria

Analysis of a Supersonic Nozzle System Effect in Gas-Cooled Lances on Slag Splashing Parameters

11:20 - 11:45

Prof. Nan Yao, Princeton University, USA

Seeing the Unseen: Decoding Atomic Adsorption, Nucleation, and Electronic Structure with Functionalized Scanning Probe Microscopy

11:45 - 12:10

Dr. N. Funda Ak Azem, Dokuz Eylül Universit, Turkey

Design Strategies for Doping Metal Oxide Nanomaterials for Enhanced Photocatalytic Performance

12:10 - 12:35

Prof. Mihaela Baibarac, National Institute of Materials Physics, Romania

Composites based on reduced graphene oxide and polydiphenylamine doped with heteropolyanions for energystorage applications

12:35 - 13:00

Mr. Catello Somma, Seroba, Italy

Targeted Radiopharmaceutical Therapy: Advances, Investment Dynamics, and Future Directions—Part 1

13:10 – 14:00 Lunch @ Restaurant

14:00 - 14:25

Miss. Şehnaz Genc, Eskisehir Technical University, Turkey

Turning Agricultural Waste into Functional Membranes: Banana Peel-Based Materials for Hydrogen Production via Alkaline Water Electrolysis

IN-PERSON

14:25 - 14:50

Dr. Thomas-Skurk, ZIEL - Institute for Food & Health, Germany

Coffee Beyond Caffeine: Human Pharmacokinetics of Coffee-Specific Biomarkers and Their Association with Acute Immunomodulatory Responses

14:50 - 15:15

Felix Zak, Technical University of Munich, Germany

From Material Characterization to System-Level Performance Prediction

15:15 - 15:40

Prof. Carlo Trigona, University of Catania, Italy

Plants as Living Sensors and Power Sources: Revealing Nature's Hidden Transducers

15:40 - 16:00

Prof. Hans-Ulrich Dodt, University of Vienna, Austria

Tissue clearing of whole organs: A challenge for chemistry

16:00 – 16:20 Refreshment Break

Day 2 Concludes

Virtual

Day 02

July 24, Friday

CENTRAL EUROPEAN SUMMER TIME (CEST)

09:00 - 09:20

Dr. Baode Zhang, Liaoning Petrochemical University, China

Probing non-covalent interactions within π-π stacking assembly by EPR Spectroscopy

09:20 - 09:40

Dr. Rongji Lai, Nanning Blood Center, China

A robust DNA walker for simplified, rapid and sensitive detection of HBV DNA in blood donors

09:40 - 10:10

Dr. Abhishek Bansal, New Era Consultancy Services, India

A Projection-Based Framework for Chemical Kinetics, Thermodynamics, and Molecular Organization

10:10 - 10:30

Miss. Krishnendu P R, Amrita school of Pharmacy, India

Molecular mechanism of sesamol in inflammatory bowel disease: Integrative computational, microbiome, andbiological evaluation targeting jak1 pathway

10:30 - 10:50

Prof. Miroslav Iliaš, Joint Institute for Nuclear Research, Russia

First-principles theoretical study of adsorption properties of heavy and superheavy elements and their compounds onselected surfaces

10:50 - 11:10

Miss. Mariia Smirnova, Valiev IPT of NRC Kurchatov Institute, Russia

Evolution stages of periodic relief on the silicon surface under ion irradiation

11:10 - 11:30

Dr. Antonina Dunina-Barkovskaya,
Moscow Lomonosov State University, Russia

Cell Membrane Cholesterol and Diseases Associated with Its Deficiency

11:30 - 11:50

Prof. Hayk Minassian, A. Alikhanian National Science Laboratory, Armenia

Revealing the quadrupole surface plasmon resonance in TI3C2TX multilayered maxine

11:50 - 12:10

Dr. Uta Rösel,
Friedrich-Alexander-Universität Erlangen-Nuremberg, Germany

Simulation-based prediction of fiber orientation in highly filled thermoset materials based on process-relevantrheological data

12:10 - 12:30

Dr. Rayya Al Balushi, A'Sharqiyah University, Oman

Conjugated Poly-Metalla-Ynes for Opto-Electronic Applications

12:30 - 12:50

Mrs. Rumeysa-Hilal-Celik, Niğde Ömer Halisdemir University, Turkey

Effect of GO Derivatives Reinforced Nanofiber Polymeric Scaffolds on Oligodendrocytes' Maturation and Myelination

12:50 - 13:10

Dr. Arzu Çankaya & Team, Kocaeli University, Turkey

Development of polyamide 6.10 composites reinforced with nickel-coated carbon fibers

13:10 - 13:30

Dr. Manfred Kircher, KADIB, Germany

Recycling Biowaste and Residuals into Chemical Products

13:30 - 13:50

Prof. Piotr R. Scheller, TU Bergakademie Freiberg, Germany

Interfaces in liquid steel processing and related effects

13:50 - 14:10

Mr. Radim Halama, Technical University of Ostrava, Czech Republic

Accelerated creep/fatigue characteristics estimation using DIC

Virtual

14:10 - 14:30

Dr. Krisna Prak, Imperial College London, UK

Insight into structure-function of Bothrops atrox snake venom LAAO and its mechanism of action on cell apoptosis

14:30 - 14:50

Dr. Flávia Assunção, University of São Paulo, Brazil

Photobiomodulation with LED Does Not Alter Antibiotic Sensitivity in ATCC and Burn-Patient Bacteria

14:50 - 15:10

Prof. Takuji Tanaka, University of Saskatchewan, Canada

Maillard Induced Pea Protein-Polysaccharide Conjugates: A Functionally Enhanced Ingredient for the Food andBeverage Industry

15:10 - 15:30

Dr. Stewart P. Lewis, Pyramid Polymers LLC, USA

15:30 - 15:50

Mr. Salahaldeen M. A. Aljafreh, Eskisehir Technical University, Turkey

Synthesis of Sugar Beet Pulp-Derived Activated Carbon for CO2/CH4 Separation from H2-Rich Syngas

UPCOMING EVENTS

ICCCE-2027
July 05-06 | Lisbon, Portugal

July 05-06, 2027 | Lisbon, Portugal & Online

6th Edition of Chemistry & Chemical Engineering conference

July 05-06, 2027 | Lisbon, Portugal & Online

4th Edition of Material Science & Engineering Conference

Day 01

Keynote Presentations

A.K. Fazlur Rahman[1,2], Don Tilley[2]

1. Department of Chemistry, Oklahoma School of Science and Mathematics, Oklahoma City, OK, USA
2. Department of Chemistry, University of California, Berkeley, CA, USA

Synthesis of a Cobalt Cube: A Potential Catalyst for Water Oxidation

ABSTRACT

This presentation outlines the synthesis, isolation, and structural characterization of four cobalt cabane complexes with potential application as catalysts in water oxidation, a key step in artificial photosynthesis. The complexes were synthesized via reactions of cobalt (II) acetate with trifluoroacetic acid and various fluorinated pyridine ligands, including CF_3-pyridine, F_2-pyridine, and per fluoropyridine. The resulting compounds were thoroughly characterized using single-crystal X-ray diffraction, nuclear magnetic resonance (NMR) spectroscopy, and electrospray ionization (ESI) mass spectrometry. These findings potentially may contribute to the development of efficient molecular catalysts for sustainable energy conversion.

BIOGRAPHY

Prof. A. K. Fazlur Rahman is the S. J. Sarkeys Professor and Chair of the Chemistry Department at the Oklahoma School of Science and Mathematics, and an Affiliated Professor of Chemistry and Chemical Engineering at the University of Oklahoma. He earned his B.Sc. (Hons.) and M.Sc. in Chemistry from Jahangirnagar University, an M.A. in Chemistry from Brandeis University, and a Ph.D. in Organometallic Chemistry from the Australian National University, followed by postdoctoral research at Ames Laboratory, the University of Tasmania, and the University of Oklahoma. He has since held research and visiting appointments at institutions including Texas A&M, Rochester, UC Berkeley, Caltech, Rutgers, Columbia, the Free University of Berlin, and Friedrich Schiller University Jena. His research spans organometallic chemistry, homogeneous catalysis, CO_2 activation and utilization, metal-stabilized carbocations, and water oxidation catalysis, with a broader focus on artificial photosynthesis and sustainable energy through molecular catalysis.

Mu-Hua Huang

School of Materials Science and Engineering,
Beijing Institute of Technology, Beijing, 100081, China

Flexible Porous Organic Polymers with Well-Defined Structures via Bottom-up Strategy for Precious Metal Recovery and Gases Separations

ABSTRACT

The porous organic polymers with sp3 C in the polymer backbone have attracted lots of attentions, owing to their unique structure and promising application potentials in many fields. The presentation will share the story of how we developed flexible POPs using the bottom-up strategy, e.g., porous polyimides (e.g., BIT-POP-12) for removal of colored impurity in Desmodur®RE (DRE), porous polypyrrolidines (e.g., BIT-POP-17) for gold recovery and polysalicylates for gas separations (Figure 1), as well as the in situ polymerization strategy to make homogeneous polymer membranes.

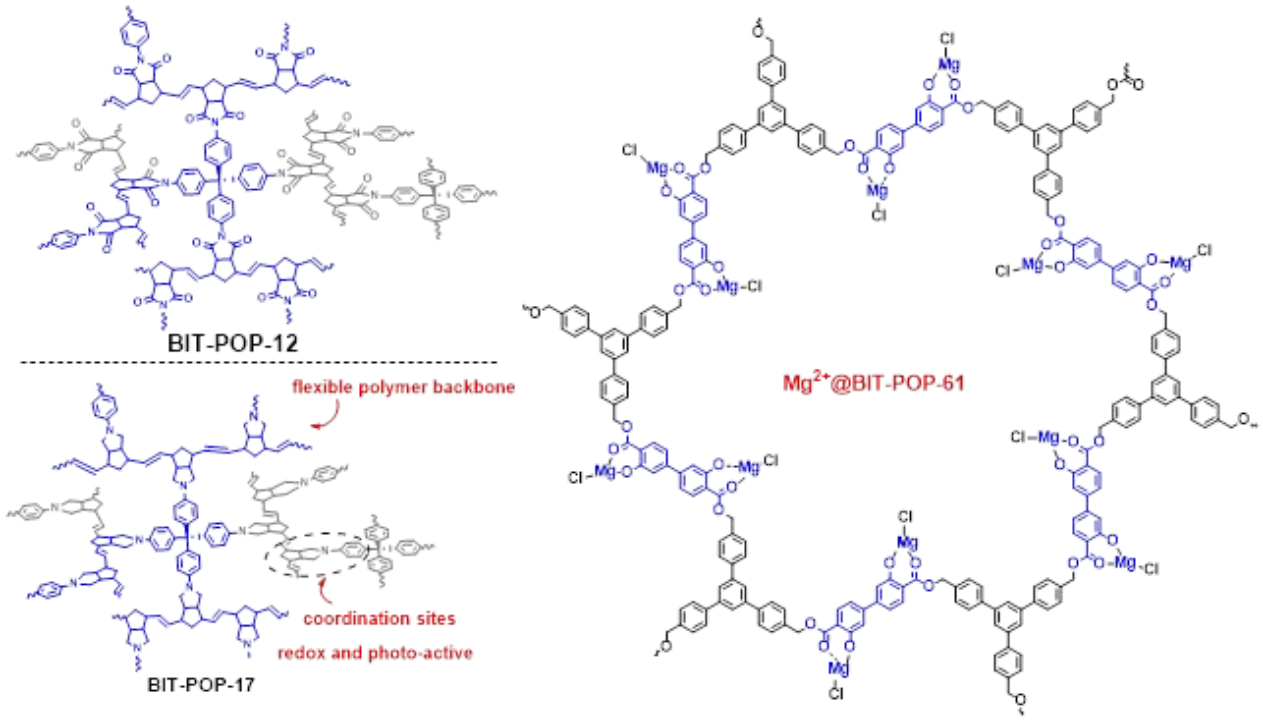

Figure 1. Flexible POPs presented in this presentation

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More importantly, the highly porous polysalicylates (named Mg@BIT-POP-60 and Mg@BIT-POP-61) with benzylic (sp3 C) ester linkage (Figure 1) was developed by a powerful "three-in-one" strategy aided by Grignard reagent. In addition, an easy processing technology named premixing-hot pressing (pm-HoP) was developed to make the nanocomposite membranes with high loadings of Mg@BIT-POP-61 (50 wt%) in polycaprolactone (PCL). The reversed H_2/CO_2 selectivity of 3.12 favoring H_2 was observed comparing with pristine PCL (0.3), as well as high H_2 permeability of 5805 Barrer. This work demonstrated a successful design of the novel porous polysalicylates by developing molecular switch, as well as the "three-in-one" strategy.

Keywords: Porous Organic Polyemrs, Flexibility, gold recovery, solid-state NMR, gas adsorption, porous polysalicylates

References:

[1] S.-Q. Peng, T. Yang, W. Fan, S. Chi, B. Kuang, L. Fan, X. Li, M.-H. Huang, Chem. Mater. 2022, 34, 5184-5193.
[2] J. Shi, S.-Q. Peng, B. Kuang, S. Wang, Y. Liu, J.-X. Zhou, X. Li, M.-H. Huang, Adv Mater 2024, e2405731.
[3] J. Zheng, B. Kuang, J.-J. Yang, J. Shi, H. Chen, J.-X. Zhou, X. Ma, M.-H. Huang, J. Membr. Sci., 2025, 731, 124232.

BIOGRAPHY

Mu-Hua Huang is a full professor in the School of Materials Science and Engineering in Beijing Institute of Technology (BIT), Beijing China. He earned his PhD degree in 2006 from ICCAS, and conducted postdoctoral researches in ETH-Zurich and University of Liverpool during 2008-2011, before he returned to China to take up a position at BIT in 2012. His current research interests include the designs, syntheses and multiple applications of porous polymer materials, energetic materials, as well as NMR technology for characterization of polymer materials. He has authored and co-authored over 50 peer-reviewed publications in the areas, including Nature Chemistry, Advanced Materials. He has also registered and filed over 40 international and domestic patents, more than 20 of them has been authorized. He was invited to give more than 20 lectures in international conferences and universities in the past 3 years. He served as the vice-president of the Spectroscopy Branch of Beijing Physical and Chemical Analysis and Testing Society, committee members including POPs2025 and BCEIA.

Day 01

Oral Presentations

Ulrika Nilsson*, Tim Åström, Awat Dostberg, Ioannis Sadiktsis, and Conny Östman

Stockholm University, Stockholm, Sweden

Automated thermal desorption-gas chromatography/mass spectrometry for rapid screening of hazardous chemicals in clothing and other textiles

ABSTRACT

Common clothing garments and other textiles on the European market have been shown to often contain numerous and high levels of, so far mostly non-regulated, but likely hazardous chemicals. Textile chemicals, non-covalently bound to the textile fibres, may migrate through sweating or rubbing and be absorbed by human skin, thus constituting a possible risk for skin sensitization or other health effects. For prevention purposes, the control of clothing and other textiles for such chemicals must therefore be improved.

