PEERS ALLEY MEDIA

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2026

MARCH 25-27

VIRTUAL EVENT

7TH EDITION OF

ADVANCED CHEMISTRY WORLD CONGRESS

SCIENTIFIC PROGRAM

DAY 01
WEDNESDAY

MARCH 25, 2026

(GMT) Greenwich Mean Time

07:35-07:40	**Welcome Note**

Analytical Chemistry | Industrial Chemistry | Agricultural Chemistry | Medicinal Chemistry | Chemical Engineering | Green Chemistry | Environmental Chemistry | Biochemistry | Organic Chemistry | Physical Chemistry | Geochemistry | Food Chemistry | Materials Science | Molecular Biology | Polymer Chemistry and Technology

Distinguished Speaker Talks

07:40-08:00	Title: Integrating Biotic and Abiotic Worlds Toward Emotional Satisfaction **Shuichi Fukuda,** *Keio University, Japan*
08:00-08:20	Title: Molecular Insights and Cytotoxic Evaluation of Newly Synthesized N-(Acridin-9-yl)-N-(2-Substituted Benzoyl) Compounds **Hemalatha Kanagarajan,** *Saveetha University, India*
08:20-08:40	Title: Plastic Waste Pyrolysis by Application of Radiation Technology **Gurbanov Muslim Axmed,** *Institute of Physics of the Ministry of Science and Education, Azerbaijan*
08:40-09:00	Title: Digital Chemistry for Smart Cities: Cross- Disciplinary Framework using AI, IoT & Chemical Sensors **Aditya Singh,** *Amrita Vishwa Vidyapeetham, India*
09:00-09:20	Title: Identification and Prioritization of Barriers to Smart Waste Management Systems in the Textile and Apparel (T&A) Industry **Monabbir Rafsan Fahim,** *Bangladesh University of Textiles, Bangladesh*
09:20-09:40	Title: Real-Time Water Quality Assessment using a Multisensor IoT Monitoring System **R. Priscilla Joy,** *Karunya Institute of Technology and Sciences, India*
09:40-10:00	Title: Morphological and Mechanical Analysis of Epoxy-Chicken Feather Fiber Composites with COMSOL-Assisted Simulation **Zainab Waheed Abdullah,** *Middle Technical University, Iraq*

REFRESHMENT BREAK 10:00-10:15	
10:15-10:35	Title: Resveratrol and Selenium Nanoparticles: A Biochemical and Molecular Assessment for the Treatment of Type 2 Diabetes and Associated Complications **Mahmoud Balbaa,** *Alexandria University, Egypt*
10:35-10:55	Title: Modeling of the Temperature Dependence of the Diffusion Characteristics of Vacancies in BCC Titanium **Madina Boboqambarova,** *National Research Nuclear University MEPhI, Russia*
10:55-11:15	Title: Spectroscopic, Structural, and Computational Characterization of a Novel Piperidyl-Sulfonyl-Thiazolidinone Derivative **M. Sarasija,** *Satavahana University, India*
11:15-11:35	Title: Investigation of Biopesticides for the Pest Control through Inhibition of the Acetylcholinesterase Purified from *Loxostege Sticticalis* (L.) (Lepidoptera: Crambidae) **Demet KIZIL,** *Bursa Technical University Central Research Laboratory, Turkey*
11:35-11:55	Title: Failure Analysis of a Heavy-Duty Fastener used in Hydraulic Systems: An Inspiring Study **Aravind P,** *AVH Innovations and Metallurgical Laboratory, India*
11:55-12:15	Title: Isotropic Phase of nematogens: Solving Landau–de Gennes Modelling Problems **Aleksandra Drozd-Rzoska & Sylwester J. Rzoska,** *Institute of High Pressure Physics "Unipress", Poland*
12:15-12:35	Title: Green Nanotechnology Approaches for Sustainable Drilling Fluid Formulations **Borkha Mech,** *Dibrugarh University, India*
12:35-12:55	Title: Future Directions of the Heterogeneous Catalysis: Polyoxometalate-Based Covalent Organic Frameworks **Arash Ebrahimi,** *Comenius University in Bratislava, Slovakia*
LUNCH BREAK 12:55-13:35	
13:35-13:55	Title: Near-Infrared Spectroscopic Detection of Chemical Signatures Associated with External Flavor Addition in Green Coffee **Jaime Daniel Bustos Vanegas,** *Universidad Surcolombiana, Colombia*

13:55-14:15	Title: Evaluation of the Effect of Precursor NMC622@TiO_2 Core–ShellPowders using a Prelithiated Anode from Fig Seeds: Spotlight on Li-Ion Full-Cell Performance **Rawdah Abduh Ghaleb Whba,** *Taiz University, Yemen*
14:15-14:35	Title: Bridging Empirical Formulations and Machine Learning Approaches For Soil Infiltration Modeling in the Mitidja Plain **Mazighi Amina,** *Higher National School of Hydraulics of Blida, Algeria*
14:35-14:55	Title: Contaminants of Emerging Concern on Microplastics Found in the *Chrysaora chesapeakei* of the Patuxent River, Chesapeake Bay, MD **Carol Adrianne Smith,** *Morgan State University, USA*
14:55-15:15	Title: Actinobacteria from Nocardiaceae Family as Nanomaterial Factories **Lucía Ortega Cabello,** *Universidad Autónoma Metropolitana, Mexico*
15:15-15:35	Title: Sulfonation Degree by different Analytical Techniques for Sulfonated Aromatic Polymers **Juan Carlos Sanchez Hiza,** *Centro de Investigación en Química Aplicada, México*
15:35-15:55	Title: Sensitive Lophine Layer for the Detection of Hydrogen Ions (H+) **Pedro Marcos Velasco Bolom & Jorge Luis Camas Anzueto,** *Tecnológico Nacional de México/Instituto Tecnológico de Tuxtla Gutiérrez, México*
15:55-16:15	Title: From Chemical Characterization to Biological Function: Bioactive Compounds from Brazilian Tropical Fruit Byproducts **Jailane de Souza Aquino,** *Federal University of Paraíba (UFPB), Brazil*
NETWORKING	
END OF DAY 1	

SCIENTIFIC PROGRAM

DAY 02
THURSDAY

MARCH 26, 2026

(GMT) Greenwich Mean Time

07:35-07:40	**Introduction**

Sessions: Analytical Chemistry | Industrial Chemistry | Agricultural Chemistry | Medicinal Chemistry | Chemical Engineering | Green Chemistry | Environmental Chemistry |Biochemistry | Organic Chemistry | Physical Chemistry | Geochemistry | Food Chemistry | Materials Science | Molecular Biology | Polymer Chemistry and Technology

Distinguished Speaker Talks

07:40-08:00	Title: Automated Multimodal Materials Analysis: A Unified Pipeline for Experimental Characterization Data with ML-Based Nanostructure Identification **Kavitha Jayaram, B N M Institute of Technology, India**
08:00-08:20	Title: Fluorescent Chemosensors in the Detection of Ultra-Trace Quantity of Toxic Hg^{2+}, Pb^{2+}, Al^{3+}, F^{-}, AsO_4^{3-} & AsO_3^{3-} in Water Towards Monitoring Humam Health and Management **Samir Kanti Datta,** *University of Calcutta, India*
08:20-08:40	Title: A Comparative Analysis of Deep Learning and Machine Learning Models for Fruit and Fruit Disease Recognition: Applications to Citrus, Guava, and Mango **Sayeda Rahnuma Akthar,** *Independent University Bangladesh, Bangladesh*
08:40-09:00	Title: Uncertainty-Based Efficient Neutrosophic Imputation Methods for Population Mean **Vishal Kumar,** *Central University of Haryana, India*
09:00-09:20	Title: Integration of Technologies to Study the Interference Effect of Coexisting Ions through Algorithmic Analysis **Parul Taneja,** *Indian Institute of Technology Guwahati, India*
09:20-09:40	Title: Synergistic *Artemisia Monosperma* with Royal Jelly: Antibacterial, Antioxidant, Antibiofilm, and Anti-Alzheimer Potential **Sally Said Ibrahim Ehmedan,** *Arish University, Egypt*

09:40-10:00	Title: Exploring the Functional Food Potential of *Grand Naine* Banana Flour (GBF) as a Prospective Weaning Formulation by Developing GBF-Based Composite Flour Mixes **Mamoni Das,** *Assam Agricultural University, India*
REFRESHMENT BREAK 10:00-10:15	
10:15-10:35	Title: Development of Herbal Toothpaste against Tooth-Associated Ailments **Sakthi Priyadarsini. S,** *SRM Institute of Science & Technology, India*
10:35-10:55	Title: The Role of Supply Chain Agility and Resilience in Enhancing Firm Performance **Esra Nur GOKHAN,** *Beykoz University, Turkey*
10:55-11:15	Title: Global Market Trends in Biomedical Sensors: Materials, Device Engineering, and Healthcare Applications **V. R. Palanivelu,** *Periyar University, India*
11:15-11:35	Title: Evaluation of Testicular Protective Effects of *Prunus Amygdalus* and Zinc Against Cadmium Induced Toxicity in Rats **Faiza Zubair,** *University of Sargodha, Pakistan*
11:35-11:55	Title: Biochemical Profiling of Freshwater Fish Species from the North-Western Himalayas **Rakesh Kumar Thakur,** *Central University of Himachal Pradesh, India*
11:55-12:15	Title: Hydrochemical Assessment and Environmental Value of Karst Springs in Vlore County, Albania **Marinela Muco & Fatlinda Shkurti,** *"Ismail Qemali" University, Albania*
12:15-12:35	Title: Recent Developments in Directed Metal-Catalyzed C-H Bond Functionalization **Hamad H. Al Mamari,** *Sultan Qaboos University, Sultanate of Oman*
12:35-12:55	Title: Analyzing Twitter and Youtube Posts for Identifying Influencers of Apple Products in the Bangalore Region: A Comprehensive Study with Sentiment Analysis **Purushottam Bung,** *RV Institute of Management, India*
LUNCH BREAK 12:55-13:35	