An automated analytical method has been developed and is suggested as a fast method for control and comprehensive screening of semivolatile hazardous chemicals in textiles. This method is based on automated thermal desorption– gas chromatography/mass spectrometry (ATD-GC/MS) and has so far been evaluated for synthetic polyester textiles, cotton as well as blends of these fibres.

The method requires very little of manual handling, no solvents and a minimum of consumables. The total run time for each sample is around 40 min, including thermal desorption, chromatographic separation, and mass spectrometric detection. For most of the studied analytes, the method quantification limit in full scan acquisition is well below 5 ppm, sufficiently low for screening of textile chemicals regulated by EU.

Keywords: Textile chemicals, automated thermal desorption-gas chromatography/mass spectrometry, skin sensitizers, hazardous chemicals

BIOGRAPHY

Ulrika Nilsson, professor in analytical chemistry, is leading the research of the ChemInTex group in the Department of Chemistry at Stockholm University. She has a long experience of developing mass spectrometric and chromatographic techniquies for both environmental pollutants and health hazardous chemicals, with a special interest in skin sensitizers.

Julien Göthel[*1,2], Uwe Pahl[1]

[1]*Rouge H2 Engineering AG, Puntigamer Straße 127, 8055 Graz, Austria*
[2]*Insitute of Iron- and Steeltechnology, Leipziger Straße 34, 09599 Freiberg, Germany*

Advanced Oxygen Carrier Materials for Clean H_2 Production and CO_2 Seperation in Chemical Looping Processes

ABSTRACT

The evolution of Chemical Looping (CL) technology has shifted from mere combustion to selective value-added production, specifically Chemical Looping Hydrogen Production (CLHP) and CO_2 capture, enabling the utilization and upcycling of various synthesis gases with reducing effects on metal oxides. This positions CL as a pivotal technology for decarbonization, Power-to-X strategies, and the integration of fluctuating renewable energies. In this framework, the solid Oxygen Carrier (OC) functions as both a transfer medium and thermochemical storage, facilitating the direct splitting of steam or carbon dioxide to generate pure hydrogen and carbon monoxide through cyclic redox reactions. While standard materials like Nickel or Copper fail due to unfavourable equilibria or thermal instability, iron oxides represent a robust industrial choice for CL applications given their cost efficiency and ability to undergo complete reoxidation by H_2O. However, natural ores succumb to extreme cyclic loads, necessitating synthetic iron oxide composites to withstand specific degradation mechanisms. These include mechanical attrition driven by significant volume changes during phase transitions, thermal sintering above 850 °C which irreversibly reduces porosity and gas diffusion, and iron migration causing particle agglomeration and defluidization. To counter these degradation pathways, active iron is embedded into chemically stable support matrices such as Al_2O_3 or ZrO_2 via methods like co-precipitation. This approach optimizes crystallite size and pore structure to absorb volumetric stress and prevent sintering. Nevertheless, challenges persist, notably the irreversible formation of inactive spinels. Consequently, advanced research focuses on catalytic doping with rare earth oxides or utilizing perovskites to enhance oxygen mobility. Ultimately, the technical realization of clean hydrogen production relies on developing synthetic iron-based composites that retain microstructural integrity and kinetic performance over thousands of severe thermochemical cycles.

BIOGRAPHY

Julien Göthel is a Metallurgy Engineer (Dipl.-Ing.) and doctoral candidate at the Institute of Iron and Steel Technology at TU Bergakademie Freiberg (Germany). His work focuses on pyro-, hydro-, and process metallurgy, specifically advancing closed-loop and low-impact circular economy solutions. As Head of Process Design in System Integration at Rouge H2 Engineering AG, he leads the engineering of integrated systems and directs supporting scientific research.

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Ivan Chodák, Hamed Peidayesh

Polymer Institute SAS, Bratislava, Slovakia

Correlation between electrical conductivity and deformation of polymeric composites

ABSTRACT

Plastics are usually applied as materials with low electrical conductivity. If higher electrical conductivity is needed, composite materials of a particular plastic or rubber is mixed with electroconductive filler to achieve higher conductivity. The concentration of electroconductive filler may increase beyond so called percolation threshold and the composite's conductivity may approach to the conductivity of metals. The reason consists in formation of electroconductive paths through the whole crossection of the material; at this filler concentration conductivity increases through several orders of magnitude within rather small increase of the filler content. On the other hand, if the material exhibits the conductivity over the percolation threshold and it is submitted to mechanical deformation, number of the conductive paths can be destroyed and the conductivity may decrease substantially. The electrical conductivity was measured together with the mechanical deformation, it was found that the conductivity never has changed monotonously with the deformation increase, but usually several extremes were identified. Moreover, all extremes on the conductivity dependence could be assigned to certain features on the stress – strain curve, e.g. monotonous conductivity decrease in Hookean region, followed by the increase up to mechanical yield point and following plastic deformation. Relaxation at constant deformation was usually represented by recovery in conductivity, but while the recovery never reached the staring conductivity, the repeating cyclic behaviour was always the same between the 2nd and any further cycles. The way of application of these observations for sensors construction is shown.

Keywords: electrical conductivity, stress-stresin curve, electroconductive composite, plastics, rubber

BIOGRAPHY

Prof Ivan Chodak is a senior scientist, former head (1982 – 2009) of Department of Composite Materials at Polymer Institute SAS. The author and coauthor of over 190 scientific papers, H-index = 38. Scientific interests: multiphase polymeric systems, electroconductive composites, polymer nanocomposites and biodegradable polymer blends. In the period 2005 - 2009 a member of Presidium of the Slovak Academy of Sciences, external teacher of Polymer Physics at Slovak Technical University and Trencin University of Alexander Dubcek. the elected member of the Slovak Learned Society (from 2012), the elected member of European Academy of Sciences and Arts (from 2024).

Višnja Vrdoljak, Edi Topić, Josipa Sarjanović, Dino Kuzman, Tomica Hrenar, Jana Pisk

University of Zagreb Faculty of Science, Department of Chemistry, Zagreb, Croatia

Engineering Nuclearity in Vanadium Assemblies: From metallosupramolecular isomerism to Tunable Oxidation Catalysis

ABSTRACT

Coordination-driven vanadium(V) assemblies were synthesized from aroylhydrazone ligands and NH_4VO_3 in the presence of various alcohols, using both conventional synthetic approaches and post-assembly structural transformations. They were systematically investigated to elucidate how reaction conditions and auxiliary alkoxide ligands control the formation of discrete tetranuclear complexes versus one-dimensional coordination oligomers, and how these structural motifs influence their stability and catalytic performance. Solid-state structures were elucidated by single-crystal and powder X-ray diffraction, supported by IR-ATR, NMR spectroscopy, and thermogravimetric analysis. Across all architectures, the monomeric building unit displays an ONO coordination environment around vanadium(V), provided by a doubly deprotonated hydrazonato ligand. Oligomerization occurs via coordination of a pyridyl nitrogen atom to the sixth coordination site of the neighbouring oxovanadium center. Assemblies with alternating syn/anti motifs are thermodynamically preferred over those composed exclusively of syn or anti units. The functional consequences of the metallosupramolecular nuclearity were evaluated in the catalytic oxidation of substituted benzyl alcohols using tert-butyl hydroperoxide. The results highlight a fundamental trade-off between catalytic activity and selectivity: highly active catalysts tend to lose selectivity due to overoxidation, whereas highly selective systems operate more slowly.

Keywords: self-assembly, hydrazone ligands, metallsupramolecular; structure–property relationships; alcohol oxidation catalysis

BIOGRAPHY

Višnja Vrdoljak obtained her PhD in Inorganic Chemistry from the Faculty of Science at the University of Zagreb in 1996. After completing a post-doctoral fellowship at the University of Trieste, Italy, she joined the Faculty of Science at the University of Zagreb, Croatia. In 2015, she was appointed as a professor at the Department of Chemistry. Her current research focuses on developing hybrid organic-inorganic polyoxometalate-based materials and metallsupramolecular architectures of molybdenum, vanadium, and copper.

Katarzyna Zielińska*, Betina Małysa, Przemysław Bartoszewicz, Jacek Kosno, Tomasz Krawczyk

Łukasiewicz Research Network – Institute for Renewable Resources Chemistry, Kędzierzyn-Koźle, Poland
Silesian University of Technology, Faculty of Chemistry, Gliwice, Poland

Non-halogenated flame retardants for various applications in advanced materials

ABSTRACT

The growing regulatory pressure on halogenated flame retardants and increasing demand for sustainable advanced materials have intensified research into effective non-halogenated fire protection systems. For several years, research activities at Łukasiewicz ICSO have focused on the development of innovative, efficient flame retardants dedicated to a broad spectrum of advanced material applications, including polyurethane foams, polymer emulsions, adhesives, resins, as well as paper-, plywood-, wood-based materials and textile fabrics.

This contribution presents non-halogenated flame retardant systems whose fire-retarding performance is based on synergistic phosphorus–nitrogen chemistry. Particular attention is given to bio-based flame retardants containing α-amino acids and phosphoric acid, characterized by a high content of phosphorus and nitrogen, while being free from harmful halogens and formaldehyde. These systems act predominantly in the condensed phase, promoting char formation and reducing heat release during combustion. To further enhance fire resistance and functional performance, selected formulations are additionally reinforced with aluminium hydroxide, which contributes to reduced flammability through endothermic decomposition and supports the formation of a stable protective layer. Importantly, the presence of inorganic components also improves the durability and stability of the interaction between the flame retardant and treated substrates, such as textile fibers.

The presented solutions can be synthesized from raw materials of natural origin, recycled feedstocks, or petrochemical sources, offering flexibility in terms of sustainability and application requirements. The results demonstrate that non-halogenated, phosphorus–nitrogen-based flame retardants can meet stringent fire safety criteria while remaining compatible with modern advanced materials and environmentally responsible design principles.

Keywords: Flame retardants, plastic additives, amino acids, organic technology, advanced materials

BIOGRAPHY

Research-driven chemist with a PhD in Chemistry and over 10 years of experience in applied chemical technology, polymer modification, and catalytic process development. Currently, I lead the Chemical Processes and Technologies Research Group at the Łukasiewicz Research Network – ICSO, where I oversee industrial and scientific R&D in the field of organic and bioorganic technologies, obtaining and implement of functional additives for polymers, chemical recycling of materials, and flame-retardant obtaining technologies as well as circular economy issues and waste water treatment.

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Mohammad Hassan Mazaherifar [1,*], Octavia Zeleniuc [1], Camelia Cerbu [2], Sergiu-Valeriu Georgescu 1, Antonela Lungu [1], and Camelia Cosereanu [1]

[1] *Faculty of Furniture Design and Wood Engineering, Transilvania University of Brasov, B-dul Eroilor nr. 29, 500036 Brasov, Romania*

[2] *Department of Mechanical Engineering, Faculty of Mechanical Engineering, Transilvania University of Brasov, B-dul Eroilor nr. 29, 500036 Brasov, Romania*

Performance of Carbon Fiber-Reinforced Date Palm Midrib Composites

ABSTRACT

This paper evaluates the performance of composites made from date palm (Phoenix dactylifera L.)midribs reinforced with carbon fiber. Two types of adhesives—unsaturated polyester and epoxy resin—were used as binder for the experimental panels. The physical properties and mechanical strength of the composites, as a function of fiber types, lamination configuration, as well as adhesive types, were determined. The density levels of the panels made using epoxy and unsaturated polyester resin were found to be 1103 kg/m3 and 1133 kg/m3, respectively. Panels made using polyester adhesive had 6.05% and 3.98% for water absorption and thickness swelling values, respectively. Corresponding values of 3.09% and 6.35% were found for the panels made using epoxy resin. Mechanical properties of the samples revealed that carbon fiber-reinforced epoxy hybrids offer superior mechanical performance, whereas polyester-based hybrids may be more suitable for impact-resistant applications. Stereo-microscopy and vertical density profile (VDP) analysis of the panels resulted in variations in layer adhesion and density distribution. Based on the findings in this work, carbon fiber-reinforced epoxy-bonded hybrid panels exhibited superior mechanical properties, while those panels made using polyester-based binder would be more suitable where impact resistance is desired. The combination of date palm fibers and carbon fiber presents significant potential for sustainable applications, offering a balance of strength and durability.

Keywords: Phoenix dactylifera; long fibers; midribs; carbon fiber; laminate; mechanical testing; dimensional stability

BIOGRAPHY

I am Mohammad Hassan Mazaherifar, a PhD candidate at Transilvania University of Brașov, Romania. My research focuses on Wood Products and Composite Materials, with an emphasis on sustainable, high-performance material development.

Harry Z. Ha

Fluor Canada Ltd, Canada

Molecular Representation and Modeling of Renewable Diesel Processing with Canola Oil

ABSTRACT

Process simulation of renewable diesel production processes is required to design and analyze key process units, such as Feed Treatment, HDO and the Hydro-Dewaxing processes. A simulation model was built to correlate the thermodynamic and transport properties of a particular process using canola oil as the feedstock. The model uses commonly identified triacylglycerols (TAGs) to represent the molecular composition of the canola oil. Correlations have been developed with available data to predict the properties for each pure compound, and thereafter the properties of mixture.

Canola oil is typically characterized by analyzing the fatty acids either as free fatty acids (FFA) or as fatty acid methyl esters (FAME) using Gas Chromatography (GC). The slates of canola oil are highly populated with 5 - 8 TAGs with C_{16}-C_{18} long chains, which constitute more than 80% of the total composition. Therefore, the canola oil can be readily represented by a limited number of compounds. In this application, 36 commonly identified TAGs are used in this study to represent the molecular composition of canola oil. The model was developed using Aspen Plus with compositions tuned to match the reported FAME analysis. To estimate the properties of canola oil, the properties of each pure component need to be estimated. Correlations have been developed to estimate the thermal-physical and transport properties of those TAG whose data are not available. The model parameters are based on reported data of several TAGs available in DIPPR database. Model predictions have been validated with reported thermal-physical and transport properties of canola oil. The proposed molecular representation successfully predicted the thermal-physical properties (density and heat capacity), and the transport properties such as thermal conductivity, viscosity, and surface tension of canola oil.

The molecular representation is further applied in the hydro-deoxygenation and hydro-dewax process to produce the renewable diesel from canola oil. The process model is calibrated and validated with available engineering data. The model can be used in similar renewable diesel projects to provide reliable design basis for engineering and operations.

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Towards a safe and sustainable recyling of elastane-containing textiles

ABSTRACT

The consumption of household textiles within the European Union (EU) is estimated to be 26 kg/citizen[1], and the global textile industry is rapidly expanding. Fast-fashion is a global challenge influenced by dynamic consumer demand for fashion trends. This introduces novel chemicals, e.g., dyes and other functional chemicals that are not yet regulated, making it hard to predict the chemical content in garments. This might diminish the overall lifespan of a garment, for example, if the colour easily fades during laundry. The amount of textile waste is also increasing, nearly 7 million tonnes in 2022 within the EU, of which 26% of the separately collected textile waste was subjected to incineration or landfilling[2]. The environmental burden is not just related to consumption, but also to the Waste Framework Directive[3], which suggests that household textile waste should be recycled before being incinerated or deposited in landfills. Thus, the hypothesis for this study is to test an alternative recycling strategy for worn-out textile apparel, aiming to develop a safe and environmentally sustainable methodology. This is evaluated by removing elastane from textiles through partial degradation, without a substantial release of health-hazardous impurities from the elastane polymer backbone. Preliminary results indicate that the dissolution of elastane does not release any detectable molecules and thus provides a safe means of removing elastane from garments. Low levels of elastane-related substances have, however, been observed following a partial depolymerization. In conclusion, the methodology may offer a promising alternative to recycle worn-out textiles via an effiencient elastane removal of second hand fashion.