13:35-13:55	Title: Unlocking the Energy Potential of Moroccan Bentonite Clay: Structural, Optical, and Thermal Insights for Advanced Applications **Noura El Ghoubali,** *Mohammed V University in Rabat, Morocco*
13:55-14:15	Title: SPH Framework for Solid–Fluid Interaction **Elías Jeffersson Santacruz Yunga,** *ESPOL Polytechnic University, Ecuador*
14:15-14:35	Title: The Chemistry of Stradivari and Guarneri—The Defining Aspect of their Excellence **Joseph Nagyvary,** *Texas A&M University, USA*
14:35-14:55	Title: Comparative Economic Analysis of Batch vs. Continuous Manufacturing in Catalytic Heterogeneous Processes: Impact of Catalyst Activity Maintenance and Materials Costs on Total Costs of Manufacturing in the Production of Fine Chemicals and Pharmaceuticals **Felix Mendoza Suarez,** *Auburn University, USA*
14:55-15:15	Title: Carbazole Derivatives as Platforms for Luminescent Organic and Hybrid Crystalline Materials **Alonso Acosta Vera,** *University of Rochester, USA*
15:15-15:35	Title: Fate of Micro- Nanoplastics in Treatment Wetlands **Amado Enrique Navarro Frómet,** *Universidad Tecnológica de Izúcar de Matamoros, México*
15:35-15:55	Title: Direct Determination of 2, 4-D in Natural Water Samples by Solid Surface Fluorescence **Maria Carolina Talio,** *INQUISAL-CONICET., Argentina*
15:55-16:15	Title: ESG Challenges in the Social Context of the Animal Protein Based Food Sector: The Brazilian Case **Juliana Damaris Candido de Lima,** *Universidade Federal Fluminense, Brazil*
NETWORKING	
END OF DAY 2	

SCIENTIFIC PROGRAM

DAY 03
FRIDAY

MARCH 27, 2026

(GMT) Greenwich Mean Time

07:15-07:20	**Introduction**

Analytical Chemistry | Industrial Chemistry | Agricultural Chemistry | Medicinal Chemistry | Chemical Engineering | Green Chemistry | Environmental Chemistry | Biochemistry | Organic Chemistry | Physical Chemistry | Geochemistry | Food Chemistry | Materials Science | Molecular Biology | Polymer Chemistry and Technology

Distinguished Speaker Talks

07:20-07:40	Title: Effects of Novel Fulvic Acid Amendments on Soil Structural Stability and Organic Carbon–Nitrogen Pools in Three Agro-Ecological Soils
	Hafeezullah Babar, *Agriculture Research Centre, Soil Fertility Research Institute, Pakistan*
07:40-08:00	Title: Chapter-Wise Question Generation from Academic Book PDFs Using Generative AI
	Dhiraj Ghanshyam Karwatkar, *TGPCET, India*
08:00-08:20	Title: Promising Materials for Optoelectronics $CdIn_2S_4$: Experimental Studies of Electronic Properties
	Zafar Kadiroglu, *Ministry of Science and Education, Republic of Azerbaijan*
08:20-08:40	Title: Application of Liquid Biofertilizers Derived from Industrial Effluents for Legumes: An Option of Sustainable Waste Management
	Sunita Chauhan, *Kumarappa National Handmade Paper Institute (KNHPI), India*
08:40-09:00	Title: Persistence of Information in the Quantum Measurement Problem
	Shantena Augusto Sabbadini, *Pari Center, Italy*
09:00-09:20	Title: cfDNA Liquid Biopsy: Revolutionizing Breast Cancer Diagnostic, Prognostic & Precision Oncology
	Heba Kamel Mahmoud Badawy, *Sinai University, Egypt*
09:20-09:40	Title: AI Driven Algorithms for Predictive Compound Design and Optimization in Drug Discovery
	Subhranil Das, *School of Computer Science UPES, India*

09:40-10:00	Title: River and Groundwater used for Irrigation of Agricultural Crops **Smailov Eltar Ablametovich & Sydykbaeva Telegey Israyilovna** *International Kyrgyz-Uzbek University named after B. Sydykov, Kyrgyzstan* *National Academy of Sciences of the Kyrgyz Republic, Kyrgyzstan*
REFRESHMENT BREAK 10:00-10:15	
10:15-10:35	Title: Contributions of Debye-Waller Factors and EXAFS to Materials Chemistry Based on Advanced Anharmonic Correlated Einstein Model **Nguyen Van Hung,** *University of Economics - Technology for Industries, Vietnam*
10:35-10:55	Title: Spatial Mapping of Soil Salinity in a Semiarid Region using a Machine Learning Model Based on Spectral Indices and Ground Data **Khalid EL BAHJAOUY,** *University Sultan Moulay Slimane, Morocco*
10:55-11:15	Title: An Innovative Way to use an Extract of the Viticulture By-Products **Zulfiya Shakiryanova,** *M. Auezov South Kazakhstan Research University, Kazakhstan*
11:15-11:35	Title: Minority Power: Driving Change through Social Influence **Imane MARGOM,** *Sidi Mohamed Ben Abdellah University (USMBA), Morocco*
11:35-11:55	Title: FasalNirog: A Multimodal AI-Driven Web Platform for Crop Disease Diagnosis and Expert-Guided Support **Sujata S. Kulkarni,** *Bhartiya Vidya Bhavans Sardar Patel Institute of Technology, India*
11:55-12:15	Title: Effects of Electron Beam Irradiation on the Physicochemical, Functional, Nutritional Properties, and Microstructure of Millet Flour (*Pennisetum glaucum* L.R.Br.) **Dely Maissa,** *University of Carthage, Tunisia*
12:15-12:35	Title: Assessment of Oropharyngeal Dysphagia in Patients with Rheumatoid Arthritis **Dina Wael Ibrahim,** *Beni-suef University, Egypt*
12:35-12:55	Title: Spatial access differentials to healthcare facilities: A secondary analysis of the Democratic Republic of Congo **Elizabeth Avosuahi Dania,** *The University of the Western Cape, South Africa*

12:55-13:15	Title: Comprehensive Physicochemical Characterisation of Bovine Bone as a Sustainable Biomaterial for High-Value Applications **Ziningi Rosebud Myeni,** *Technology Innovation Agency, South Africa*
13:15-13:35	Title: Livelihood Transformation of Tribals through SHG and Water Hyacinth Product Entrepreneurship: A Case in West Bengal **Dipanwita Chakraborty,** *Giri Institute of Development Studies, India*
13:35-13:55	Title: AI Meets Reality: Detecting Rice Diseases in Benin — A Bibliometric and Field Perspective **HOUNGUE Y. Pélagie Elyse,** *Université d' Abomey-Calav-IMSP, Bénin*
13:55-14:15	Title: Catalytic Functions for Hydrogen Production and Storage **Ernest Ilisca,** *Storage of Hyperfine Hydrogen for Transport, France*
14:15-14:35	Title: Discovery of a Novel Small Molecule Degrader of Mutant Estrogen Receptors using DNA Encoded Libraries **Murugesan Palaniappan,** *Baylor College of Medicine, USA*
14:35-14:55	Title: Effective Preparation for STEM Learning in Early Childhood **Jabari Mahiri,** *University of California Berkeley, USA*
14:55-15:15	Title: Multiphysics Simulation and Machine Learning for Intelligent Optimization of Coffee Roasting Processes **Jaime Daniel Bustos Vanegas,** *Universidad Surcolombiana, Colombia*
NETWORKING	

PEERS ALLEY MEDIA

DAY 01

VIRTUAL EVENT

7TH EDITION OF

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MARCH 25-27, 2026

SPEAKER TALKS

Integrating Biotic and Abiotic Worlds Toward Emotional Satisfaction

Shuichi Fukuda

System Design and Management Research Institute, Keio University, Japan

Our current world is the Industrial Society and it is product-based. What characterizes humans is we can think about the future. Anthropoids taught us if we get off the ground, we can create movements as wish. 4 legged animals can walk stably, but the center of their body gravity keeps the same distance from the ground. So, they cannot create movements as they wish. They have to compromise with the current environment and situation. But Anthropoids or apes jumped on trees and found out if they get away from the ground, they can create movements as they wish. Living things are called “Creatures”, because they create movements. Movement is indispensable for living. Thus, Humans became aware that if they keep away from the ground, they can create “Life” as they desire. In other words, they can challenge to make their dreams come true. As Deci and Ryan pointed out in their “Self Determination Theory”, humans get the maximum happiness and the feeling of achievement when they do the job internally motivated in their own way. Humans enjoy the challenges and the processes ignite their challenging spirit. Brain is getting wide attention these days. But when true death is sentenced. Even when our brains stops working, death is not announced. Death comes when our hearts stop working. Yes, if our hearts keep working, blood flows and all our organs, except brain, keep working. And we should know that brains can process only smaller amount of information than hearts. Remember Wordsworth’s poem “Rainbow in the sky”. If we see rainbows in the sky, our heart leaps up. Same occurs with babies. Who teach them to crawl, walk and speak. They express their feelings with their bodies and they explore the environments and they start to crawl and then walk. We, adults, often misunderstand that linguistic communication is needed to communicate. But as Facebook shows us many examples of different species of animals become friends. This is biotic world. But the current Industrial Society is abiotic. In the current society, biotic world and abiotic worlds are separated. But this framework is going to an end. Every society shifts from one to another with time. And when the society is coming to a close, many issues emerge. In the current Industrial Society, the greatest problem is the excessive consumption of energy. Energy resources are running out. AI is

expected to be a solution. But AI consumes a large amount of energy. Thus, it works the other way. It worsens the situation. And another big problem is rapidly decreasing workforce due to decrease of childbirth and increase of elders. In the Industrial Society, Engineering and technology are considered important. But they are completely different. Engineering means to “cultivate” or “explore”. Technology focuses on reproducibility. It pursues efficiency and cost performance. It is the world of “Control”. But the real world is changing every minute, so we cannot control it. Learning to swim provides a good example. Water changes every minute. So, we cannot identify parameters and we cannot apply mathematical approaches. We have to learn by ourselves. Learning to swim is an exploration. It is the world of discovery. We discover how to swim by ourselves or with the inborn tool, or instinct.