Keywords: Fast-fashion, Textile recycling, Sustainability, Efficiency, Elastane removal

BIOGRAPHY

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Enhancing SpentDialysate Regeneration: The Role of Magnetic Nanoplatforms and Advanced Membranes

ABSTRACT

Hemodialysis remains the principal treatment for end-stage renal disease, but its high consumption of ultrapure water and dialysate creates major environmental and economic burdens. This work presents a more advanced and sustainable dialysateregeneration strategy based on the integration of cellulose acetate/silica monophasic hybrid membranes with superparamagnetic iron oxide nanoparticles functionalized by silica. The proposed system combines membrane selectivity, nanoparticle adsorption, and magnetic recovery to improve urea removal while enabling dialysate reuse.

The monophasic hybrid membranes were prepared by a sol–gel assisted phase inversion route, producing asymmetric structures with tunable porosity and mechanical strength. Structural characterization by ATR-FTIR and SEM confirmed the successful formation of homogeneous CA/SiO_2 membranes. In parallel, core-shell nanoparticle were synthesized by co-precipitation followed by silica-based surface functionalization, yielding uniform core–shell particles with good colloidal stability and superparamagnetic behavior. This coating enhanced dispersion and surface functionality while preserving magnetic retrievability.

The current stage of the project focuses on validating the integrated membrane–nanoparticle regeneration platform under conditions relevant to dialysis applications. Experimental investigations have demonstrated the compatibility of the membrane and magnetic nanomaterials, the efficient recovery of nanoparticles after the adsorption stage, and the operational feasibility of the sequential adsorption–magnetic separation–membrane filtration process. Ongoing studies are evaluating the overall regeneration performance of the complete system, and a comprehensive assessment will be reported in future publications.

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This work represents a significant step beyond our previous membrane-based approach by introducing a recoverable and integrated nanoplatform designed for sustainable dialysate regeneration. The proposed strategy provides a scalable foundation for next-generation hemodialysis technologies while supporting reduced resource consumption and improved process sustainability.

Keywords: Spent dialysate regeneration, SPIONS, core-shell silica nanoparticles, adsorption, Separation technology.

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BIOGRAPHY

Fahimeh Zare is a PhD in Chemical Engineering and researcher specializing in membrane technology, nanoparticle synthesis, and porous thin film characterization. She contributes to the HORIZON PHOTONGATE project, focusing on advanced photonic multi-sensing systems. Fahimeh has presented at various international conferences and published four peer-reviewed articles, with another under review. Her work appears in top journals like Membranes, Sensors, and Hydrogen Energy. She received several honors, including the BIC France-Portugal scholarship. Her research targets advanced membrane materials, uremic toxin removal, SPIONS and core-shell Nanoparticles, and hydrogen production technologies, aiming to drive innovation in separation science and sustainable energy through collaborative, high-impact research.

Prof. Norman Chiu

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Towards Standard-free Quantitative Profiling of RNA Modifications Using Mass Spectrometry

ABSTRACT

Although selected RNA modifications have been extensively studied, the functions of many other modifications within the epitranscriptome remain largely unknown. This is partly due to the limited availability and high cost of RNA standards, which hinder the development of robust analytical methods for comprehensive and quantitative profiling. Theoretically, the interplay among different RNA modifications can influence RNA functions, thus highlighting the importance of accurate profiling for biomarker discovery. Using mass spectrometry as a universal platform, recent advances have enabled untargeted analysis of RNA modifications. In our study, using the glioblastoma epitranscriptome as a model system, we introduce a practical approach to address the lack of standards and correct the bias in the electrospray ionization of different ribonucleosides. Our developed method has shown to improve quantitative accuracy and reproducibility. With the ability to determine the accurate quantity of each RNA modification, we extended our study on the chemical stability of modified nucleosides under various experimental conditions. If unaddressed, these factors can introduce significant bias and lead to erroneous conclusions in quantitative studies of epitranscriptomes.

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Comparison of the interactions of 18-membered lanthanide macrocycles with G-quadruplexes

ABSTRACT

Cancer remains the second most common cause of death worldwide. New compounds that could be applied in cacner therapy are still sought. One of the approaches proposed in the literature is the selective stabilization of G-quadruplexes (GQs) in particular genome regions of cancer cells. The GQ is a non-canonical four-stranded secondary structure of nucleic acids formed by guanine-rich sequences. Macrocyclic complexes of lanthanides represent an interesting group of compounds specially designed for targeting nucleic acids, yet the influence of subtle diamine scaffold variations on GQ interaction remains insufficiently defined. The presentation will concern the template synthesis, characterisation and comparative evaluation of La^{3+}, Dy^{3+} and Pr^{3+} macrocyclic complexes derived from dicarbonyl derivatives of pyridine and aliphatic or alicyclic diamines, focusing on topology-dependent interactions with telomeric GQs (Tel26, Tel22), promoter GQs (Pu22, hTERT) and duplex DNA (a control). The reasearch methodology includes i.a. GQ thermal stability measurements, circular dichroism experiments and fluorimetric titrations. The results highlight unique structure-activity relationships in lanthanide macrocycles and provide a rare complement to prior studies on lanthanide-DNA interactions. Overall, these findings contribute to a comparative framework for understanding how subtle structural modifications in lanthanide macrocycles influence topology-dependent GQ recognition, providing guidance for the rational tuning of future ligand architectures.

Keywords: lanthanide, macrocycle, complex, DNA, G-quadruplex

BIOGRAPHY

I am a second year doctoral candidate at the Faculty of Chemistry, Adam Mickiewicz University in Poznań. My scientific interests focus on the synthesis of macrocyclic complexes and studying their interactions with biomolecules. Apart from chemistry, I am interested in learning foreign languages, especially French. My other hobbies include reading, hiking and baking sweets.

Alexander A. Kamnev [1,2]

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Microbial reduction of selenite with the formation of Se(0) nano-structures

ABSTRACT

Microbial transformation of soluble toxic selenium oxyanions is widespread; Se(0) nano-structures (SeNS) are the main products. Such biogenic nano-sized Se(0) particles have wide applications in nanobiotechnology, food and medical industry, etc. Studying the bioreduction in situ (in bacterial biomass) is challenging; much information can be obtained using Raman spectroscopy sensitive to the chemistry and allotropic states of SeNS [1]. For luminous photobacteria, selenite also influences their bioluminescence [2], which can be used as a toxicity test, while selenite bioreduction to Se(0) is a way to detoxify it [1, 2]. In this talk, examples of these processes will be illustrated and discussed. (Supported by grant # 26-14-20001 from the Russian Science Foundation and Krasnoyarsk Regional Fund of Science, Krasnoyarsk, Russia.)

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Keywords: soil bacteria, photobacteria, selenium oxyanions, Se nanoparticles, biospectroscopy

BIOGRAPHY

Prof. Kamnev graduated with a MS in chemistry from Saratov State University (SSU), Russia (1980). He studied physicochemical and electrochemical properties of 3d-metal hydroxides in alkaline media at SSU and received his Cand.Sci./PhD in 1992 from SSU. In 1992, he moved to the title Institute (Russian Academy of Sciences, Saratov), and since then he has been leading scientific projects at the Laboratory of Biochemistry, developing molecular spectroscopic approaches in biochemistry/microbiology. In 2002, he obtained a DSc in physical chemistry from SSU. He has published over 140 articles in SCI(E)/Scopus journals, serving also in Editorial/Advisory Boards of three international journals (of quartiles Q1).

Day 02

Keynote Presentations

Ernst Wagner

Ludwig-Maximilians-Universität (LMU),
Pharmaceutical Biotechnology, Munich, Germany

Chamaeleon Nanocarriers for RNA Delivery and Genome Editing

ABSTRACT

Improved and targeted delivery of RNA drugs remains a key requirement. Our lab focuses on a bio-inspired chemical evolution strategy. We incorporate artificial amino acids such as tetraethylene pentamino succinic acid (Stp) or lipo amino fatty acids (LAF) into xenopeptide (XP) libraries. These sequence-defined libraries are subjected to a 'Chemical evolution' process tailored for a specific delivery application, enabling identification of new RNA carriers. Refinement of carriers is supported by molecular dynamics and machine learning. Several rounds of chemical evolution identified double pH-responsive LAF-XPs as small molecules that can be assembled in few (4-8) simple coupling steps into different topologies (U-shapes, Bundles) and display outstanding RNA delivery, even in full serum and at very low mRNA dose (activity at only ~2 nanoparticles/cell). Enhanced escape out of intracellular acidic vesicles (endosomes) into the cytosol turned out to be the key delivery advantage. The effect is based on two separate molecular aspects: i) depending on the carrier topologies, formation of novel fusogenic lipid phases (as analyzed by SAXS); and ii) a drastic pH-dependent distribution from lipid phase (at physiological pH) to lipid/water interface (at endosomal pH), as analyzed by change in logD (octanol/water) and supported by molecular dynamics. The pH-dependent polarity of LAF units is implemented by a central tertiary amine within the lipidic domain, which upon protonation disrupts the hydrophobic character. Applications include mRNA expression upon systemic administration, in vivo gene silencing by siRNA LNPs with superior activity in liver endothelial cells or, with PEG-cRGDfk targeting coat, in tumor endothelial cells. Potent carriers for CRISPER Cas9/sgRNA trigger genome editing in cell culture and in vivo in muscle and brain.

Keywords: Cas9, genome editing, LNP, mRNA, polyplex, targeted delivery

BIOGRAPHY

Prof. Ernst Wagner is Chair of Pharmaceutical Biotechnology, Department Pharmacy, LMU Munich (since 2001). He was Director Cancer Vaccines, Boehringer Ingelheim 1992-2001 (world-wide first polymer-based gene therapy in 1994), 1987-1995 Group Leader at IMP Vienna and VUB, 1985-1987 postdoc at ETH Zurich, 1985 PhD in chemistry (TU Vienna, Austria). He is Academician of European Academy of Sciences, Controlled Release Society College of Fellows, Honorary Professor at Sichuan U. He authored 527 publications, with ≥ 55 800 citations, h-index 119 (GS). Under his supervision 105 doctoral students graduated successfully, and 20 academics under his former received a professorship.

Bin FEI [a], Xin HU, Wei CAI

A School of Fashion and Textiles,
Hong Kong Polytechnic University, Hong Kong, China

Environmental Photonic Energy Manipulation with Fire Safety Coatings

ABSTRACT

Through incorporating thermochromic microcapsules, boron nitride nanosheets and montmorillonite nanosheets, an advanced polyurea-based composite coating was fabricated. The chameleon-inspired color change and admirable IR emissivity were achieved in the composite coatings, which adaptively adjusted the solar absorption and reflection in daytime while enabling radiative cooling throughout the day. The montmorillonite and BN nanosheets formed a ceramic protective layer and suppressed combustion behavior of polyurea coatings. In this work, we firstly introduced Si-O and B-O bonds onto the surface of thermochromic microcapsules (TCMs) to decrease their fire hazards, by synthesizing a Si/B-containing shell. Then, we further combined BN and montmorillonite (MMT) nanosheets with polyurea (PUA) resin to prepare flame-retardant composite coatings, by a solvent-free approach. Such designed composite coatings would spontaneously adjust their absorption and reflection of solar light upon the critical change of environment temperature. Meanwhile, the synergistic effect of BN and MMT nanosheets can suppress the fire hazards of PUA coating. More importantly, it is expected that the hydroxyl group of MMT nanosheets and the amino group of BN nanosheets, as well as the carbamido group of PUA molecule will affect the C─O─C bonds to increase the dipole moment, and support more IR emission [1,2]. After all, the integration of chameleon-inspired, dipole moment-increasing, and fireretardant strategies significantly promotes the practical application of radiative cooling coating [3], by meeting the aesthetic demand, admirable IR emissivity, and high fire safety.

Keywords: flame retardancy, IR emissivity, radiative cooling, thermochromic coating

BIOGRAPHY

Prof. Bin FEI obtained BSc (1996) from the University of Science & Technology of China and PhD (2003) from the Changchun Institute of Applied Chemistry, Chinese Academy of Sciences. After postdoctoral researches, he joined ITC of PolyU in 2010, and became full Professor in 2023. His current research interests fall in functional fashion and smart yarn, regenerative biomaterial and green nanotechnology, biomimic catalysis and sustainable energy.

Day 02

Oral Presentations

Nezihe Ayas

Eskisehir Technical University, Iki Eylul Campus,
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26555, ESKISEHIR/TURKEY

Biomass as Both Feedstock and Functional Material for Hydrogen Production: A Dual Role in Sustainable Energy

ABSTRACT

Efficient hydrogen production from renewable resources requires catalytic routes capable of converting biomass derivatives and waste feedstocks into hydrogen-rich gas, as well as low-cost materials capable of supporting the downstream steps of conversion, storage, and carbon management. Biomass can contribute to both fronts, serving as a renewable feedstock to be catalytically upgraded into hydrogen-rich gas and as a precursor for the functional materials that enable the wider hydrogen chain. Both roles are addressed here within a single research framework on sustainable energy.

The work on the production side spans the full hydrogen chain, from feedstock conversion through gas upgrading to end-use. Catalytic steam reforming, gasification, and supercritical water gasification have been investigated for a range of renewable inputs, including model bio-oil oxygenates, ethanol, microalgae oil, and agricultural residues. Catalyst development has centered on transition metals such as Ni and Co, often combined with promoters such as La, on natural mineral and engineered oxide supports. Within this framework, acetic acid steam reforming has served as a particularly informative model reaction for bio-oil valorization, providing a benchmark against which the same catalyst-design principles can be evaluated across other feedstocks. Downstream of these reforming and gasification steps, complementary studies on CO2 capture by biomass-derived activated carbons and MOFs address gas purification, while work on alkaline water electrolysis, PEM fuel cell electrocatalysis, and electrochemical hydrogen storage closes the chain at the conversion and end-use stages.

In parallel, biomass is used not only as a feedstock but as a source of functional materials within hydrogen production and conversion systems. Recent work in this direction includes the development of biomass-derived composite membranes from banana peel, incorporated into a polysulfone matrix as a low-cost alternative to commercial Zirfon® for alkaline water electrolysis, where the bio-derived membranes showed improvement in ionic transport performance over the commercial reference. This direction extends biomass valorization beyond hydrogen generation, into the materials that make up the surrounding production and conversion infrastructure.

ABSTRACT

Taken together, these studies position biomass as a chemically diverse platform that supports both sides of the hydrogen chain, linking catalytic conversion of renewable feedstocks with the design of bio-derived functional materials for sustainable energy systems.

BIOGRAPHY

Prof. Dr. Nezihe Ayas is a distinguished academic and researcher in Chemical Engineering at Eskişehir Technical University, Türkiye. Her research interests encompass hydrogen energy, fuel cells, renewable energy, biomass conversion, biofuels, gasification, catalytic processes, and sustainable energy technologies. She has made significant contributions to scientific research through numerous publications and academic projects, particularly in the development of sustainable approaches for energy production and biomass valorization. Prof. Ayas is actively involved in postgraduate education and research, contributing to the advancement of innovative and environmentally sustainable chemical engineering technologies.

Pedro Silva
Lumar Metals, Austria

Analysis of a Supersonic Nozzle System Effect in Gas-Cooled Lances on Slag Splashing Parameters

ABSTRACT

The paper is devoted to the analysis of a supersonic nozzle system effect in a gas-cooled lances on the technological parameters of slag splashing in an oxygen converter. Simulation calculations were carried out taking into account the parameters of nozzles used in the technological lines of the converter steel plants in Ukraine and Brazil. The problems were solved in several stages. The simulation results of the first stage revealed the influence of different nozzle diameters dcr, dex and inlet pressure before nozzle P0 on the nitrogen consumption per one nozzle Vн. There were also presented results of calculations showing the influence of critical dcr and output dex of nozzle diameter and nitrogen flow through one nozzle Vн on the power of injected nitrogen N1 and the depth of penetration of the stream hx into the liquid slag. The second stage was dedicated to numerical simulation of the slag splashing process, including an array of results for the first stage. The thermodynamic and physical parameters were calculated using our own computer program, whereas 3D simulations were conducted using the ANSYS Fluent program.

Keywords: numerical modelling; recycling of waste material; supersonic jets; thermodynamic parameters of splashing; optimization of process

BIOGRAPHY

Dr. Pedro Silva is a materials engineering professional and researcher with more than 15 years of international experience in metallurgy, materials science, and industrial technology. He holds a PhD in Materials Engineering from the Max Planck Institute for Iron Research in Germany, where his research focused on interface characterization, mechanical properties, and chemical interdiffusion in advanced steel materials. Currently associated with Lumar Metals in Vienna, Austria, Dr. Silva contributes to the development of innovative technological solutions for the steelmaking industry. His expertise spans advanced materials characterization, steel processing, industrial innovation, and sustainable metallurgical technologies.

Nan Yao

Princeton Materials Institute, PrincetonUniversity, Princeton, New Jersey, 08540, USA

Seeing the Unseen:Decoding Atomic Adsorption, Nucleation, and Electronic Structure with Functionalized Scanning Probe Microscopy

ABSTRACT

Recent improvements in scanning tunneling microscopy (STM) and non-contact atomic force microscopy (NC-AFM) allow us to study surface structures, molecule adsorption, and electronic stateswith exceptional clarity.This study combinesexperiments and theoryusing CO-functionalized AFM tips on qPlus sensors to investigate key processes that affect molecular adsorption, ice nucleation, and electronic structure on metal surfaces.

We first reveal that CO adsorption on Cu(111) saturates at ~26%, well below the 33% expected for the √3×√3R30° structure, independent of dosing and deposition temperature, indicating an intrinsic thermodynamic constraint. Statistical analysisand first-principles calculations show that nanometer-scale, substrate-mediated interactions (~5.3 nm), arising from surface-state electron confinement and elastic strain,suppress higher coverageand enforce a self-limiting adsorbate density.

Next, we demonstrated that CO-tip AFM can distinguish individual transition-metal atoms in molecular structures. Fe and Co atoms in metal phthalocyanines show different imaging contrasts and force signatures, indicating variations in orbital occupation above them.

Third, we demonstrate the presence of a commonwater cluster on both hydrophilic Pt(111) and hydrophobic Cu(111) surfaces, thereby observing the onset of ice nucleation. We identified a critical nucleus of 15 water molecules, with growth patterns that depend on surface properties.

In summary, these findings highlight how CO-functionalized scanning probe microscopy can reveal important interactions, structural details, and electronic properties that influence surface chemistry and phase changes at the atomic level.

BIOGRAPHY

Prof. Nan Yao is Professor of the Practice at the Princeton Materials Institute, Princeton University, USA, and the founding Director of Princeton's Imaging and Analysis Center. He is an internationally recognized expert in materials characterization, advanced microscopy, nanomaterials, and complex materials. His research integrates advanced imaging, diffraction, spectroscopy, in-situ techniques, and computational modeling to investigate materials at the atomic and nanoscale levels. Prof. Yao has authored more than 340 scientific publications and two books, and has contributed to landmark discoveries including the first natural quasicrystal. He is a Fellow of the AAAS, Materials Research Society, Microscopy Society of America, and Royal Microscopical Society.

N. Funda Ak Azem

Dokuz Eylül University, Faculty of Engineering, Department of Metallurgical and Materials Engineering, Buca, 35390, Izmir, Türkiye

Dokuz Eylül University, The Graduate School of Natural and Applied Sciences, Department of Nanoscience and Nanoengineering, Buca, 35390, Izmir, Türkiye

Design Strategies for Doping Metal Oxide Nanomaterials for Enhanced Photocatalytic Performance

ABSTRACT

Photocatalytic metal oxide nanomaterials have attracted significant attention for environmental remediation and sustainable energy applications because of their chemical stability, non-toxicity, and strong photocatalytic potential. However, their practical efficiency is often limited by wide band gaps, insufficient visible-light absorption, and rapid electron-hole recombination. This keynote highlights doping and codoping as strategic approaches for overcoming these limitations and advancing visible-light-responsive photocatalytic nanomaterials. Particular emphasis is placed on how dopant engineering modifies the structural, electronic, and surface properties of metal oxides to improve photocatalytic activity. Doping introduces defect states and alters electronic structures, enabling band-gap narrowing, enhanced light absorption, oxygen vacancy formation, and improved charge carrier dynamics. Nevertheless, single dopant incorporation may also generate recombination centers that restrict photocatalytic efficiency. Consequently, codoping has emerged as a more effective strategy because the simultaneous incorporation of multiple dopants creates synergistic interactions that stabilize defect states, promote efficient charge separation, and optimize surface reaction pathways. Recent studies employing controlled sol-gel synthesis demonstrate that codoping frameworks can systematically regulate dopant concentrations, leading to developed nanostructures with enhanced visible-light responsiveness and accelerated photocatalytic degradation of organic pollutants. Characterization techniques, including XRD, SEM, FTIR, XPS, UV–Vis, and photoluminescence analyses, reveal the direct relationship between defect engineering and photocatalytic performance. Overall, this keynote demonstrates how the transition from conventional doping to synergistic codoping establishes a robust framework for designing next-generation metal oxide nanomaterials for sustainable environmental and energy-related applications.

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BIOGRAPHY

Funda Ak Azem received her Ph.D. in Metallurgical and Materials Engineering from Dokuz Eylul University in 2008. She began her academic career as a research assistant in 1999 and was promoted to associate professor in 2023. Her research focuses on semiconductor and metal oxide nanomaterials for photocatalytic, optical, and biosensing applications, as well as carbon-based nanomaterials, biomaterials, and corrosion science. Her work emphasizes the design of advanced nanostructures through doping, defect engineering, and morphology control to enhance functional performance in environmental and energy-related applications.

Mihaela Baibarac* and M. Cercel, A. Nila, A. Udrescu, C. Bartha, C. Negrila

National Institute of Materials Physics, Magurele, Romania

Composites based on reduced graphene oxide and polydiphenylamine doped with heteropolyanions for energy storage applications

ABSTRACT

The synthesis of hybrid nanomaterials that unite conducting polymers with redox-active inorganic units and carbon-based nanostructures has become a central strategy for improving next-generation energy-storage technologies. This work examines how nanocomposites built from polydiphenylamine (PDPA), heteropolyanions, and reduced graphene oxide (rGO) evolve in terms of structure and electrochemical behavior, aiming to clarify how rGO influences charge-transfer dynamics within these systems. Expanding upon earlier investigations of PDPA–heteropolyanion materials, the present study incorporates rGO into the hybrid framework and employs spectroscopic and electrochemical analyses to uncover the resulting interfacial phenomena. The addition of rGO introduces new interaction pathways at the nanoscale, altering charge-distribution processes and modifying the redox characteristics of the polymer–inorganic network. Distinct spectroscopic features reveal how PDPA, heteropolyanions, and rGO interact and organize, offering insight into the mechanisms governing electron mobility and interfacial coupling. By correlating morphological features with electronic and electrochemical responses, the study identifies synergistic effects that enhance capacitive performance and improve long-term cycling stability. These findings demonstrate that PDPA-based hybrids containing rGO can serve as active materials for energy-storage applications and emphasize the critical role of engineered interfaces in the development of advanced polymer-derived nanostructures.

Keywords: conducting polymer, reduced graphene oxide, optical properties, energy storage

BIOGRAPHY

Dr. Mihaela Baibarac is a senior researcher at the National Institute of Materials Physics, specializing in advanced nanomaterials, optical techniques, and interfacial electrochemistry. Her work focuses on the design and characterization of hybrid polymer-inorganic systems for energy storage. She is the author of over 200 scientific papers, has contributed to multiple national and international research projects, and holds several patents in the field of functional materials. Her research integrates optical spectroscopy, electrochemistry, and carbon nanostructured materials to develop high-performance energy platforms. She is also a supervisor of PhD students, contributing to the development of the next generation of scientists.

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Targeted Radiopharmaceutical Therapy: Advances, Investment Dynamics, and Future Directions—Part 1

ABSTRACT

Radiopharmaceuticals have emerged as a transformative modality in precision oncology, with growing potential in non-oncologic indications, such as severe autoimmune diseases and rheumatology, because of their capacity for targeted therapeutic delivery. As radiopharmaceutical therapy continues to evolve, advancements in radiochemistry, radionuclide production, and clinical applications are reshaping the field. This article is the first of a 2-part series, offering a comprehensive analysis of recent developments in radiopharmaceutical therapy, examining both scientific innovations and investment trends that are driving industry growth. The paper outlines emerging trends, success factors, and strategic considerations from an investment perspective. Venture capital and strategic investors are reshaping the competitive landscape and enabling innovation. Supply chains, production capacity, and clinical trial infrastructure are key to scalability. As the field matures, aligning innovation, commercialization, and regulation is critical. Radiopharmaceuticals face executional challenges but offer significant opportunities for investors, patients, and health systems.

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Turning Agricultural Waste into Functional Membranes: Banana Peel-Based Materials for Hydrogen Production via Alkaline Water Electrolysis

ABSTRACT

This study presents the development of a sustainable, low-cost composite membrane for hydrogen production via alkalinewater electrolysis usingbanana peel (BP) as a biomass-derived additive. The membranes were synthesized using polysulfone and polyvinylpyrrolidone (PVP) in N,N-dimethylacetamide, incorporating ground BP particles (<112µm) at varying loadings to evaluate their influence on membrane structure, transport properties, and electrochemical performance. A systematic investigation was conducted by varying BP content (0.1-0.4 g and up to 40 wt.% relative to PVP), while maintaining constant polymer composition. Structural and morphological characteristics were analyzed using FTIR and SEM, confirming successful incorporation of BP and its role in modifying pore structure. Electrochemical performance was assessed through electrolysis testing by measuring cell voltage and current and electrochemical impedance spectroscopy (EIS). The results demonstrated that BP incorporation does not prohibit ionic transport and membrane performance. Optimized membranes exhibited charge transfer resistance as low as 0.27-0.28 Ω, compared to 1.05-1.10 Ω for the commercial Zirfon® membrane, corresponding to a 70-75% improvement in ionic conductivity. Additionally, membranes with lower BP loading achieved electrolysis performance comparable to commercial membranes under identical conditions. Overall, this work highlights the potential of agricultural waste-derived materials as functional membrane additives, offering a sustainable pathway for enhancing alkaline water electrolysis systems and advancing green hydrogen production technologies.

Keywords: Hydrogen, Alkaline WaterElectrolysis, Membrane, Sustainability

BIOGRAPHY

Şehnaz GENÇ is a PhD candidate and research assistant in Chemical Engineering at Eskişehir Technical University. She holds a B.Sc. degree from Middle East Technical University. Her research focuses on hydrogen production via alkaline water electrolysis, membrane development, and adsorption-based gas separation. Her work combines experimental studies with process modeling for sustainable energy applications.

Thomas Skurk

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Coffee Beyond Caffeine: Human Pharmacokinetics of Coffee-Specific Biomarkers and Their Association with Acute Immunomodulatory Responses

ABSTRACT

Coffee consumption has consistently been associated with a lower risk of cardiometabolic diseases, yet the biological mechanisms responsible for these benefits remain incompletely understood. Our work combines findings from two randomized human intervention studies investigating both the biological activity and the pharmacokinetics of coffee-specific compounds. In a randomized crossover trial, healthy volunteers received coffee, an aqueous caffeine solution, or water. Serial blood sampling demonstrated that coffee and caffeine differentially modulated circulating cytokines. Pure caffeine induced a stronger suppression of several pro-inflammatory cytokines, whereas coffee produced a distinct immune response, indicating that the coffee matrix substantially modifies caffeine-mediated effects. These findings provide novel evidence that bioactive compounds beyond caffeine contribute to the acute immunological effects of coffee.

In a complementary intervention study, targeted UHPLC-MS/MS analysis characterized the pharmacokinetics of coffee-derived atractyligenin metabolites. Atractyligenin and its 19-O-β-D-glucuronide were rapidly absorbed, remained detectable in plasma for up to 24 hours, and proved to be robust biomarkers of Arabica coffee intake independent of brewing method. These biomarkers offer objective tools for assessing coffee exposure in nutritional and epidemiological studies.

Our research demonstrates that coffee exerts biological effects extending beyond caffeine alone while providing validated biomarkers for objective exposure assessment. Combining pharmacokinetic profiling with functional immune phenotyping contributes to a more comprehensive mechanistic understanding of the health effects associated with habitual coffee consumption.

Keywords: Coffee, caffeine, atractyligenin, biomarkers, immunomodulation, pharmacokinetics

BIOGRAPHY

Thomas Skurk is Professor of Nutritional Medicine and Head of the Core Facility Human Studies at the ZIEL Institute for Food & Health, Technical University of Munich (TUM), Germany. His research focuses on human nutrition, metabolic diseases, and clinical nutrition, with particular emphasis on diabetes, obesity, and precision nutrition. He leads translational human intervention studies integrating advanced metabolic phenotyping, biomarkers, and nutritional interventions to investigate diet–health interactions. Prof. Skurk studied medicine at the Universities of Regensburg and Würzburg and completed his habilitation in Nutritional Medicine at TUM. He has authored more than 350 scientific publications and serves on several national expert committees in nutritional medicine.

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From Material Characterization to System-Level Performance Prediction

ABSTRACT

A persistent challenge in materials development is the limited ability of conventional characterization methods to predict performance under realistic service conditions. While intrinsic material properties can be measured with high precision, the actual performance of materials and functional coatings is strongly influenced by interactions occurring within the complete tribological system.