Chemistry is very different from other industries. It makes clear how current resources can be utilized to produce another product. It is the world of invention. Other industrial fields are the world of innovation.

They are making efforts to develop tactics. Chemistry, on the other hand, is strategic. Or it would be better to say “Pragmatic”. What is important is you can cross the boundary and move ahead toward the new frontiers. Chemistry opens the door to the new world. And it should be emphasized that chemistry is associated with sensing deeply. Wireless telecommunication is getting wide attention these days. But most of them discuss only its speed and the amount of information. But if our smart phones convey such signals as smells, etc., we can share the atmosphere and share the feelings. Suppose if you walk by the wall, and it senses you are very happy, it creates music that resonance with your spirit. And when chemistry provides you with the new frontier, then you can dream about tomorrow and enjoy challenging. This will provide a bright tomorrow for the elderly. As life is expected to be 120 years soon. The elderly can have bright tomorrow and enjoy their “Self” life.

Presenter:
Shuichi Fukuda
Keio University, Japan

Molecular Insights and Cytotoxic Evaluation of Newly Synthesized N-(Acridin-9-yl)-N-(2-Substituted Benzoyl) Compounds

Hemalatha Kanagarajan and **Madhivadhani K**

Department of Pharmaceutical Chemistry, Saveetha College of Pharmacy, Saveetha Institute of Medical and Technical Sciences, Saveetha University, India

The novel set of N-(acridin-9-yl)-N-(2-substituted benzoyl) derivatives was designed and these compounds were subjected to docking studies against topoisomerase II and the result of docking studies revealed that all the compounds possess significant to moderate interaction with the targeted enzyme. Among the docked compounds, compound AB7 possesses significant docking score -8.7 kcal/mol when compared to standard drug doxorubicin. The compound AB7 shows four NH-pi interaction with amino acid residues such as Gly437, Ala 753 and Trp 754 and van der Waals bond with Ser 432, Ser 433, Ser 438, Glu 750, Lys 751 and Asp 757. The remaining docked compound shows a docking score range from 7 to 8.7 kcal/mol along with one or two hydrogen bond interactions. Based on the docking score the derivatives AA2, AA3, AB3, AB7, AB7, AF6, AF10, AP7, AP10 and APZ7 are selected for the synthesis by conventional method. These compounds are subjected to *in-vitro* cytotoxicity study by MTT assay method with MCF-7 cell lines. All the tested compounds displayed an IC_{50}> 125 µg/mL at a concentration range of 30–250 µg/mL. Among the tested compounds, derivative APZ7 substituted with chlorobenzene and pyrrole ring shows a significant IC_{50} value (46.402 µg/ml) and followed by compound AP10 substituted with chloro benzene and pyridine moiety (59.42 µg/ml) shows good inhibition in breast cancer cell line.

Presenter:
Hemalatha Kanagarajan
Saveetha University, India

Plastic Waste Pyrolysis by Application of Radiation Technology

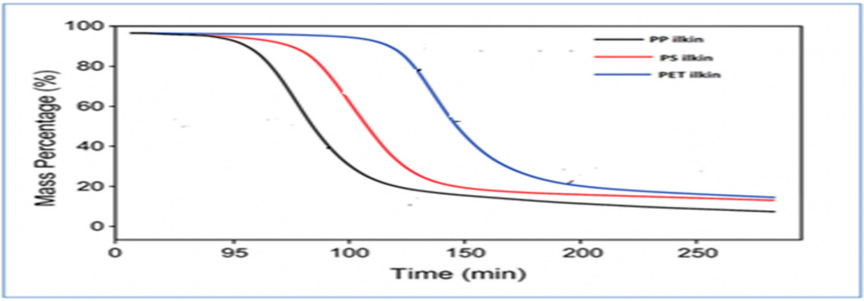
Gurbanov M.A and **Gulieva U.A**

Institute of Physics of the Ministry of Science and Education, Azerbaijan

Despite the studies on the chemical composition, structure and morphology changes of polymer materials and post-consumer waste, the effect of ionizing radiation on the thermal decomposition of plastic waste has been poorly studied. The recombination of various radicals and fragments formed in the polymer matrix as a result of irradiation, as well as their reactions at high temperatures, allow for changes in the output ratios of gaseous, liquid and solid products formed during the pyrolysis process and allow the pyrolysis process to be carried out at relatively low temperatures.

The aim of the work is to study the effect of pre-irradiation on the thermal decomposition process of PP, PS and PET plastic waste using various methods (FTIR, EPR, Thermogravimetric). Irradiation of the samples was carried out using γ-rays of the 60Co isotope under static conditions, at room temperature and under vacuum. The research work was carried out in 2 directions: Initially, the pyrolysis process of PP, PS and PET plastic waste at different doses was studied individually using the above methods. In the 2nd stage, the effect of pre-irradiation on the pyrolysis process of mixed waste (PP-PS, PP-PET) was studied.

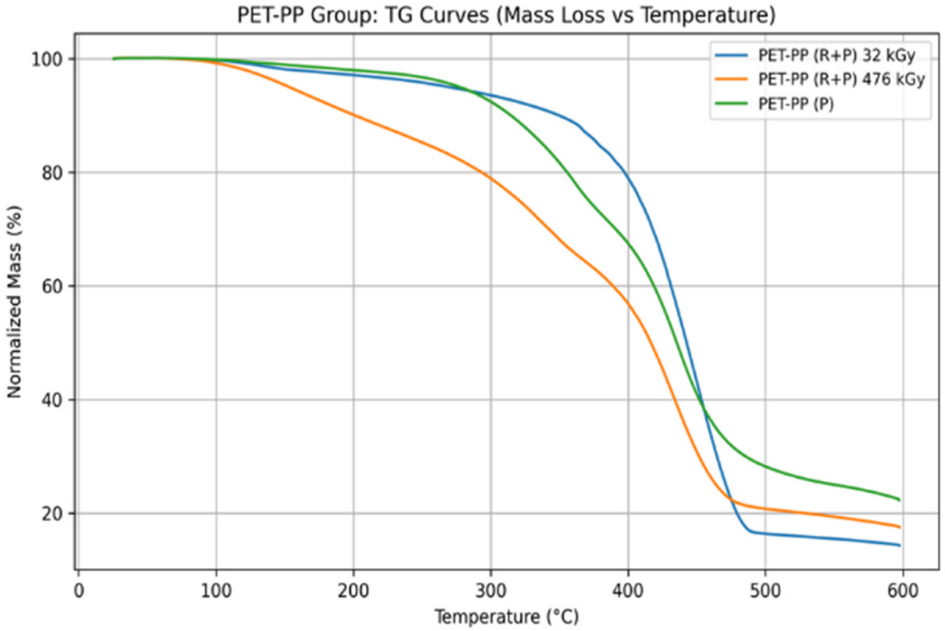
Figure 1 shows the TG curves of the samples



As can be seen, the pyrolysis process of PP waste (ΔT/Δt =5°C/sec) starts earlier than the decomposition of other wastes. The amount of solid residue decreases from 14.5 m% (PET) to 6.5 m% (PP), depending on the type of waste.

The activation energy values at different doses (32-1500 kGy) decrease as the dose increases.

Figure 2 shows the TG curves of the pyrolysis processes of mixed wastes (PP-PET and PP-PS) at different doses (32-476 kGy).



As can be seen, in both cases, at low values of radiation dose, the pyrolysis process begins at higher temperatures. At high doses, the decomposition appears to occur at lower temperatures.

Presenter:
Gurbanov Muslim Axmed
Institute of Physics of the Ministry of Science and Education, Azerbaijan

Digital Chemistry for Smart Cities: Cross-Disciplinary Framework Using AI, IoT & Chemical Sensors

Aditya Singh
Amrita Vishwa Vidyapeetham, India

Over the years, technological advancements have improved the development, which has been contributing towards the growth of Smart Cities. This also includes the development in the field of Chemistry, especially by digital technologies. This study will talk about the concept of Digital Chemistry, as well as a paradigm which will be interdisciplinary in nature while incorporating not only Chemical Sensors, but also IoT & AI technologies in order to discuss various aspects in Smart City Infrastructures like Environmental Monitoring and Urban Sustainability in addition to Public Health. Conventionally Chemistry focusses on laboratory settings, but on the other hand, Digital Chemistry is able to carry chemical insight into the real-world system at real time with the assistance of intelligent automation, networked sensing, and data fusion. The study will discuss a framework which could describe the ways chemical data streams produced from waste, air, and industrial sources, as well as water, to be digitized, analyzed, in addition to acted upon through sensor networks and ML. Then, the chemical sensors which are implanted in urban infrastructures like in water pipelines, smart grids, waste facilities, and transport systems will be talked about to allow dynamic environmental diagnostics along with proactive policy interferences. Such insights are essential for pollution mitigation, circular economy, climate resilience, and disaster response pathways. Then, gaps in the current literature based on the published papers will be considered, and the ways the current advancement of Smart Cities could be enhanced through this study. Then, some real-life examples and graphical analysis will be covered to support this study as well as understand the future of Digital Chemistry in the context of Smart Cities.

Presenter:
Aditya Singh
Amrita Vishwa Vidyapeetham, India

Identification and Prioritization of Barriers to Smart Waste Management Systems in the Textile and Apparel (T&A) Industry

Md. Golam Sarower Rayhan[1], Md. Masum[1], Saifur Rahman Tushar[1], Monabbir Rafsan Fahim[1,2] and **Koppiahraj Karuppiah[3]**

[1]Bangladesh University of Textiles, Bangladesh.
[2]Sonargaon University, Bangladesh
[3]Saveetha School of Engineering, India

The textile and apparel (T&A) industry is prominently criticized for extreme waste generation, deteriorating environmental sustainability. This esteemed fashion industry must incorporate a smart waste management system (SWMS) to restructure the manufacturing processes. This study attempts to demonstrate the critical barriers to implementing SWMS in the traditional T&A industry of Bangladesh. An extensive literature review and expert validation assisted in selecting the most suitable barriers for the SWMS in Bangladesh's T&A industry. A hierarchical influential model has been developed through Fuzzy Total Interpretive Structuring Modeling (TISM), and a causal relationship has been constructed using the Fuzzy Decision Making and Trial Evaluation Laboratory (DEMATEL) method. The TISM modeling identified that "Lack of strategic planning" and "Inadequate stakeholder awareness" have the highest driving power and least dependence power among all the barriers. In addition, the TISM modeling indicated that "Lack of government supervision" and "Lack of IT infrastructure" have the highest dependence power and lowest driving power. Conversely, the DEMATEL analysis signified "Lack of government regulatory policies" as the most impactful barrier and "Lack of IT infrastructure" as the least impactful one. The extensive literature survey of relevant works revealed that there is no concrete research on identifying the barriers or obstacles to the implementation process of SWMS in Bangladesh's T&A industry. This study first seeks to construct a double model evaluation to validate the crucial barriers to shaping the sustainable future of Bangladesh's T&A industry.

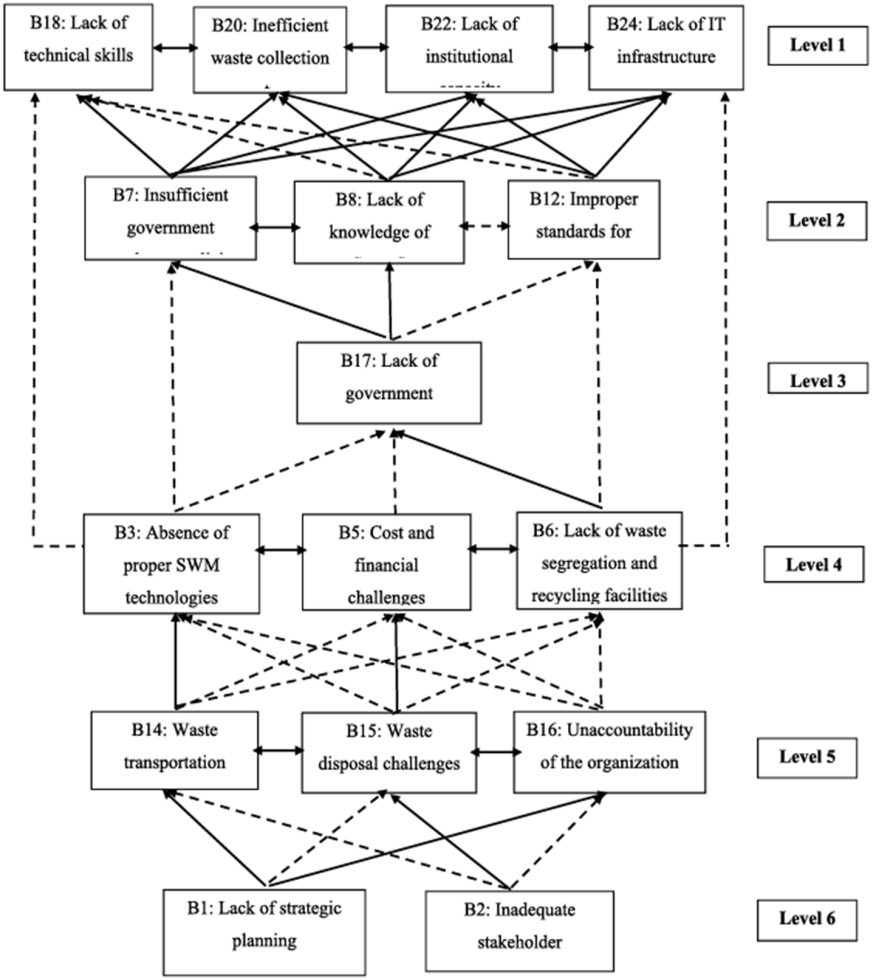


Figure: Hierarchy of the SWMS Barriers

Presenter:
Monabbir Rafsan Fahim
Bangladesh University of Textiles, Bangladesh

Real-Time Water Quality Assessment using a Multisensor IoT Monitoring System

R. Priscilla Joy[1], Immanuel Johnraja[1] and **Mary Metilda[2]**

[1]Karunya Institute of Technology and Sciences, India
[2]Sri Ramakrishna Engineering College, India

Clean drinking water is often taken for granted until a sudden change in taste, colour, or odour alerts a community to a potential contamination issue. Laboratory testing, though accurate, tends to be slow, and in many smaller towns the nearest testing centre may be several kilometres away. This study explores whether a small, sensor-based IoT setup can fill this gap by monitoring key chemical parameters of water in real time and offering early indications of quality deterioration.

The system developed here uses a combination of pH, electrical conductivity, turbidity, temperature, and nitrate sensors, all connected to an ESP32 microcontroller. Readings are pushed periodically to a cloud platform using Wi-Fi and stored for trend analysis. Three different sites were chosen for field testing: a groundwater well that feeds local households, a small storage tank, and a distribution tap. These locations naturally experience different patterns of contamination, making them suitable for observing real-world variations.

During the monitoring period, the system successfully captured increases in turbidity following heavy rainfall and recorded noticeable shifts in conductivity whenever the water level in the well dropped. Nitrate fluctuations were also more pronounced near agricultural areas, something that often goes unnoticed with occasional manual testing. Comparison with laboratory measurements showed that the sensors remained fairly reliable, generally agreeing within 91–96% across parameters.

The results suggest that such an IoT-based approach can provide a practical layer of early warning, especially for communities that depend on shared water sources. While it does not replace laboratory testing, it offers a steady stream of information that can prompt quicker action whenever water quality begins to drift outside safe limits.

Presenter:
R. Priscilla Joy
Karunya Institute of Technology and Sciences, India

Morphological and Mechanical Analysis of Epoxy-Chicken Feather Fiber Composites with COMSOL-Assisted Simulation

Zainab Waheed Abdullah, Zeina Talib Kareem and **HeyamRazaq Atwan**

Department of Applied Mechanics Engineering, Technical College of Engineering, Middle Technical University, Iraq

Chicken feathers represent a category of waste materials. Feathers can be recycled through incineration or burial. Both recycling methods are detrimental to the environment, contributing to increased air pollution and slow decomposition, respectively. The most prominent and successful initiative was the development of new material systems that were both cost-effective and environmentally sustainable to reduce waste materials. This study utilized epoxy as a matrix for biocomposites reinforced with waste chicken feather fibers (CFF), which were produced by a manual mixing technique. Various loadings of CFF of 0.5, 1, 1.5, and 2wt% were utilized following chemical treatment. Optical and scanning electron microscopy were employed to examine the morphological structure of biocomposites. Additionally, tensile, bending, impact, and hardness tests were conducted to assess the mechanical properties of biocomposites. The tensile strength of biocomposites increased by 25, 12.5, and 4% as the CFF loadings were raised from 0.5 to 1.5wt%. The tensile strength of biocomposites with 2wt% loading was found to be lower than that of pure epoxy. Similar behavior was recorded for young's modulus, flexural strength, impact strength and hardness which is attributable to better dispersion and integration of CFF within the epoxy matrix, as corroborated by morphological images. Furthermore, the simulated results aligned well with the experimental tensile outcomes that showed a homogeneous stress distribution with the applied load greatest value occurring at the center of the gauge length and gradually diminishing along the sample. The eco-friendly materials developed in this study could serve alternative applications, significantly reducing chicken feather waste in the environment and mitigating pollution issues.

Presenter:
Zainab Waheed Abdullah
Middle Technical University, Iraq

Resveratrol and Selenium Nanoparticles: A Biochemical and Molecular Assessment for the Treatment of Type 2 Diabetes and Associated Complications

Mahmoud Balbaa, Aya Y. Soliman and **Nihal Elguindy**
Faculty of Science, Department of Biochemistry, Alexandria University, Egypt

Dietary polyphenols, such as resveratrol (Res) and elemental selenium nanoparticles (SeNPs), are increasingly being studied for their therapeutic potential in the treatment and management of type 2 diabetes mellitus. In this study, we evaluated a novel therapeutic method using chitosan-stabilized Res/SeNPs (CS/Res/SeNPs) in a mouse model of T2DM induced by a high-fat diet (HFD) combined with multiple low-dose streptozotocin (STZ) injections. We used biochemical, histological, and molecular docking investigations to determine the impact of these nanoparticles on glucose and insulin levels, oxidative/antioxidant balance, apoptotic and anti-apoptotic gene expression, and inflammatory mediators. Treatment with free Res, CS/Res/SeNPs-5, CS/Res/SeNPs-10, and Metformin (Met) alleviated hyperglycemia, insulin resistance (IR), and dyslipidemia while normalizing increased liver and kidney biomarkers. These therapies also shown anti-inflammatory, antioxidant, and anti-apoptotic properties. CS/Res/SeNPs-10 demonstrated the strongest hepatoprotective and anti-diabetic benefits. The docking results revealed that Res binds to key insulin signaling proteins, such as phosphatidylinositol 3-kinase (PI3K)/protein kinase B (AKT)/mammalian target of rapamycin (mTOR). Overall, our findings show the therapeutic potential of CS/Res/SeNPs in controlling T2DM problems and propose a low-cost strategy for improving diabetic patients' health outcomes and quality of life.