This work presents application-oriented experimental tribology as a methodology for bridging the gap between laboratory characterization and field performance. Modern tribological test systems enable the simulation of realistic operating conditions through flexible motion configurations and time-dependent control of key parameters such as load, temperature, speed, acceleration, lubrication state, and environmental media.

A key aspect is the shift from evaluating individual materials towards characterizing complete tribological systems. This approach captures the interactions between materials, counter bodies, lubricants, and environmental influences that ultimately govern application performance. Consequently, tribological system testing provides more relevant information for material selection and optimization than isolated material characterization alone.

System responses are monitored using multiple in-situ measurement channels, including friction force, electrical contact resistance, acoustic emission, temperature, and displacement signals. These data support both rapid ranking of material concepts during early-stage screening and deeper understanding of degradation and failure mechanisms through analysis of time-resolved responses. Complementary post-test methods such as microscopy and surface spectroscopy further enable the correlation of observed system behavior with material modifications and wear processes.

The presented approach positions experimental tribology as a predictive development and qualification tool that supports accelerated materials innovation, reduces uncertainty regarding field performance, and enables more informed decisions during the development of advanced materials and functional coatings.

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Keywords: Tribology, Tribotesting under extreme conditions

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- since 2025, Lead Applied Tribology Testing & Method Development

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Tissueclearing of whole organs: A challenge for chemistry

ABSTRACT

Since the first chemical clearing of a mouse brain (Dodt et al., Nature Methods, 2007), tissue clearing has grown exponentially as a method for investigating the three-dimensional and anatomy of organs in small animalssuch as mice and zebrafish. The technique enablesthe imaging of intact organsin their entirety using light-sheet microscopy combined with fluorescence labelling of structures of interest. However, attempts to render brains of larger animals fully transparent have so far been reportedonly sporadically, and primarily for rat brains. Extending these investigations to larger species — with the ultimate goal of clearingand imaging human brains (Oakes-Klein et al., Communications Biology, 2026) in three dimensions — would therefore represent a significant advance.

To this end, we have substantially improved our clearing technology and can now routinely produce optically transparent whole pig brains. Our approach relies predominantly on chemical methods; yet neither our group nor the vast majority of researchers active in the clearing field have a formal background in chemistry. Engaging chemists in this area would therefore be highly beneficial. A precise, chemically informed elucidation of human organs in 3D at cellular resolution holds the potential for breakthroughs in both fundamental research and clinical applications.

Dodt, H.-U., et al. (2007). Ultramicroscopy: three-dimensional visualization of neuronal networks in the whole mouse brain. Nature Methods, 4, 331–336.

Oakes-Klein, et al. (2026).activeDISCO enables large-scale exploration of human brain anatomyby light sheet microscopy. Communications Biology, doi: 10.1038/s42003-026-09935

Virtual Presentations

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Probing non-covalent interactions within π-π stacking assembly by EPR Spectroscopy

ABSTRACT

π-π stacking interactions play a fundamental importance for the further development of supramolecular chemistry, materials science and tuning and prediction of the crystal structures by controlling self-assembly and molecular recognition. however, the nature of π-π stacking interactions remains unclear. In order to elucidate the insight, Electron Paramagnetic Resonance (EPR) measurement was carried out to investigate the insight of the interactions within π-π stacking assembly. Carbon nanotubes (CNTs) exhibit extended π electron clouds, while the phenyl rings in the polyimide (PI) show localized π electrons. Since the introduction of CNT into aromatic PIs is accompanied by the recombination or movement of unpaired electron, EPR should be a powerful method for probing the paramagnetic products of the introduction of CNT into polyimides process. EPR measurement results indicate that the resonance line parameters of g = 2.003±0.001 and peak-to-peak linewidth lpp = 7 ± 1 G is generated for the polyimide films. Polyimide samples with CNT have a second resonance at slightly larger magnetic field values and has a g = 2.008 ± 0.001. Neat PI displays a symmetrical and relatively higher intensity EPR signal in comparison to CNT/PI nanocomposites. Intensity ratio of PI central resonance aroused by aromatic group of PI between the neat PI and CNT/PI nanocomposites indicating that these paramagnetic centers are influenced by the electronic structure of CNT surface. Compared with neat PI nanocomposites, CNT/PI nanocomposites show almost less than one third of intensity at the central PI resonance, which indicates a decreased generation of unpaired electrons originated from imide group in the presence of CNT. The findings are significant to elucidate the nature of non-covalent interactions within π-π stacking assembly.

Keywords: Non-covalent interactions, π-π stacking, EPR, Carbon nanotubes, Polyimides

BIOGRAPHY

I hold PhD at 2013 from Harbin Institute of Technology (one of top nine C9 League of Chinese Universities). In 2016, I was affiliated with the school of mathematics and physics of University of Freiburg as a Post doctor; Currently, I am working at Liaoning petrochemical University as a professor. Research interests focus at non-covalent interactions, nanomaterial construction, polymer science and composite materials

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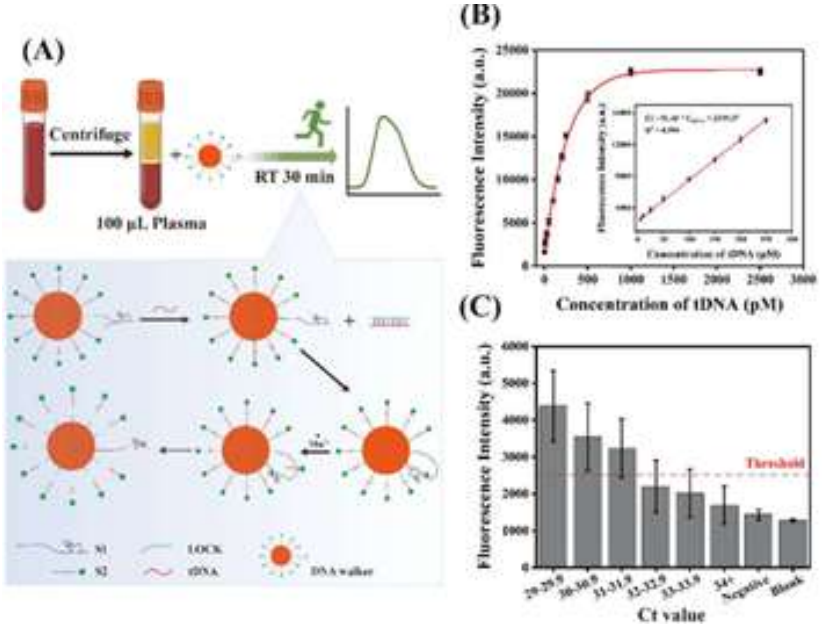
A robust DNA walker for simplified, rapid and sensitive detection of HBV DNA in blood donors

ABSTRACT

Background: Although preventive vaccine is available, HBV infection continues to be a global health challenge, especially in rapid and accurate screening in resource-limited regions due to underdeveloped infrastructures.

Aim: This study aimed to address the pressing need for efficient and user-friendly diagnostic technologies in resource-limited regions as a point-of-care testing (POCT).

Method: We developed a self-powered DNA walker system integrating AuNPs and DNA strands for direct detection of HBV DNA in the blood.



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The lock strand (LOCK) was first hybridized with the walking strand (S1) to a S1-LOCK duplex, which blocked the DNAzyme activity on S1. Then the S1-LOCK and fluorophore-labeled substrate strand (S2) were modified onto AuNP surfaces, constructed a DNA walker system. Upon the target HBV DNA (tDNA) presence, strand displacement reactions between tDNA and S1-LOCK were triggered to release DNAzyme, which subsequently mediated cleavage of S2 with Mn2+ cofactors autonomously and progressively, generating amplified fluorescent signals.

Figure 1. (A)Principle of HBV DNA detection by DNA walker in the plasma. (B) Response fluorescence intensity at series concentrations of target. Inset: Linear calibration range (5–250 PM). (C) Clinical performance evaluation using HBV DNA-positive (n=22) and negative (n=3) plasma samples.

Result: This DNA walker system enabled rapid detection within 30 minutes at room temperature, demonstrating a sensitivi- ty of 3.6 PM with a linear range of 5-250 pM (R2 = 0.999, Fig. 1B). Clinical validation using 22 HBsAg-/HBV DNA+ (OBI) plasma samples from blood donors revealed a strong negative correlation (r = -0.86) between fluores- cence signals and qPCR Ct values, with a detection limit of Ct <32 (approximately 20,000 IU/mL, Fig. 1C), that con- sistent with the WHO-recommended viral load threshold for initiating nucleos(t)ide analogue therapy.

Cited this work: Lai R, et al. A robust DNA walker for simplified, rapid, and sensitive detection of HBV DNA in blood. Mikrochim Acta. 2025;192(7):422. Published 2025 Jun 13.

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A Projection-Based Framework for Chemical Kinetics, Thermodynamics, and Molecular Organization

ABSTRACT

Chemical kinetics, thermodynamics, and biochemical organization are traditionally treated as distinct layers of chemical science, each described using its own set of empirical laws and models. While these approaches are highly successful, a unified conceptual framework connecting microscopic molecular dynamics to observable chemical behavior remains incomplete.

In this work, I propose a projection-based framework for chemical and biochemical systems, in which observable quantities such as reaction rates, activation barriers, free energy, and equilibrium states are interpreted as context-dependent manifestations of underlying molecular processes. Within this perspective, reaction rates correspond to effective fluxes between observable states, activation barriers reflect constraints on accessible pathways, and thermodynamic quantities describe the structure of accessible configurations under given environmental and experimental conditions.

The framework provides a unified interpretation of classical chemical concepts, including Arrhenius and non-Arrhenius kinetics, transition state theory, tunneling effects, enzyme catalysis, stochastic kinetics, master equation approaches, diffusion, solvent effects, and nonequilibrium irreversibility, without modifying established physical laws. Reaction networks are described as reduced representations of molecular dynamics, and entropy production is associated with changes in accessible configurations under nonequilibrium conditions.

This approach extends naturally to biochemical systems, where metabolic pathways, protein folding, membrane formation, and genetic stability emerge as structured outcomes of coupled kinetic and thermodynamic constraints. By linking chemical reactivity, transport, and biological organization within a single conceptual structure, the framework offers a coherent perspective on how complex chemical systems arise from underlying molecular processes.

The results suggest new directions for interpreting reaction mechanisms, guiding chemical design, and understanding the transition from chemistry to biology.

Keywords: Chemical kinetics, Thermodynamics, Reaction mechanisms, Nonequilibrium systems, Molecular transport, Biochemical systems

BIOGRAPHY

Abhishek Bansal is an independent consultant, researcher, and amateur scholar whose recent work reflects over 20 years of fully self-funded, self-directed research. He has proposed novel B-Equations and related engineering frameworks for impedance analysis, transformers, inverters, generators, pumps, solar systems, machinery, turbines, batteries, SMPS, and short-circuit analysis. In biomedical science, he has formally claimed Novel Bansal-NonLinear Theory and Novel Bansal-Biology Theory with nine frameworks, including B-Phy, B-Chem, B-Disease, B-Pharma, B-AI, and B-Prosthetics. He has developed free BVidAL Clinical Software Suite(beta version) and BVidAL RTOS (Real Time Operating System) for biomedical analysis, simulation, imaging, signals, and medical-device research.

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Molecular mechanism of sesamol in inflammatory bowel disease: Integrative computational, microbiome, and biological evaluation targeting jak1 pathway

ABSTRACT

Inflammatory bowel disease (IBD) is a chronic inflammatory disorder driven by impaired intestinal barrier function, gut dysbiosis, immune dysregulation, and oxidative stress. The JAK-STAT signalling pathway plays a central role in promoting pro-inflammatory cytokine responses in IBD. This study aimed to comprehensively elucidate the therapeutic potential of sesamol, a natural lignan with potent antioxidant and anti-inflammatory properties, through an integrative computational, microbiological, and biological approach. Potential sesamol-associated targets were identified using network pharmacology and protein-protein interaction analysis. Gene Ontology and KEGG pathway enrichment analyses highlighted the significance of JAK-STAT signalling. Molecular docking, molecular dynamics simulations, and MM-GBSA binding free energy calculations (Schrödinger V14.1.38) demonstrated that sesamol exhibits strong binding affinity towards JAK1, forming a highly stable complex compared to JAK2. In vivo validation was performed using the dextran sulfate sodium (DSS)-induced micex colitis model. Sesamol treatment significantly ameliorated clinical symptoms, reduced inflammatory cytokine levels, normalized elevated JAK1 expression in colonic tissue, and restored intestinal barrier integrity. Additionally, 16S rRNA sequencing revealed that sesamol effectively modulated the gut microbiome by increasing beneficial genera such as Lactobacillus and Bifidobacterium, decreasing pathogenic taxa, and improving microbial diversity, thereby reversing dysbiosis. These findings collectively demonstrate that sesamol exerts multi-target protective effects in IBD by inhibiting JAK-STAT signalling, reducing inflammation and oxidative stress, restoring gut barrier function, and positively modulating the intestinal microbiome. Sesamol emerges as a promising natural multi-target candidate for IBD management.

Keywords: Sesamol, Inflammatory bowel disease, JAK1, Network pharmacology, Gut microbiome, Molecular dynamics

BIOGRAPHY

Krishnendu P R is a Research Scholar in the Department of Pharmaceutical Chemistry at Amrita School of Pharmacy, Amrita Viswa Vidyapeetham, Kochi. Her research interests include medicinal chemistry, natural compounds, prodrug design, and computational drug discovery. Currently, she is focused on the computational and experimental evaluation of natural compounds for the management of inflammatory bowel disease, with emphasis on JAK-STAT signalling and gut microbiome modulation. She has expertise in network pharmacology, molecular modelling, and in vivo disease models.

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First-principles theoretical study of adsorption properties of heavy and superheavy elements and their compounds on selected surfaces

ABSTRACT

Gold and Quartz are materials coating detectors that are used in the preparation of superheavy elements in so-called atom-at-a-time experiments. Within them, synthesized atoms and their possibly formed molecules adsorb onto the surface, and experimentalists estimate their adsorption enthalpy. In my online talk, I give a review of several first-principles theoretical studies on the adsorption properties of heavy and superheavy elements and their compounds on the above-mentioned surfaces. Such predicted results provide assistance to experimentalists concerning the identification of adsorbed species. The main computational apparatus was the relativistic periodic DFT, as implemented within the AMS BAND program suite. To name a few of our studies, in [1], we investigated the adsorption properties of group 1 and 2 elements Cs, Fr, E119, Ba, Sr, and E120, as well as group 1 hydrides and hydroxides on hydroxylated quartz surfaces. In [2], adsorption energies, E_{ads}, of a superheavy element (SHE), Lv, and its lighter homologue, Po, as well as those of their oxides, hydrides, and hydroxides, on hydroxylated quartz surfacesare calculated. It was shown that elemental Po and Lv should be the most volatile out of all the considered species over the quartz surface, with Eads on the order of van der Waals bond energies. Likewise, in [3], E_{ads} of oxides and oxyhydrides of the superheavy element Ts and its lighter homologue At on the gold surface are predicted and discussed.