Presenter:
Mahmoud Balbaa
Alexandria University, Egypt

Modeling of the Temperature Dependence of the Diffusion Characteristics of Vacancies in Bcc Titanium

Madina. Boboqambarova and **Andrei. Nazarov**
National Research Nuclear University MEPhI, Russia

Body centered cubic (bcc) titanium (β-Ti) demonstrates significant potential as a highly promising structural material for high-temperature applications and intense radiation exposure. Due to its exceptional ductility, phase transformation stability (up to 1155 K), and compatibility with various alloying elements, β-Ti represents a promising material for next-generation alloys used in advanced energy technologies, aerospace, and nuclear industries. Predicting the kinetics of structural and property changes in metals under extreme conditions requires a fundamental understanding of atomic-scale defect dynamics.Crystal lattice defects, particularly vacancies, play a crucial role in processes such as atomic diffusion, solid-state phase transformations, radiation-induced cluster formation, and radiation damage. The thermodynamic characteristics of vacancies, including their formation energy and formation volume, are essential inputs for predictive multiscale modeling of material degradation and recovery processes. However, experimental determination of these temperature-dependent parameters, especially at elevated temperatures, presents significant challenges due to technical limitations.

This study employs atomistic modeling using a model of natural thermostat [1] based on a combination of molecular dynamics (MD) and modified molecular statics (MMS) [2] methods to investigate vacancies in bcc titanium in high temperatures range. The model accounts for thermal expansion and elastic relaxation around defects, enabling determination of structure in the vicinity of the vacancy and their temperature-dependent evolution. An embedded atom method potential is used in the simulations. The temperature dependences of vacancy formation energy and vacancy formation volume are obtained, and these data, the temperature-corrected parameters provide a foundation for more accurate prediction of structural evolution in titanium and its alloys under severe operating conditions.

Presenter:
Madina Boboqambarova
National Research Nuclear University MEPhI, Russia

Spectroscopic, Structural, and Computational Characterization of a Novel Piperidyl-Sulfonyl-Thiazolidinone Derivative

M. Sarasija[1] And **D. Ashok**[2]

[1]Green and Medicinal Chemistry Laboratory, Department of Chemistry, Satavahana University, India
[2]Department of Chemistry, Jawaharlal Nehru Technological University, India

For more than a century, heterocycles have constituted one of the largest areas of research in organic chemistry. They have contributed to the development of society from a biological and industrial point of view as well as to the understanding of life processes and to the efforts to improve the quality of life. Among the approximately 20 million chemical compounds identified by the end of the second millennium, more than two-thirds are fully or partially aromatic and approximately half are heterocyclic. The presence of heterocycles in all kinds of organic compounds of interest in biology, optics, pharmacology, material sciences and so on is very well known. Between them, sulfur and nitrogen-containing heterocyclic compounds have maintained the interest of researchers through decades of historical development of organic synthesis. However, heterocycles with other heteroatoms such as oxygen, phosphorus and selenium also appears. Many natural drugs such as papaverine, theobromine, quinine, emetine, theophylline, atropine, procaine, codeine, reserpine and morphine are heterocycles. Almost all the compounds we know as synthetic drugs such as diazepam, chlorpromazine, isoniazid, metronidazole, azidothymidine, barbiturates, antipyrine, captopril and methotrexate are also heterocycles.

This study presents the design and synthesis of a novelheterocyclic compoundfeaturing three pharmacophores: piperidyl, sulfonyl, and thiazolidinone. The objective was to evaluate its structural features and pharmacokinetic potential for medicinal applications. The compound was synthesized *via* a stepwise route starting with piperidone hydrochloride, followed by tosylation, condensation with thiosemicarbazide, andcyclization with dimethyl acetylenedicarboxylate. The final product was purified and characterized using high-performance liquid chromatography, Fourier-transform infrared spectroscopy, ultraviolet-visible spectroscopy, nuclear magnetic resonance spectroscopy, and high-resolution mass spectrometry. Computational anal-

ysis was performed using the SwissADME platform.Thespectroscopic and in silico findings confirm that the compound has a well-defined structure and favourable physicochemical properties.

Presenter:
M. Sarasija
Satavahana University, India

Investigation of Biopesticides for the Pest Control Through Inhibition of the Acetylcholinesterase Purified from *Loxostegesticticalis* (L.) (Lepidoptera: Crambidae)

Demet KIZIL

Bursa Technical University Central Research Laboratory, Turkey

Acetylcholinesterase (AChE) is a cholinergic enzyme called acetylcholine acetylhydrolase.Acetylcholinesterase inhibition is one of the prominent methods in studies on pest controlmanagement. In this study, AChE was purified 103.7-fold from *Loxostegesticticalis* (L.)using an Edrophonium-Sepharose 6B affinity column, and some kinetic properties wereinvestigated. The molecular weight of the purified enzyme was determined by Sodium-Dodecyl Sulfate–Polyacrylamide Gel Electrophoresis (SDS-PAGE). Inhibition studies ofAChE were realized with tacrine, edrophonium chloride, and cypermethrin, which areknown inhibitors of AChE, as well as aqueous extracts of certain plant leaves. The subunit molecular weight of purified AChE was estimated to be approximately 56 kDa by SDSPAGE analysis. The maximum activity of Loxostege sticticalis AChE was specified at 40.0 °C and pH 8.0. Vmax, Km, and kcat values of the AChE were determined as 243.9±15.7EU/mg protein, 0.122±0.06 mM, and 13.7±2.7 min−1, respectively. In the inhibition studies, the IC50 values of tacrine, edrophonium chloride and cypermethrin were found to be 3.4±0.5, 0.08±0.006 and 85.0±4.1 µM, respectively. Besides, the IC_{50} values of aqueous extracts of olive leaf, alder leaf, walnut leaf, cherry laurel leaf, and plane leaf were as 12.0±0.6, 15.2±1.3, 32.1±1.5, 58.3±1.9, and 75.2±2.8 µg dry matter/mL, respectively. In addition, the oleuropein and phenolic substance amounts of these plant extracts weredetermined and correlated with the IC_{50} values. Consequently, the plant extracts used inthis study may be recommended as an alternative biopesticide source to control such pestsvia AChE inhibition.

Presenter:

Demet KIZIL

Bursa Technical University Central Research Laboratory, Turkey

Failure Analysis of a Heavy-Duty Fastener used in Hydraulic Systems: An Inspiring Study

P. Aravind[1], K. H. Harsha[1], M. Vinod Kambli[1], C.D. Parasurama[1], P. Sampath Kumaran[2] and **T. S. Srivatsan[3]**

[1]AVH Innovations and Metallurgical Laboratory [AVH], India
[2]Department of Mechanical Engineering, Sambhram Institute of Technology, India
[3]Professor (Emeritus), Department of Mechanical Engineering, The University of AKRON, USA

Background: A cone point set screw is a headless screw with a sharp, conical point that bites into a shaft with the prime purpose of ensuring a permanent setting. The "M30" cone screw refers to a specific type of fastener with a metric thread size of 30mm and is often chosen for use as an anchor component in the industries spanning 'civil' construction and 'heavy-duty' machinery. In this connection, a M30 cone screw that was subjected to a static load of 2.5-ton kg and was repeatedly used multiple times during a construction. This did necessitate a need to systematically assess both the material properties and its conformance with product specifications for the purpose of its selection and use.

Objective: Around a batch of 300 numbers of the M30 cone screw were subject to repeated use in a specific construction site and all of the chosen screws were subjected to the same loading condition. However, one of the M30 cone screws did fail by complete fractured and broken immediately following after 8 hours of its installation at a specific construction site. The primary purpose of this inspiring research Investigation was to focus on assessing the underlying factors that contributed towards catastrophic failure of the M30 cone screw failure at the construction site. Results aided by careful observation and concomitant analysis does provide a useful knowledge specific to the prevention of such failures while concurrently ensuring reliability in the industry specific to "civil" construction industry and ensuring its service for the indented application.

Methods: In this innovative and inspiring research study, a failed M30 cone screw was retrieved from a construction site and a series of tests were performed in a systematic and methodical manner. The tests included the following: (i) Hardness Test, (ii) Chemical composition, (iii) Microstructure characterization, (iv) Inclusion content, (v) scanning electron microscopy (SEM)

observation, (vi) Energy Dispersive X-ray (EDAX) analysis, and (vii) Radiography Test. These tests were performed to carefully assess both properties and characteristics based on the requirements of the desired product.

Results:

- Chemical composition of the M30 cone screw sample was analysed with the standard specification of the steel grade 10.9 of IS 1367 (P-3) -17

- The Hardness test results did reveal the “value” to be beyond the maximum limit. This does reveal a greater tendency for failure by brittle fracture and does have a detrimental effect and/or influence on overall mechanical properties and performance of the bolt

- Careful and comprehensive examination of the microstructure did clearly reveal a banded matrix of tempered martensite both at and near the vicinity of the cracked region. The presence of the banded matrix did cause structural stress differences at the fine microscopic level, thereby the existence of a high degree of anisotropic characteristics at the “local” level . This is an undesirable property development which does have a potential negative impact on overall performance of the specific bolt.