[1] M. Iliaš, V. Pershina, Mol. Phys., 2024, https://doi.org/10.1080/00268976.2023.2293229
[2] V.Pershina, M.Iliaš, Mol.Phys., 2025, https://doi.org/10.1080/00268976.2025.2573831
[3] A. Ryzhkov, V. Pershina, M. Iliaš, and V. Shabaev, Phys. Chem. Chem. Phys, 2024, https://doi.org/10.1039/D3CP05645G

Keywords: adsorption energy, surfaces, superheavy elements, theoretical predictions, DFT

BIOGRAPHY

Miroslav Iliaš (https://orcid.org/0000-0002-8038-6489) finished his PhD. studies at Comenius University Bratislava in 2002. He is working in the field of Theoretical and Computational Chemistry. His research interests are applications of computational chemistry methods for assisting experiments of superheavy elements synthesis

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Evolution stages of periodic relief on the silicon surface under ion irradiation

ABSTRACT

To date, extensive experimental and theoretical data have been accumulated regarding the formation of wavy relief on solid surfaces during ion irradiation. Most experimental works have examined the regularities of wavy relief formation and its parameters depending on the ion beam incidence angle, ion energy, and ion species. In particular, it was established that the formation of wavy relief on the surface occurs within a certain range incidence angles and upon reaching a critical fluence, the values of which differ by orders of magnitude for ions of chemically active and inert gases. The current study provides an analysis of the factors governing the nucleation and evolution of periodic structures on silicon surfaces under ion irradiation. The findings are based on a comprehensive analysis of literature data and the results of our own experiments on the formation of such structures via ion bombardment with gallium ions. This type of ion is notable because, on one hand, implanted gallium ions do not form chemical compounds with silicon atoms, so they can be treated as inert gas ions. On the other hand, these ions are present in the near-surface layer in the form of precipitates, which can be regarded as model systems for silicon-ion complexes with chemically active gas species located near the surface under oblique ion beam incidence.The experimental part of the work was carried out using scanning electron microscopy (SEM), transmission electron microscopy (TEM), and secondary ion mass spectrometry (SIMS). The formation of periodic structures in the form of wavy and terraced relief is considered within the framework of a nonlocal surface erosion model proposed by the authors of this work. The work was carried out within the framework of the state assignment to the National Research Centre “Kurchatov Institute”.

Keywords: silicon, sputtering, periodic relief, ion beam

BIOGRAPHY

Our research group investigates the underlying mechanisms and regularities of both sputtering processes and nanostructure formation on semiconductor surfaces, using a focused ion beam as the primary tool.

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Cell Membrane Cholesterol and Diseases Associated with Its Deficiency

ABSTRACT

This review considers the significance of cell membrane cholesterol for health from the perspective of cell biology. The cell of an animal organism is a unique system in which the functioning of its constituent molecules is interdependent and coordinated, and any disruption of this coordination is fatal to the cell. One example of such coordination and mutual regulation is the functioning of membrane proteins, whose activity depends on their interaction with membrane lipids. With a given genome and corresponding set of proteins, this lipid component provides a wide range of regulation of cellular functions. Cholesterol is one of the most important lipids in cell membranes, and many membrane proteins are cholesterol dependent. For effective cell function, optimal cholesterol concentration is required, and deviations from this optimal level in either direction reduce the efficiency of cell processes. We examine the role of cholesterol in microbial infections and certain other conditions in which the pathogenesis is associated with a loss of cholesterol by cells. Considering the role of cholesterol in the pathogenesis of diseases and understanding the mechanisms of interactions between cholesterol and proteins are important resources for the development of drugs that target interactions between proteins and cholesterol and normalise cholesterol-dependent cell functions.

Keywords: cell membrane, cholesterol, cholesterol-dependent proteins, diseases

BIOGRAPHY

Born in Moscow in 1952, graduated from the Biology Department of the Moscow Lomonosov State University in 1975; worked at the Belozersky Research Institute, Moscow Lomonosov State University from 1975 to 2022. Collaboration with University College London, Amsterdam University, Stuttgart University, NIH. Areas of interest: intercellular communications; gap junctions; cell membranes, cholesterol-dependent proteins and processes; Five grandchildren

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Revealing the quadrupole surface plasmon resonancein TI3C2TX multilayered maxine

ABSTRACT

MXenes have demonstrated strong potential for optoelectronic applications owing to their diverse elemental compositions and tunable structural properties. However, in the Vis-NIR part of the spectrum, the optical properties of even the most studied TI3C2TX remain only partially understood. Although the observedresonance at 1.5 eV in the absorption spectrum of single- or few-layer samples is confirmed to result from interband transitions, the case of multilayer samples requires further study. In experiments [1,2], another resonance appeared in the absorption spectrumof multilayer Mxene with lineardimensions of a few micrometers at around 1.3 eV. In [3], this resonance was attributed to quadrupole surface plasmon (QSP) oscillations arising due to the roughness of the flake surface. Consequently, in large samples with dimensions comparable to the wavelength of the incidentradiation, the charge carriers in nanoparticles experience an inhomogeneous electric field with some phaseretardation. Under these conditions, the QSP mode,as well as higher multipoles, appear as new bands in shorter wavelengths. Contrary to multilayered MXenes, in mono - and a few-layer particles, the QSP cannot be exited, since in this case, in one of the spatial dimensions, the particle size is much less than the wavelength of incident light.

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In this communication, we present experimental results (spectrophotometer in transmission mode) and COMSOL Multiphysics simulations of the absorption spectra of Ti3C2TX in the Vis-NIR range. Transmission of prepared on silica glass MXene particles of linear sizes of 1-3 μk were performed with the spectrophotometer Cary 7000 UMS. Experiments and simulations clearlydemonstrate the existence of a maximumcorresponding to QSP resonance at around 950 nm, alongside a resonance at shorter wavelengths (around 800 nm) due to interband transitions. The study advances understanding of the origin of MXene spectral resonances.

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3. M. Gonçalves et al. Interband, Surface Plasmon and Fano Resonances in Titanium Carbide(MXene) Nanoparticles in the Visible to Infrared Range, Photonics 2021, **8**, 36.

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Simulation-based prediction of fiber orientation in highly filled thermoset materialsbased on process-relevant rheological data

ABSTRACT

This studypresents the development of a simulation model for highlyfilled thermoset materialswith a focus on predicting fiber orientation under processing conditions. For the first time, the rheological properties, required for the model and highly privotal for the consistence of model and reality, were determined using a high-pressure capillary rheometer, enabling material characterization under process-relevant conditions in terms of the shear rate. This approach allows a more realistic representation of the flow behavior of highly filled thermoset material systems compared to conventional rheological measurement methods. The study was based on epoxy and phenolic resin with glass and carbon fibresas well as a filler grade between40 and 60 vol.-%. The simulation results were subsequently validated by comparing the predicted fiber orientations with the actual filler orientation measured after injection molding. Further, the filler orientation was correlated with the thermal conductivity of samples. The comparison demonstrates a good conformity between simulation and experimental observations, highlighting the capability of the proposed model to accurately describe fiber orientation in highly filled thermosets. Authors also revealed that the conformity increases in terms of displacement flow whereas mixed flow conditions in highly filler thermosets are more unlikely to be predicted precicly. The presented methodology improves the predictive qualityof fiber orientation simulations by incorporating process-near rheological data and provides a valuable tool for understanding and optimization of highly filled thermoset materials. Within the study,the a thermal conductivity of up to 2 $W \cdot m^{-1} \cdot K^{-1}$ was reached. Further,authors were able to predict the filler orientation and with that created the possibility of predicting the thermal conductivity relative to the fibre orientation.

Keywords: simulation, highly filler thermosets, fibre orientation, thermalconductivity

BIOGRAPHY

The author studiedMechanical Engineering at Friedrich-Alexander University (FAU) Erlangen–Nuremberg, earning a Bachelor’s degreein 2016 and a Master’s degreewith distinction in 2018. During this period,the author was supported by a Max Weber Programscholarship. Since 2019, the author has been a research assistant at the Institute of Polymer Technology at FAU and has headed the Processing division of the institute since 2021. The author completed a doctoral degree with distinction in 2023 and has held the positionof Academic Councillor since then. In 2024,the author became the deputy of the head of the institute.

Rayya Al Balushi and Ahsanul Haque

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Conjugated Poly-Metalla-Ynes for Opto-Electronic Applications

ABSTRACT

Conjugated polymers are an exciting class of materials with wide-ranging opto-electronic (O-E) applications. Among them, poly(aryleneethynylene)s (PAEs) are valued for their extended π-conjugation and structural rigidity. However, their luminescence is typically limited to fluorescence from singlet states. To overcome this, we introduced Pt(II) centers into the polymer backbone, forming poly(metallaynes) with enhanced spin–orbit coupling that enables efficient triplet-state emission. These Pt(II)-based polymers, often referred to as Pt-poly-ynes, exhibit near-unity phosphorescence quantum yields at low temperatures and retain strong emission at room temperature. In this talk, I will present the design, synthesis, and characterization of new conjugated Pt(II) poly(metallayne) systems. These materials are processable, thermally stable, and show promising optical properties for applications in LEDs, photocells, nonlinear optics, and display technologies. The study also offers insights into triplet-state engineering in conjugated systems, which can be extended to all-organic analogues.

Keywords: Pt(II) poly-yne, conjugated, polymer, O-E applications, poly(metallayne)s

BIOGRAPHY

Dr. Rayya Al Balushi is an Associate Professor of Chemistry and Head of the Basic and Applied Sciences Department at A'Sharqiyah University. She also chairs the university research ethics and biosafety committee. She received her Ph.D. in Chemistry from Sultan Qaboos University. Her research focuses on the design and synthesis of metalla-yne and poly(metalla-yne) materials and study their structure-property relationships for optoelectronic and catalytic applications . She has published extensively in high-impact journals and received multiple awards for excellence in research, teaching and scientific contributions.

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Effect of GO Derivatives Reinforced Nanofiber Polymeric Scaffolds on Oligodendrocytes' Maturation and Myelination

ABSTRACT

Graphene oxide (GO) and its derivatives have attracted significant attention in neural tissue engineering due to their extraordinary properties (1-5). GO derivatives may differentially regulate cellular behaviour (1, 4, 6-8), yet their comparative influence on myelination and cell proliferation within fibrous polymeric scaffolds remains insufficiently explored. This study investigates the effects of GO and two chemically reduced GO derivatives (ascorbicacid reduced/a-rGO, and hydrazine reduced/h-rGO) (7, 9, 10) incorporated into nanofiber tissue scaffolds (8, 11, 12) on human oligodendroglioma cells' maturation and myelination. Scaffolds were fabricated via electrospinning of PCL polymer reinforced with GO, a-rGO, or h-rGO nanoparticles (11-13) and evaluated using the human oligodendroglioma cell line (HOG/SCC163) (14-16). Cells were cultured in differentiation medium (14, 16) to promote oligodendrocyte maturation. The effects of GO derivatives and their concentrations on cell proliferation and myelination-related activity were assessed through Ki67 and myelin basic protein (MBP) immunostaining. Comparative analyses demonstrated that higher concentrations of GO and its derivatives generally increased MBP expression while reducing Ki67-positive cell populations, indicating enhanced cellular maturation and reduced proliferative activity. Cell viability remained above 65% in all groups. Among the tested materials, h-rGO-reinforced scaffolds exhibited the strongest MBP expression, suggesting a favorable microenvironment for myelination-related processes. GO-containing scaffolds provided the highest cell viability but showed comparatively moderate effects on MBP expression.

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In contrast, a-rGO scaffolds displayed concentration-dependent increases in MBP expression accompanied by reduced cell viability. These findings demonstrate that the reduction method and resulting properties of graphene derivatives significantly influence oligodendrocyte behavior. Tailoring the type of graphene derivative incorporated into fibrous scaffolds enables selective regulation of proliferation and myelination-associated markers, offering a promising strategy for the development of advanced neural tissue engineering platforms targeting remyelination and nerve regeneration.

Keywords: graphene oxide, reduced graphene oxide, oligodendrocyte maturation, myelination, neural regeneration

BIOGRAPHY

I am a PhD candidate in the Nanoscience and Nanoengineering Program at Istanbul Medeniyet University, Türkiye. My research focuses on neural tissue engineering, myelination, and the development of advanced biomaterials for regenerative medicine. I am currently involved in a TÜBİTAK-funded research project (project no:221Z372) investigating graphene-based biomaterials and their interactions with neural cells to promote myelination from oligodendrocytes. My work combines experimental studies with computational approaches, including molecular dynamics simulations and the modeling of inorganic nanomaterials such as polymers and GO derivative nanoparticles. My research interests include graphene oxide derivatives, biomaterial–cell interactions, myelination, and the application of nanomaterials in neural regeneration.

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Development of polyamide 6.10 composites reinforced with nickel-coated carbon fibers

ABSTRACT

The rapid development of electric vehicles and electronic systems has increased problems related to electromagnetic interference (EMI), making the development of materials with electromagnetic interference shielding (EMI shielding) capability increasingly important. The EMI shielding properties of electrically conductive materials also increase. Therefore, in this study, conductive composites were developed using nickel-coated carbon fibers (Ni-CF) as a conductive reinforcement in a PA6.10 matrix, an engineering thermoplastic known for its good mechanical properties, high chemical resistance, and partially biobased structure. The composites were produced by melt compounding in a twin-screw extruder, and test specimens were prepared via injection moulding. Composites containing 10, 20, and 30 wt.% Ni-CF were fabricated, and their morphological, thermal, mechanical, and electrical properties were investigated. Morphological micrographs revealed good interfacial compatibility between the Ni-CF and the PA6.10 matrix. Thermal analysis results indicated that although the Tdeg10 values slightly decreased with increasing Ni-CF content, the Tdeg50 values improved. In addition, the residual mass at 800 °C increased with the increasing Ni-CF content. According to the mechanical test results, the tensile strength of neat PA6.10 was 61 MPa, which increased to 82 MPa, 116 MPa, and 131 MPa for composites containing 10, 20, and 30 wt.% Ni-CF, respectively. Electrical conductivity results showed that the composite containing 10 wt.% Ni-CF exhibited semiconductive behavior with a conductivity of 1.32×10^{-2} S/cm, whereas the composites containing 20 and 30 wt.% Ni-CF reached conductivity values of 4.86 S/cm and 24.18 S/cm, respectively, indicating a transition to metallic conductive behavior. These findings demonstrate that Ni-CF reinforced PA6.10 composites are promising material alternatives for electromagnetic interference shielding applications.

Keywords: Polyamide, Nickel-Plated Carbon Fiber, EMI Shielding, Electrical Conductivity.

BIOGRAPHY

Dr. Sema Samatya Yılmaz is both a Mechanical Engineer and a Textile Engineer. She completed her master's degree in Textile Engineering and conducted project- and laboratory-based graduate research in the Màster Universitari en Enginyeria de Tecnologies de Materials Fibrosos program at Universitat Politècnica de Catalunya, Spain. She received her PhD in 2022 from the Department of Polymer Science and Technology at Kocaeli University, Türkiye. Her research interests include polymer processing, polymer blends, electrospun nanofibrous structures, wound dressings, biomedical applications, conductive nanocomposites, and active food packaging. Dr. Sema Samatya Yılmaz currently works as a lecturer at Kocaeli University.