- It is evident from the SEM-EDAX analysis carried out near the cracked region to reveal a healthy population of second-phase particles, or inclusions, i.e., the manganese-sulphide (Mn-S), that favour the early initiation of fine microscopic voids at the local level. Coalescence of the fine microscopic voids results in the formation and presence of microscopic cracks in the microstructure of the cone screw sample.

- The radiography test results clearly reveal the presence of slag inclusions near the region of the fine microscopic cracks and this was confirmed through EDAX analysis

Conclusions: In essence the reason for failure of the bolt screw can be attributed to the conjoint and mutually interactive influences of the following: (i) high hardness, (ii) presence of second-phase particles in the microstructure, (iii) presence of manganese-sulphide (MnS) inclusions in the microstructure, and (iv) a banded matrix microstructure of tempered martensite in the immediate vicinity of the fine microscopic cracks. Based on the above-mentioned findings failure of the chosen and studied M30 cone

screw occurred with respect to other bolts that belonged to the same lot, which were all subjected to the same loading (2.5 metric ton) and exposed to the same environment.

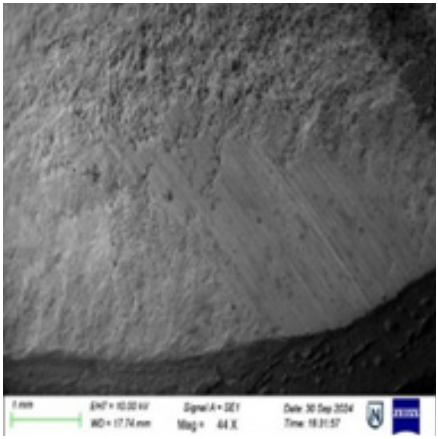


Figure 1a (Macro region - Crack Initiated @ 44 x)

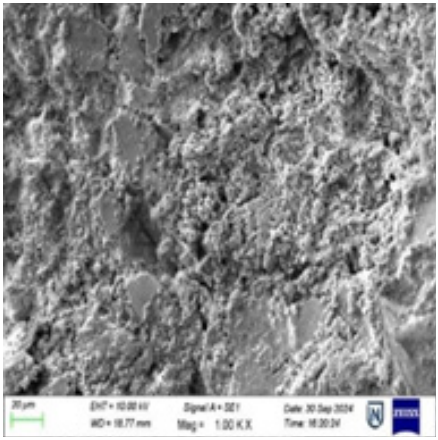


Figure.1b (SEM micrograph @ 1000 x)

Presenter:
Aravind P
AVH Innovations and Metallurgical Laboratory, India

Isotropic Phase of nematogens: Solving Landau–de Gennes Modelling Problems

Aleksandra Drozd-Rzoska and **Sylwester J. Rzoska**
Institute of High Pressure Physics "Unipress", Poland

The Landau–de Gennes model is an essential fundamental framework in the *Physics of Liquid Crystals and Soft Matter Physics*. Basically, it is validated by the universal parameterisation of the Cotton–Mouton effect, the Kerr effect, and light scattering in the isotropic phase of nematogenic liquid crystals. However, as early as 1974, de Gennes identified the first two puzzling problems of this model. Over the following decades, this list has expanded.

This report presents the first comprehensive analysis of these issues, with the explicit experimental reference. It also recalls the poorly discussed pretransitional changes in the dielectric constant and the extension under a strong electric field (E): the *Nonlinear Dielectric Effect* (NDE). Notably, there are distinct pretransitional forms of pretransitional effects, depending on molecular structural features such as permanent dipole moment loci or steric hindrance. It is tested for 5CB, 5*CB, and MBBA: nematogenic liquid crystalline materials that differ in the above features.

The presented results reveal the interplay between observation and pretransitional fluctuation timescales, leading to a new, coherent model that explains puzzling issues in line with experiments. The question of whether this approach can be linked to the Landau–de Gennes canonical model picture arises.

Acknowledgement: This research was funded by the National Center for Science (NCN, Poland), grant number NCN OPUS 2022/45/B/ST5/04005

Presenter:
Aleksandra Drozd-Rzoska and Sylwester J. Rzoska
Institute of High Pressure Physics "Unipress", Poland

Green Nanotechnology Approaches for Sustainable Drilling Fluid Formulations

Borkha Mech and **Debashree Dutta**

Department of Petroleum Technology, Dibrugarh University, India

Objective and Scope: Green nanotechnology offers a sustainable pathway for improving drilling fluid performance while minimizing environmental impact. The synthesis of green nanoparticles (GNPs) using plant-derived extracts is an emerging approach that combines eco-friendliness with cost-effectiveness. Plant sources act as natural reducing and stabilizing agents due to their diverse phytochemical constituents, including phenols, flavonoids (such as quercetin), and primary amines. These biomolecules enable controlled synthesis of nanoparticles by serving as both capping and reducing agents. By utilizing such renewable resources, green nanotechnology promotes the development of drilling fluid additives that are both environmentally benign and functionally efficient.

Methodology: In pursuit of sustainable drilling fluid formulations, this study employed extracts from Tea, Mango, Curry, Neem, Tulsi, and Guava leaves to synthesize iron oxide, copper oxide, and silver nanoparticles. The nanoparticles were characterized using a particle size analyzer and scanning electron microscopy (SEM) to assess their size distribution and morphology. Their performance was evaluated by incorporating them into water-based drilling fluids, followed by rheological and filtration testing to determine the impact of GNPs on fluid behavior and efficiency.

Results: Characterization results confirmed successful synthesis of all three types of nanoparticles, with copper oxide nanoparticles exhibiting the smallest particle size. Rheological studies revealed a notable improvement in plastic viscosity, particularly with nanoparticles derived from tea leaf extract, where viscosity increased from 15 cP (base fluid) to 18 cP. Filtration tests further demonstrated enhanced performance, with significant reduction in fluid loss observed upon the addition of copper oxide nanoparticles synthesized from tea and mango leaf extracts.

Conclusion: Green nanoparticles enhance the rheological and filtration performance of water-based drilling fluids, improving drilling efficiency. This highlights the potential of green nanotechnology to develop sustainable formulations that minimize dependence on synthetic additives while meeting environmental and economic goals.

Presenter:
Borkha Mech
Dibrugarh University, India

Future Directions of the Heterogeneous Catalysis: Polyoxometalate-Based Covalent Organic Frameworks

ArashEbrahimi, LukášKrivosudský, SaeedKhodabakhshi, Masoud Khaleghiabbasabadi, Masoud Sadeghi and Martin Motola

Faculty of Natural Sciences, Department of Inorganic Chemistry, Comenius University in Bratislava, Slovakia

The emerging polyoxometalate-based covalent organic frameworks (POMCOFs)—a cutting- edge class of futuristic porous compounds—has significantly broadened the practical scope of the state-of-the-art heterogeneous catalysis. The aforementioned crystalline materials have exhibited their extraordinary performances in miscellaneous catalytic exploitation involving redox reaction, organic processes, water splitting, and environmental preservation. The integration of the individual features of both polyoxometalates (POMs) and covalent organic frameworks (COFs) provides POMCOFs with a united system possessing improved functionalgroups,betterchargetransformationandenhancedcatalyticefficiency.Continuing studies will not only expand their flexibility and competence, but also direct new possibilities forschemingthefuture generation of catalytic platformsable tocatalyzeawidespread range of chemical reactions. This demonstration presents the most recent synthetic methods and catalytic capabilities of POMCOFs, systematizes their categorization, and proposes a forward-looking viewpoint on evolving these areas of material chemistry.

Presenter:
Arash Ebrahimi
Comenius University in Bratislava, Slovakia

Near-Infrared Spectroscopic Detection of Chemical Signatures Associated with External Flavor Addition in Green Coffee

Jaime Daniel Bustos-Vanegas[1], Andrés Felipe Bahamon[1], Nelson Gutiérrez-Guzmán[1] and **Leonardo Henao[2]**

[1]Universidad Surcolombiana, Colombia
[2]Café Santa Bárbara SAS, Colombia

The growing commercialization of green coffees subjected to external flavor addition during fermentation has generated the need for objective analytical tools capable of differentiating naturally processed coffees from chemically flavored counterparts. Although these products are often referred to as “infused” or “co-fermented,” the underlying process typically involves the deliberate addition of natural or artificial flavoring agents during fermentation. In this study, near-infrared (NIR) spectroscopy coupled with chemometric modeling was investigated as a non-destructive approach to detect chemical signatures associated with such flavoring practices. A dataset comprising 25 flavored green coffee samples and 79 non-flavored wet-processed coffees was analyzed in diffuse reflectance mode (log(1/R)), with five replicate measurements per sample. Spectral preprocessing included interpolation to a common grid, median-based quality control using an interquartile range (IQR) criterion, and standardization prior to modeling. Supervised classifiers were evaluated within a unified pipeline, with logistic regression providing stable discrimination between flavored and non-flavored coffees (AUC = 1.00 in internal validation). A dataset comprising 25 flavored green coffee samples and 79 non-flavored wet-processed coffees was analyzed in diffuse reflectance mode (log(1/R)), with five replicate measurements per sample. Spectral preprocessing included interpolation to a common grid, median-based quality control using an interquartile range (IQR) criterion, and standardization prior to modeling. Supervised classifiers were evaluated within a unified pipeline, with logistic regression providing stable discrimination between flavored and non-flavored coffees (AUC = 1.00 in internal validation). Unsupervised clustering within the flavored subset revealed multiple chemometric subgroups, suggesting variability in flavor carrier concentration, chemical composition of the flavoring agents, or differences in application protocol. These findings demonstrate that NIR spectroscopy is sensitive not only to the presence of externally added flavoring compounds but also to composi-

tional heterogeneity within flavored green coffees, supporting its potential as a rapid screening tool for authenticity and chemical profiling.