Dr. Manfred Kircher

KADIB, Germany

Recycling Biowaste and Residuals into Chemical Products

ABSTRACT

The shift from fossil fuels to renewable carbon sources is not only a technical challenge for the chemical industry, but also raises the question of future raw material availability. Primary biomass from agriculture and forestry already contributes to the supply of raw materials for the chemical industry, but it is foreseeable that primary biomass will be limited in the long term due to demand for food and feed, energy production, and industrial uses. For this reason, biogenic residues, waste, recycled materials, and CO2 are attracting increasing attention. Processes for their utilization are currently being developed and piloted. These potential raw materials are suitable to varying degrees for different classes of chemical products (bulk, specialty, and fine chemicals). They require specific production systems in companies that can rely on adapted public infrastructure, e.g., in terms of logistics and energy supply.

The presentation will outline the current status of the raw materials transition in the chemical industry, the options for non-fossil carbon sources, and examples of the product and process pipeline. Finally, the conditions for an economically and ecologically successful raw materials transition in the chemical industry will be discussed.

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Interfaces in liquid steel processing and related effects

ABSTRACT

Iron- and steelmaking processes are running in the temperature range between 1300°C and 1700°C. In all process steps the separation of liquid and solid phases plays a crucial role besides chemical reactions. The interfacial tension is a key property for phase separation which in turn is a result of running chemical reactions, local chemical and electrochemical potentials. In situ measurements and observations as well as in laboratory experiments and in the industrial processes will be presented.

The presentation will cover following topics:

-Effect of chemical reactions on interfacial tension between liquid steel and liquid slag
On both sides of the interface high concentration gradients of all elements exists in the range of approx. 150 nm in steel and 400 nm in slag. The molar mass flow rate of oxygen through the interface decreases the interfacial tension locally down to zero.

-Interfacial flow caused by local gradients of interfacial tension
The interfacial convection always occurs under industrial process conditions and increases the mass transport in the boundary layer. The maximum flow velocity in the boundary layer in liquid slag was estimated to 25^{-3} m/s.

-Non-metallic precipitations with different mineralogical composition – behaviour in liquid steel
The behaviour of different types of precipitations was examined in situ using confocal scanning laser microscope. Alumina particles attract strongly each other and agglomerate. Particles with other mineralogical composition do not attract and agglomerate.

-Effect of chemistry and external electrical potential on interfacial tension between liquid steel and liquid slag

Effect of slag and steel chemistry – basicity and O and S activities, respectively – on interfacial tension was experimentally investigated using the drop weight method. Additionally the effect of applied external electric potential was measured. O and S have a strong effect on interfacial tension and the zero charge potential is influenced by the slag chemistry.

Keywords: liquid steel, liquid slag, interfacial tension, precipitations, electric potential

Radim Halama

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Accelerated creep/fatigue characteristics estimation using Digital Image Corelation (DIC)

ABSTRACT

Evaluating cyclic plasticity and creep characteristics of structural materials traditionally requires conducting multiple time-consuming mechanical tests. To address this, this study presents an accelerated evaluation methodology utilizing Digital Image Correlation (DIC) to estimate cyclic and creep properties from a reduced number of specimens. The primary objective is to determine the cyclic stress–strain curve (CSSC) from a single low-cycle fatigue (LCF) test and to explore accelerated creep characterization. By applying 3-D DIC measurements on specimens with varying cross-sections, such as curved or hourglass geometries, a continuous distribution of strain amplitudes is obtained along the gauge length. Evaluation is fully automated using custom Python-based tools. The methodology was validated under uniaxial, torsional, and nonproportional loading paths using additively manufactured AlSi10Mg, SS316L, and R7T railway wheel steel. Results show that the DIC-reconstructed CSSC closely matches data from conventional multi-specimen testing. However, when applying a similar approach to creep testing using the Norton power law on hourglass specimens of SAC305 and 3D printed AlSi7Mg, the minimal creep strain tended to be overestimated on lower stress levels. Consequently, while the DIC-based fatigue characterization technique provides a reliable and highly accelerated alternative to traditional testing, its application in creep is better suited for validating advanced constitutive models than direct parameter estimation.

Keywords: Digital Image Correlation, Low-cycle fatigue, Cyclic stress–strain curve, Creep testing, Additive manufacturing, Solders

BIOGRAPHY

Radim Halama is a Professor at the Department of Applied Mechanics, FME, VŠB-Technical University of Ostrava, Czech Republic. He specializes in computational and experimental mechanics, focusing on cyclic plasticity, low-cycle and multiaxial fatigue, creep, and digital image correlation. Currently, he leads the Low-Cycle Fatigue working group (WG 4.7) within the EU COST Action FABER (CA23109). He has co-authored several book chapters and numerous peer-reviewed journal articles. Additionally, he formerly served as the university's Vice-Rector for International Relations and Social Affairs, and was also responsible for industrial cooperation and technology transfer.

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Insight into structure-function of Bothrops atrox snake venom LAAO and its mechanism of action on cell apoptosis

ABSTRACT

Snakebite is a major health issue worldwide with long-lasting impairment of patient income and the quality of life. There is currently a poor understanding of the cellular mechanisms triggered by snake toxins underpinning the devastating symptoms during envenomation. LAAO is a highly toxic enzyme that oxidises L-amino acids and participates in tissue necrosis. Kinetic analyses and mechanistic studies using recombinant LAAO reveal key catalytic residues and striking cellular defects preceding cell death. LAAO wild-type increases oxidative stress levels and inhibits autophagic flux, reducing lysosome number and size. Higher mitochondrial fission indicates that LAAO impairs mitochondria dynamics and function, leading to mitophagy. However, mitochondrial clearance is prevented by the lysosomal defects. These phenotypes are accompanied by a shutdown of cell respiration and energy production. Thus, LAAO cytotoxicity targets co-ordinately the function of essential organelles and compromises cell metabolism and fitness prior to cell death. Our work highlights potential steps to reverse LAAO toxicity and facilitate adaptive cellular responses to restore homeostasis.

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Photobiomodulation with LED Does Not Alter Antibiotic Sensitivity in ATCC and Burn-Patient Bacteria

ABSTRACT

Photobiomodulation (FBM) has been used in different specialties in the health field, with an emphasis on the interaction of light with microbiology in recent years. Represented by Laser and LED (Light Emitting Diode), research in the context of inhibiting bacterial growth has been explored, since they are bacterial species that commonly colonize the skin, and can generate occurrences. For the treatment of infections, the therapeutic use of antibiotics is recommended, which, over the years, has made the population resistant to many of them. On the other hand, the use of FBM in the treatment of skin lesions has increased, and little is investigated about the effects on the interaction of FBM by LED with the use of antibiotics in bacterial cultures. Thus, this study aims to verify bacterial inhibition and the profile of sensitivity to antibiotics with the use of LEDs at different wavelengths (465 and 630 nm) and doses (30, 40 and 50 J/cm^2) in Staphylococcus aureus and Pseudomonas aeruginosa, ATCC type and bacteria collected from burn patients. 300 µl of saline with bacterial suspension in concentrations between 0.5-0.63 were irradiated with LEDs using the McFarland scale, after five serial dilutions, and distributed in transparent flat-bottomed microtubes. Before and after irradiation, pH and temperature variables were controlled. The cultures were placed in an oven at 37ºC for 24 hours for later counting of colony forming units (CFU). To check the sensitivity profile, a qualitative method (Disc diffusion) were adopted. To quantify oxidative stress, assessments were performed using Malondialdehyde (MDA) and antioxidant action using glutathione (GSH). All data were discovered using the Shapiro-Wilk normality test and comparisons between groups using the single-factor ANOVA test, with Tukey's post hoc with a 95% confidence interval. Differences between the irradiated groups were found, however, without statistical significance or representing a change in the sensitivity profile of the bacteria investigated. The highest production of oxidative stress was at 465 nm (30 J/cm^2), and no glutathione production was detected. LED irradiation was found to be safe for application to bacterial colonies, as it did not modify their antibiotic susceptibility profile, despite inducing oxidative stress.

Keywords: Photobiomodulation, Light Emitting Diode, Pseudomonas aeruginosa, Staphylococcus aureus, Escherichia coli, Drug Resistance, Bacterial.

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Maillard Induced Pea Protein-Polysaccharide Conjugates: A Functionally Enhanced Ingredient for the Food and Beverage Industry

ABSTRACT

Pea proteins are increasingly recognized as a cost-effective, sustainable source of legume proteins with a well-balanced amino acid profile. The primary goal of this research was to enhance the functional properties of pea proteins by combining enzymatic hydrolysis with Maillard conjugation. Pea protein-enriched flour was hydrolyzed using trypsin and papain to achieve low to medium degrees of hydrolysis (2% – 15%). These hydrolysates were then conjugated with residual starch within the PPEF through heat conjugation (Maillard reaction). Molecular weight analysis indicated a shift towards higher molecular weights. The resulting conjugates showed improved functional properties compared to the raw samples with enhanced stability at acidic pH. Followingly conjugates having higher degrees of hydrolysis (above 15%) were examined with additional carbohydrate hydrolysis using α-amylase. The trypsin-hydrolyzed conjugates outperformed papain-hydrolyzed ones across a range of pH levels, demonstrating superior foaming, emulsifying, water- holding, and oil-holding properties. Contrary to previous findings in the literature, the research showed that extensive hydrolysis, when combined with Maillard conjugation, did not impair functionality but enhanced it. In the further study, protein- and starch-rich flour preparations were independently hydrolyzed using trypsin and α-amylase, respectively, and then were conjugated. Functional evaluations showed high solubility and improved foaming and emulsifying properties, particularly at acidic pH, with notable enhancements across all pH levels. Overall, this research demonstrated the potential of conjugation to enhance the functional properties of pea proteins which can be used to improve the texture and stability of foams and emulsions or to improve sensory attributes in alternate meat products. The process not only adds value to starch fractions typically used for animal feed but also promotes eco-friendly, cost-effective solutions for food and beverage applications.

Keywords: Legume proteins, green label, food ingredients, lysine-hydroxygroup conjugation, enzymatic hydrolysis.

BIOGRAPHY

Dr. Takuji Tanaka is professor in Department of Food and Bioproduct Sciences, University of Saskatchewan. His research fields are mainly in enzymology, including structure-function relationships of enzyme using X-ray crystallography to utilization of enzymes in value-added applications. His research program further extends to the utilization of fermentation, especially modification of proteins through fermentation and combinations of fermentation and insect culture to generate novel sources of food and feed materials.

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Research of the physicochemical properties of biodiesel from grape seed oil as an alternative energy source

ABSTRACT

In order to reduce fossil fuel consumption and harmful emissions to the environment, the oil obtained from grape seeds, which is separated as waste after wine production, was used as a raw material for biodiesel production as an alternative fuel at "GANJA SHERAB-2" operating in Azerbaijan. 60.0% mass petroleum-based diesel was obtained from the hydrocracking of fuel oil, and 92.9% biodiesel was obtained from the transesterification of grape seed oil. B20, B40, B60 compositions were prepared from diesel and biodiesel. The cetane number of the diesel fraction was determined to be 50.4 units. The addition of grape seed oil biodiesel led to an increase in the cetane number. The cetane number of the B20 composition is 51.8, the B40 composition is 53.2 and the B60 composition is 54.7. The kinematic viscosity of diesel, biodiesel, B20, B40 and B60 fuels is 3.1121, 3.2611, 3.4321, 3.5811, 4.7645 mm^2/s, respectively. Kinematic viscosity of fuels: petroleum-based diesel, B20, B40 and B60 meets the requirements of the PN-EN-590 standard, while the kinematic viscosity of grape seed oil biodiesel meets the requirements of the PN-EN 14214 standard. According to the international standard PN-EN ISO 3104, the viscosity range for biofuels should be between 1.9 and 6.0 mm^2/s. It was shown that the kinematic viscosity of B20, B40 and B60 biodiesel compositions corresponds to this range. Grape seed oil can be used as an economically viable and environmentally friendly natural raw material source in the production of biodiesel as an alternative fuel. At the same time, it is recommended to add the obtained biodiesel as an ecological component to diesel fuels and use it as an environmentally friendly fuel in vehicles.

Keywords: biodiesel, diesel, transesterification, grape seed, fuel oil, cetane number

BIOGRAPHY

PhD (engineering), associate professor Suleymanova Aisha works as the head of the "Oils and Ointments" laboratory at the Institute of Bioresources of the Ministry of Science and Education of the Republic of Azerbaijan (Ganja). She was awarded the scientific degree of Doctor of Philosophy in Engineering in the specialty of Petrochemistry. With a prolific academic record of approximately 53 published research articles, her scientific work has made significant contributions to advances in the fields of biofuel production from agro-industrial waste as an alternative energy source, green chemistry, biofuel production, environmental sciences, and biofuel applications.

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Synthesis of Sugar Beet Pulp-Derived Activated Carbon for CO_2/CH_4 Separation from H_2-Rich Syngas

ABSTRACT

Türkiye is one of the top producers of sugar beets pulp (SBP) worldwide with a 7-8 million tons of fresh pulp produced every year. In order to advance waste biomass valorization aligned with "zero-waste" strategies. Activated carbons derived from SBP, an abundant agro-industrial waste, were synthesized via one-step and two-step KOH activation. The effects of activation strategy, biomass:KOH ratio (1:1, 1:2, and 1:3), and activation temperature (700-900 ºC) on structural properties and gas adsorption performance were systematically investigated. will be used to improve the separation efficiency, purity of hydrogen, and hydrogen-rich gas production by biomass gasification and steam reforming processes. The synthesized ACs were characterized using XRD, FT-IR, SEM, and BET analysis. As a result, the two-step activated carbons exhibited significantly higher CO_2 adsorption capacities than the one-step samples. The highest uptake was achieved by Two-AC-2-800 (5.2 mol/kg at 2 bar and 25 ºC), followed by Two-AC-1-800 (4.9 mol/kg), whereas the best one-step sample, One-AC-1-600, reached only 3.4 mol/kg, while excessive KOH loading significantly reduced adsorption performance, with One-AC-3-800 exhibiting only 0.8 mol/kg and Two-AC-3-800 only 2.5 mol/kg. CO_2 adsorption is observed to be very high compared to CH_4 and H2 adsorption levels from 0-6 bar at 25 ºC. The adsorption of CO_2 increases from 1.4 mol/kg at 1 bar to about 8.9 mol/kg at 6 bars while that of CH_4 is 4.6 mol/kg and H2 < 0.4 mol/kg.

Keywords: Sugar beet pulp, Activated carbon, CO_2 adsorption, Biomass valorization, Zero-waste strategy

BIOGRAPHY

Salahaldeen M. A. Aljafreh is a PhD Candidate in the Department of Chemical Engineering at Eskişehir Technical University, Türkiye. His research focuses on sustainable energy and environmental technologies, particularly biomass-derived activated carbons, adsorption-based gas separation, hydrogen purification, and carbon capture. His work includes Pressure Swing Adsorption (PSA) and Vacuum Pressure Swing Adsorption (VPSA) for hydrogen purification and methane upgrading, adsorption isotherms and kinetics, biomass gasification, biodiesel and green diesel production, and alkaline water electrolysis systems.

Stewart P. Lewis

Pyramid Polymers LLC, USA

ABSTRACT

Silicon based compounds containing a basic heteroatom attached to Si (e.g., siloxanes, alkoxy silanes) form hydrocarbon soluble complexes of aluminum chloride. They are highly active for the polymerization of olefins in absence of chlorinated solvents up to the ceiling T. Reaction can be conducted in neat monomer or in alkanes and the molecular weight temperature performance of these systems are superior to their ethereal analogs or aluminum bromide under otherwise identical conditions. In the case of hexamethyldisiloxane as the coordinating agent the identity of the resultant adduct was found to be determined by the polarity of the solvent it is formed in. In low polarity alkanes it consists of dimeric aluminum chloride bound to one mole siloxane {i.e., $(Me_3Si)_2O{\cdot}Al_2Cl_6$) whereas it is monomeric in both acid and hexamethyldisiloxane {i.e., $(Me_3Si)_2O{\cdot}AlCl_3$} when formed in aromatic solvents. The activity of these complexes is tunable by adjusting the mole ratio of the coordinating agent to the acid and if aromatic solvent is included. The ability to adjust the activity of the resultant complexes allows for polymerization to be conducted safely under demanding reaction conditions (e.g., solventless, high T).

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Poster Presentations

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Spintronic potential of Co/Cr_2O_3 interfaces: oxidation and exchange bias effects

ABSTRACT

As CMOS-based electronic scaling approaches its fundamental physical limits, spintronics emerges as a compelling alternative to conventional semiconductor paradigms. This study investigates the electrical, magnetic, and optical properties of cobalt (Co) thin films as the ferromagnetic (FM) component, focusing on functional degradation induced by oxidation. Utilizing high vacuum (HV) physical vapor deposition (PVD), Co films (1–10 nm) were synthesized to evaluate the evolution of their transport properties under controlled oxidation. To mitigate this degradation, a chromium (Cr) passivation layer was introduced, where the resulting chromium oxide (Cr_2O_3) acts as an antiferromagnetic (AFM) layer. The results indicate that oxidation kinetics follow a layer-by-layer growth mechanism consistent with Cabrera–Mott theory [1], with Co reaching saturation at higher air pressures compared to Cr. This differential kinetic behavior enables precise control of the oxidation flux within the Co/Cr_2O_3 bilayer, optimizing the stability of the ferromagnetic phase. Moreover, the FM/AFM interface exhibits exchange bias effects [2], providing enhanced magnetic anisotropy and stability crucial for spintronic applications. Finally, the incorporation of a gold (Au) capping layer is proposed to establish a FM/AFM/NM trilayer architecture. In this system, Au serves a dual role: acting as a chemical passivation barrier and, leveraging its strong spin–orbit coupling [3], functioning as a strategic component for spin current manipulation and spin–orbit torque phenomena.

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2. Nogués, J., & Schuller, I. K. (1999). Exchange bias. Journal of Magnetism and Magnetic Materials, 192(2), 203–232. Leonardo Vergara has been a teacher at primary, secondary, and university levels since 2009. In 2020, he enrolled in the M.Sc. program in Physics at Universidad Técnica Federico Santa María (UTFSM), and in 2024 he was admitted to the Ph.D. program in Physics at the same institution. Alongside his teaching activities, he has been involved in scientific research projects funded by the Chilean National Agency for Research and Development (ANID). His research interests include the synthesis of nanostructured materials, electrical, electronic, and surface characterization, and metal oxide semiconductor-based gas sensors (MOS).

3. Kent, A. D., & Worledge, D. C. (2015). A new spin on magnetic memories. Nature Nanotechnology, 10(3), 187–191. https://doi.org/10.1038/nnano.2015.24 Leonardo Vergara has been a teacher at primary, secondary, and university levels since 2009. In 2020, he enrolled in the M.Sc. program in Physics at Universidad Técnica Federico Santa María (UTFSM), and in 2024 he was admitted to the Ph.D. program in Physics at the same institution. Alongside his teaching activities, he has been involved in scientific research projects funded by the Chilean National Agency for Research and Development (ANID). His research interests include the synthesis of nanostructured materials, electrical, electronic, and surface characterization, and metal oxide semiconductor-based gas sensors (MOS).

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Structural and morphological tuning of CuO thin films for enhanced ethanol gas sensing

ABSTRACT

Gas sensors are devices that detect changes in the environment and convert them into electrical signals. Thin copper films, 20 nm thick, have been fabricated in a high-vacuum thermal evaporation system on mica substrates. Growth parameters such as substrate temperature were modified. After deposition, the samples were oxidized in air at 300 °C for 3 h through an annealing process. Raman and UV-Vis spectroscopy were performed on all samples. The characteristic peak corresponding to CuO (296 cm^{-1}) appears clearly. The Kubelka-Munk function, as a function of photon energy, yields a band gap of 1.78 eV. Temperature-dependent electrical resistance tests show semiconductor-like behavior with an activation energy of 467 meV. The performance of the samples as a gas sensor was tested, measuring the electrical resistance of the films in presence of ethanol gas at low pressure (from 10^{-3} to 10^{3} Pa). Results show that the samples are sensitive and exhibit selectivity to ethanol gas.

The films were exposed to controlled surface decoration process. Ultrathin chromium films with varying thicknesses (0.1–1 nm) were evaporated on copper oxide surfaces. The characteristic Cr_2O_3 peak (550 cm^{-1}) appears in the films. Finally, the performance of the samples as gas sensors was tested, again, by measuring the electrical resistance of the films in the presence of low-pressure ethanol gas. Resistance changes of up to 50% were measured. The chromium layer exhibits an effect on this behavior, which is discussed using a gas adsorption model in p-type semiconductors.

Keywords: CuO, sensors, thin-films, oxidation, semiconductor, characterization

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Development of Titanium Dioxide-Free Drotaverine 80 mg Film-Coated Tablets and Validation of HPLC Methods for Assay and Impurity Determination

ABSTRACT

Titanium dioxide (TiO_2, E171) has long been widely used in pharmaceutical film coatings due to its ability to provide opacity and protection against ultraviolet radiation. Following growing concerns regarding its safety and the ban on its use as a food additive within the European Union, increasing attention has been directed toward the development of alternative formulation approaches for medicinal products. The aim of this study was to formulate titanium dioxide-free 80 mg drotaverine hydrochloride film-coated tablets and to validate HPLC analytical methods for the determination of active pharmaceutical ingredient assay and impurities in accordance with current regulatory requirements. Drotaverine, a phosphodiesterase type 4 (PDE4) inhibitor, is a widely used antispasmodic agent indicated for the treatment of disorders associated with smooth muscle spasms. In the formulation developed by F1 Pharma, titanium dioxide was replaced with iron oxides, while maintaining the required functional properties of the film coating. In parallel, high-performance liquid chromatography (HPLC) methods for assay and impurity determination were developed and validated in accordance with ICH Q2(R2) guidelines. The final product was subjected to stability studies under accelerated (40°C/75% RH), intermediate (30°C/65% RH), and long-term (25°C/60% RH) storage conditions. The obtained results demonstrated that the titanium dioxide-free coating had no adverse effect on the quality or stability of the medicinal product. The validated HPLC methods enabled reliable monitoring of both active substance content and impurity profiles, providing a robust tool for routine quality control and stability assessment. The findings confirm that TiO_2 can be successfully replaced in drotaverine hydrochloride film-coated tablets while maintaining the required quality attributes and ensuring compliance with anticipated future regulatory requirements.

Keywords: Titanium-free formulation, Drotaverine, HPLC, method validation

BIOGRAPHY

Dr. Magdalena Strzebońska is an Assistant Professor at the Department of Environmental Protection, Faculty of Geology, Geophysics and Environmental Protection, AGH University of Krakow, Poland. She specializes in analytical chemistry, with particular emphasis on liquid chromatography (HPLC) and instrumental analysis. She has extensive experience in laboratory research, with expertise in the development and validation of analytical methods compliant with GMP, GLP, and European Union regulations. Her scientific activity also includes the development and implementation of analytical methods in environmental studies, with a focus on the analysis of water, wastewater, and sediments. From 2001 to 2009, she worked as a Quality Control Specialist at Pliva Kraków, where she was responsible for analytical method validation, documentation, and ensuring compliance and quality of medicinal products within the pharmaceutical industry.

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Nanoparticle-Assisted Sustainable Regeneration of Spent Dialysate

Introduction

Background:
Hemodialysis is a life-saving therapy for patients with end-stage renal disease, but it is resource-intensive, especially regarding water consumption and dialysate preparation.

Challenge:
Conventional dialysate regeneration methods are not sustainable, and selective removal of urea and other solutes remains a significant technical hurdle.

Objective:
To develop a sustainable, efficient, and scalable platform for dialysate regeneration by integrating advanced nanomaterials and membrane technologies (Figure 1).

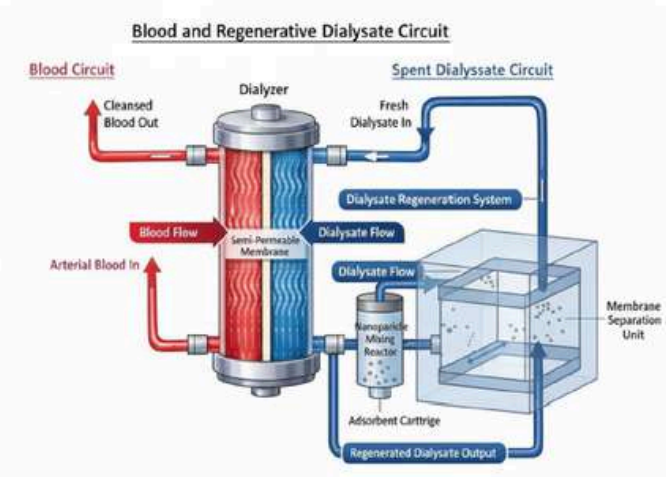

Figure 1. Schematic Procedure for Urea Removal and Regeneration of Spent Dialysate.

Results

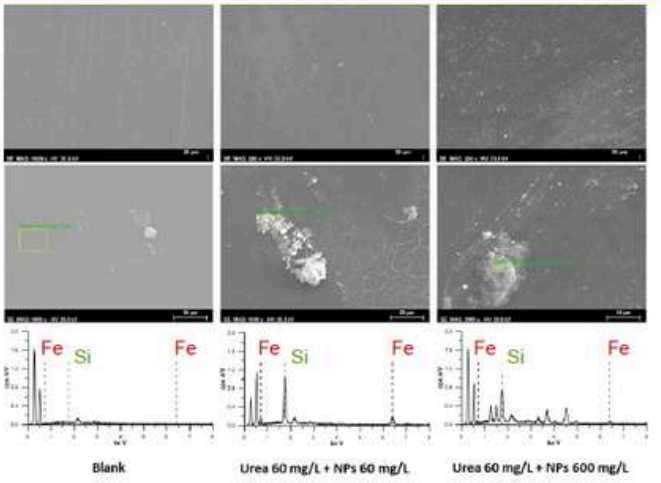

Figure 2. SEM-EDX analysis on the NPs and membrane used in the mixture experiments

- The successfully fabricated MHM features a dense and highly compact top surface with a Si–O–C hybrid network, effectively acting as a physical barrier against nanoparticle passage.
- The successful synthesis and characterization of Core-Shell NPs, confirms the formation of a well-defined hybrid structure exhibiting superparamagnetic behavior.
- The results showed that the Integrated system can remove urea effectively, especially at higher nanoparticle loading.

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Experimental Work

- Optimization of Monophasic Hybrid Membrane (MHM) property for improved flux and selectivity.
- Functionalization of the Nanoparticles (NPs) to achieve greater selectivity at their surface.
- Testing the system using simulated spent dialysate and measuring urea removal by UV-Vis spectrophotometry at different nanoparticle concentrations and pH values.

Future Work

- Recovery and Reutilization of NPs.
- Transition from batch to continuous dialysate loops.

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Highly efficient nanosized $Sn_{0.96}Y_{0.02}M_{0.02}O_2$ (M = Mo, Zr) photocatalysts for mineralization of methyl green and chlorpyrifos waste

ABSTRACT

In the modern era, industrial wastewater problem is a global issue related to human health and environmental bioactivity. Thus, water recycling with removal of organic pollutants is crucial for water shortage compensation and preserving living organisms. In this work, highly crystalline SnO_2, $Sn_{0.96}Y_{0.02}Mo_{0.02}O_2$ and $Sn_{0.96}Y_{0.02}Zr_{0.02}O_2$ nanoparticles were effectively synthesized via a coprecipitation route and characterized using many physical techniques. Analysis of X-ray diffraction (XRD) proved the high purity and crystallinity of SnO_2-based compositions with low crystallite size. The TEM images illustrated that the size of the particles of SnO_2 powder was decreased after incorporation of Y, Mo and Zr ions. The distribution histograms of SnO_2, $Sn_{0.96}Y_{0.02}Mo_{0.02}O_2$ and $Sn_{0.96}Y_{0.02}Zr_{0.02}O_2$ samples reveal that the mean particles size of these samples are 31, 14 and 12 nm, respectively. Based on Tauc plot method, the energy band gap was estimated to be 3.48, 2.99 and 3.03 eV for SnO_2, $Sn_{0.96}Y_{0.02}Mo_{0.02}O_2$ and $Sn_{0.96}Y_{0.02}Zr_{0.02}O_2$ powders, respectively. X-ray photoelectron (XPS) measurements of (Y, Mo) replaced SnO_2 nanoparticles show well recognized binding energy peaks of Sn, O, Y and Mo elements with oxidation state of +4, -2, +3 and +6, respectively. Energy-dispersive X-ray (EDX) analysis detected the existence and distribution of Sn, Y, Mo and O element in $Sn_{0.96}Y_{0.02}Mo_{0.02}O_2$nanoparticles. Nanosized $Sn_{0.96}Y_{0.02}Mo_{0.02}O_2$photocatalyst with low band gap energy demonstrates a degradation efficiency of 97.3% and 94.5% for methyl green and chlorpyrifos contaminants within 60 min and also facilitate their mineralization to carbon dioxide and water. Furthermore, the nanosized $Sn_{0.96}Y_{0.02}Mo_{0.02}O_2$powders revealed high photo-stability and reusability for photocatalytic activities.

Keywords: Global health and environment; Wastewater; Industrial pollutants; Photo-catalysis; Sunlight irradiation; SnO_2-based photocatalysts

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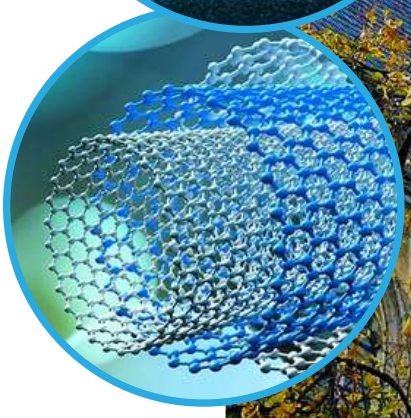

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