Presenter:
Jaime Daniel Bustos Vanegas
Universidad Surcolombiana, Colombia

Evaluation of the Effect of Precursor NMC622@ TiO_2 Core–Shell Powders Using a Prelithiated Anode from Fig Seeds: Spotlight on Li-Ion Full-Cell Performance

Rawdah Whba[1,2], Ebru Doğan[2], Iqra Moeez[3], Ali Hussain Umar Bhatti[3], Muhammad Akbar[3], Kyung Yoon Chung[3], Emine Altin[4], Mehmet Nurullah Ates[5,6], Sebahat Altundag[2], Radostina Stoyanova[7], Sevda Sahinbay[8] and **Serdar Altin[2]**

[1]Faculty of Applied Sciences, Department of Chemistry, Taiz University, Yemen
[2]Physics Department, Inonu University, Türkiye
[3]Energy Storage Research Center, Korea Institute of Science and Technology, Republic of Korea
[4]Vocational School of Health Service, Inonu University, Turkey
[5]Chemistry Department, Bogazici University, Turkey
[6]TÜBİTAK Rail Transport Technologies Institute, Energy Storage Division, TÜBİTAK Gebze Campus, Turkey
[7]Institute of General and Inorganic Chemistry, Bulgarian Academi of Sicences, Bulgaria
[8]Istanbul Technical University, Department of Physics Engineering, Turkey

In this study, innovative electrode materials for lithium-ion batteries (LIBs) were developed and extensively characterized, resulting in notable improvements in electrochemical performance. The cathode material, NMC622@ TiO_2, was synthesized using a wet-chemical method with titanium(IV) ethoxide as the titanium source. Advanced structural analyses confirmed the successful formation of a core@shell architecture, where the TiO_2 coating effectively minimized cation mixing (Li^+/Ni^{2+}) at the NMC622 surface. This structural refinement was directly linked to enhanced electrochemical properties, including improved reversibility and stability. In parallel, a sustainable approach was adopted for anode development, utilizing biomass-derived precursors—specifically fig seeds—to produce carbon-based materials through high-temperature carbonization under an argon atmosphere. Raman spectroscopy indicated a graphitic nature of the resulting material, with an ID/IG ratio of 0.5, suggesting favorable conductivity. Electrochemical performance was evaluated using half-cell configurations, and the TiO_2 coating process was optimized through diffusion coefficient measurements obtained from galvanostatic intermittent titration technique (GITT) experiments. Among the tested variants, the NMC622-T2 condition emerged as

optimal, offering the best coating integrity and electrochemical results due to minimized Li^{+}/Ni^{2+} mixing in the a–b plane. Subsequently, full-cell designs were developed incorporating a prelithiation strategy for the fig-seed-derived carbon anodes, implemented *via* a direct contact method. Unlike prior studies that focused on half-cell prelithiation, this work emphasized full-cell galvanostatic testing, yielding more realistic insights into device-level performance. The combination of prelithiated carbon anodes with TiO_2-coated NMC622 cathodes led to superior cycling stability and capacity retention, outperforming cells with uncoated cathodes over 500 cycles. This research demonstrates the synergistic potential of biomass-based anode materials and engineered cathode surfaces for high-performance, sustainable LIBs.

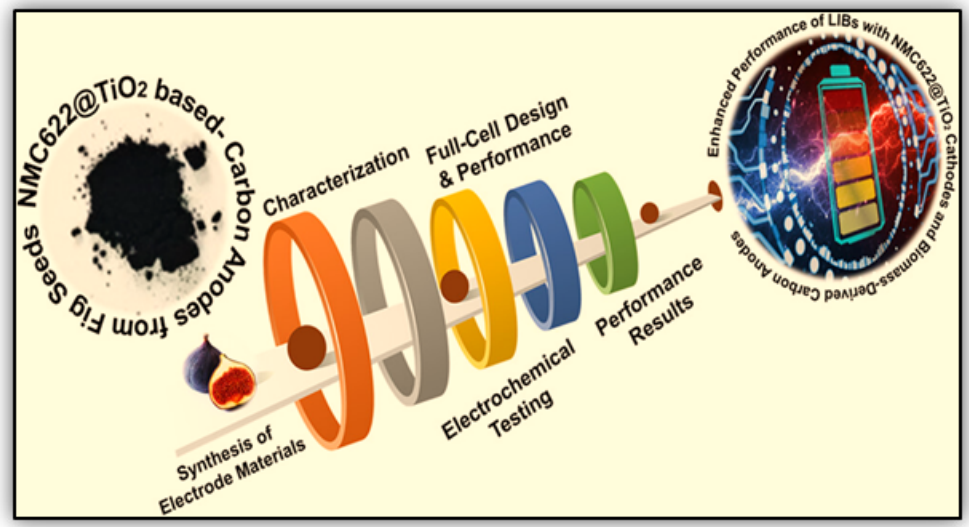


Fig.1 Full-cell performance of NMC622@TiO_2 with prelithiated fig-seed anodes, showing enhanced capacity and stability.

Presenter:
Rawdah Abduh Ghaleb Whba
Taiz University, Yemen

Bridging Empirical Formulations and Machine Learning Approaches For Soil Infiltration Modeling in the Mitidja Plain

MAZIGHI Amina, MEDDI Mohamed and **MEDDI Hind**
Higher National School of Hydraulics of Blida, Algeria

Accurate characterization of soil infiltration processes is a critical prerequisite for effective water resource management in the Mitidja plain, a key agricultural zone in Algeria. This study evaluates the performance of empirical and machine learning models in simulating infiltration, based on experimental data collected from seven sites with contrasting soil conditions. Two widely used empirical models, Kostiakov and Horton, were compared against two data-driven algorithms: Random Forest (RF) and Light Gradient Boosting Machine (LightGBM). Model performance was assessed using multiple statistical criteria, including the Nash–Sutcliffe Efficiency (NSE), Normalized Root Mean Square Error (NRMSE), Correlation Coefficient (CC), RMSE-observations Standard Deviation Ratio (RSR), and Percent Bias (PBIAS). Results indicate that the Horton model provided the best performance among empirical formulations. However, RF achieved superior accuracy overall, with higher NSE and CC values and notably lower PBIAS compared to Horton, highlighting its ability to better capture the nonlinear dynamics of infiltration. LightGBM showed competitive but slightly weaker results than RF. These findings demonstrate the potential of machine learning, particularly RF, to surpass traditional empirical models, offering more reliable predictions for infiltration modeling and supporting improved water management strategies in semi-arid agricultural regions.

Presenter:
MAZIGHI Amina
Higher National School of Hydraulics of Blida, Algeria

Contaminants of Emerging Concern on Microplastics Found in the *Chrysaora Chesapeakei* of the Patuxent River, Chesapeake Bay, MD

Carol A. Smith[1], Natalie Drichko[2], Miranda Lorenzo[2] and **Saroj Pramanik[1]**

[1]Department of Biology, Morgan State University, USA
[2]Department of Physics and Astronomy, Johns Hopkins University, USA

Microplastics are emerging pollutants that are increasingly found in every layer of our biosphere, impacting human health, agriculture, and ecosystems. Their effects are complex and depend on factors such as particle size, additives used, the hydrophobic surface layer, plastic type, and concentration. In previous research, we reported a series of volatile organic compounds, both toxic and non-toxic, identified from microplastics extracted from the gelatinous layer of jellyfish (Chrysaora chesapeakei) collected from Chesapeake Bay (MD, USA) using gas chromatography-mass spectrometry (GC-MS). In the current study, we advance our investigation by exploring the critical interaction between the hydrophobic surfaces of microplastics and adjacent waters contaminated with insoluble toxic chemicals.

This interplay significantly amplifies microplastic toxicity beyond their initial state, with specific consequences varying by plastic type. By employing Raman spectroscopy and analyzing spectra with Wiley's KnowItAll Software, we identified a wide range of contaminants, including pesticides, pharmaceuticals, minerals, food derivatives, chemicals from wastewater treatment, hormones, and recreational drugs. These findings underscore the emerging environmental concerns about microplastics. To safeguard our ecosystems and public health, we must urgently pursue further research and only by comprehensively understanding and addressing the ecological threats posed by the coexistence of microplastics and these harmful contaminants can we hope to mitigate their impact.

Presenter:
Carol Adrianne Smith
Morgan State University, USA

Actinobacteria from Nocardiaceae Family as Nanomaterial Factories

Lucía Ortega Cabello[1], Aída Hamdan Partida[2], Liliana Hernández Vázquez[1], Diego Arroyo Peralta[3], Ana C. Zárate Jiménez[3] and **Bella S. Jacuinde Chacón[4]**

[1]Departamento de SistemasBiológicos, Universidad Autónoma Metropolitana, México
[2]Departamento de Atención a la Salud, Universidad Autónoma Metropolitana, México
[3]Maestría en Ciencias Farmacéuticas, Universidad Autónoma Metropolitana, México
[4]Universidad Abierta y a Distancia de México, México

Recently, the production of nanomaterials has become of great interestdue to the diversity of applications, from electronics to health; regarding health there have been interesting applications, such as imaging due to the optic properties of nanomaterials, and as possible alternative treatments for cancer and antibiotic resistance. However, the conventional methods, even though the advantages that these methods present, there are several disadvantages such as the difficulty of reaching extreme reactions conditions and the generation of hazardous residues; as alternative, plants and microorganisms due to their enzymatic systems (such as oxidoreductases), as well as their secondary metabolites (such as flavonoids, terpenoids and alkaloids), have become a medium to obtain nanomaterials in an ecofriendly manner. In this regard, actinobacteria such as *Rhodococcus ruber* and *Dietzia mar* is were used for the extracellular synthesis of silver nanoparticles (AgNPs) for antibiotic resistance and cervical cancer, secondary metabolites were extracted and characterized through metabolic screening and enzymatic kinetics were also carried out, reduction of silver nitrate was carried out at 30°C, 150 rpm for 5 days, AgNPs were characterized through spectroscopy and microscopic techniques, Kirby-Bauer was carried out for antibacterial activity and MTT assay was carried out for cellular viability in HeLa cervical cancer cell line.Enzymatic activity was evaluated as well as different secondary metabolites were detected (tannins, flavonoids, carbohydrates, coumarins, alkaloids, glycosides, proteins, and anthraquinones) polyhedricAgNPs were obtained ranging from 3 to 40 nm, with good antibacterial activity in resistant bacteria and a 40% inhibition of cervical cancer cell line. Actinobacteria from the Nocardiaceae family may be used for the extracellular synthesis of AgNPs, which presented good antibacterial activity and antineoplastic activity, further optimization for AgNPs production should be carried out as well as evaluation of antineoplastic activity in other cancer cell lines.

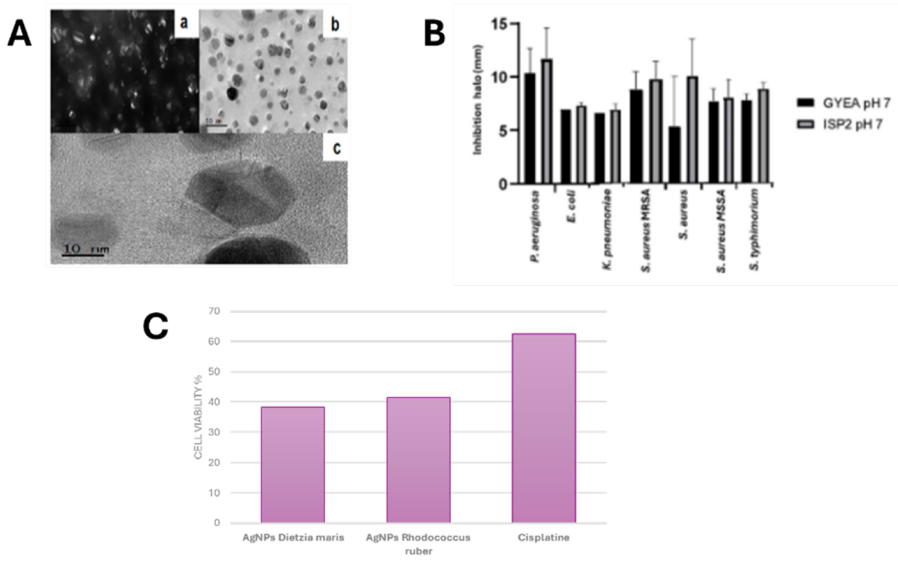


Figure 1. Results obtained from this research: A: microscopical characterization; B: inhibition halos from Kirby-Bauer test; C: cell viability test.

Presenter:
Lucía Ortega Cabello
Universidad Autónoma Metropolitana, México

Sulfonation Degree by Different Analytical Techniques for Sulfonated Aromatic Polymers

J.C. Sanchez Hiza[1], R. Benavides[1], D. Morales Acosta[1], L. Da Silva[1] and **L. Francisco Vieira[2]**

[1]Centro de Investigación en Química Aplicada, México
[2]Instituto Nacional de Investigaciones Nucleares (ININ), México.

Sulfonated aromatic polymers (SAPs) are highly versatile materials useful for a wide range of applications. Extensive research has recently focused on the modification of styrene derivatives to obtain SAPs; however, the determination of the degree of sulfonation (DS), the average number of sulfonic groups grafted per aromatic unit may vary significantly depending on the structure of the polymer matrix.In this work, several analytical techniques were employed to determine the DSof ionomers obtainedby homogeneous sulfonation of HIPS, as well as ionomeric membranes prepared from these materials. The sulfonation process was carried out using acetyl sulfate as a mild sulfonating agent, for the modification of HIPSin solution, and the ionomer obtained was prepared as membrane by dissolving in methyl ethyl ketone (MEK) as a solvent. The DS was determined using three analytical techniques: Proton Nuclear Magnetic Resonance (^{1}H NMR) and Thermogravimetric Analysis (TGA) for the ionomers and ion exchange capacity (IEC) measurements for the membranes.The DS determined by ^{1}H NMR showed values of approximately 10%, whereas TGA analysis yielded a DS of about 16 %. The higher DS obtained by TGA isattributed not only to sulfonic acid groups but also to side reaction events, such as sulfone-type crosslinking (Ar–SO_2–Ar), occurring during the sulfonation process.The DS determined in the membranes by IEC was approximately 8%, which is in good agreement with the values obtained by ^{1}H NMR, although slightly lower. This difference is attributed to the availability of sulfonic groups during membrane preparation. Establishing a direct comparison among results obtained by different analytical techniques is challenging; however, through our methods, the obtained values are consistent with the analyzed structure, whether ionomer or membrane.

Presenter:
Juan Carlos Sanchez Hiza
Centro de Investigación en Química Aplicada, México

Sensitive Lophine Layer for the Detection of Hydrogen Ions (H+)

Pedro Marcos Velasco Bolom and **Jorge Luis Camas Anzueto**
Tecnológico Nacional de México/Instituto Tecnológico de Tuxtla Gutiérrez, México

This work presents results relating the behavior of lophine molecules to hydrogen ions in water. Spectroscopic results are presented, specifically showing the dependence of absorbance changes on pH levels in water. The results demonstrate that the material exhibits a hyperchromic shift, opening the door to its direct application in a fiber-optic sensor. In this case, we found that lophine has a dynamic pH range of 5 to 11.3. Furthermore, we present satisfactory results when lophine was deposited on a thinned optical fiber. In this case, an intrinsic fiber optic sensor configuration was used, achieving a sensitivity of 0.27 dB/pH. work. One figure and one table can be included in your results and discussions.

Presenter:

Pedro Marcos Velasco Bolom and **Jorge Luis Camas Anzueto**
Tecnológico Nacional de México/Instituto Tecnológico de Tuxtla Gutiérrez, México

From Chemical Characterization to Biological Function: Bioactive Compounds from Brazilian Tropical Fruit Byproducts

JailanedeSouzaAquino[1,2,3], LuanaClementinoSantos[1,2], Jordania Candice Costa Silva[1,2], Kamila Sabino Batista[1,3], JanuseMílliaDantas de Araújo[1,4], and **Alana Natalícia Vasconcelos de Araújo[1,4]**

[1]Experimental Nutrition Laboratory, Department of Nutrition, Federal University of Paraíba (UFPB), Brazil
[2]Secretariat for Health and Environmental Surveillance, Ministry of Health, Brazil.
[3]Post Graduate Program in Food Sciences and Technology, Federal University of Paraíba (UFPB), Brazil
[4]Post Graduate Program in Nutrition Sciences, Federal University of Paraíba (UFPB), Brazil

Brazilian tropical fruits constitute a chemically diverse yet underexplored source of bioactive compounds, particularly when agro-industrial byproducts such as peels, seeds, and residual pulps are considered. Within a circular economy framework, these matrices represent valuable resources that can be transformed into high-value functional ingredients. The objective of this lecture is to demonstrate how chemical characterization of tropical fruit byproducts can be directly linked to their biological functions and health-related effects, supporting sustainable valorization strategies. The scope of this presentation includes Brazilian fruits such as acerola (*Malpighia emarginata*), cajá (*Spondias mombin*), Malayapple (*Syzygium malaccense*),and jaboticaba (*Myrciaria jaboticaba*).The methodological approach integrates detailed compositional analyses—phenolic profiling, carotenoids, organic acids, vitamin C, dietary fibers, and fermentable substrates—using chromatographic and spectrophotometric techniques, combined with *in vivo* experimental models of diet-induced metabolic dysfunction. Biological outcomes wereassessed through metabolic, inflammatory, and oxidative stressmarkers, as well as parameters related tolipid and glucose metabolism, hepatic steatosis, and gut–liver interactions. The results consistently demonstrate that fruit byproducts are chemically enriched in polyphenols and structurally complex fibers, often at higher concentrationsthanediblefractions.These chemicalfeaturestranslate intosignificant biologicaleffects,includingreductionsinserumlipidsandglycemia,attenuationofhepaticfat accumulation,enhancementofantioxidantdefenses,modulationofbileacidmetabolism,and beneficialshiftsininflammatoryparametersandgutmicrobiota–derivedmetabolitesalongthe enterohepaticaxis(Table1).Inconclusion,linkingchemical-

compositiontobiologicalfunction provides a robust scientific basis for the valorization of Brazilian tropical fruit byproducts. By integratinganalytical-chemistry,nutritionalbiochemistry,andphysiology,thislecturehighlights their potential as sustainable, high-value bioactive resources for functional food and nutraceutical development, fully aligned with circular economy principles.

Table1. ChemicalCompositionofBrazilianTropicalFruitByproducts.

Fruit	By product	Major Bioactive Compounds	Soluble and Insoluble Dietary Fiber	KeyReported Biological Effects	Main References
Acerola (*Malpighia emarginata*)	Peel, seeds, residual pulp	Polyphenols, vitaminC, carotenoids, organicacids	High	Hypolipidemic, hypoglycemic, antioxidant,anti- inflammatory; enterohepatic modulation	Batista et al.,2023a; Batista et al.,2023b
Cajá (*Spondiasmombin*)	Pulp and peel	Phenolic compounds, carotenoids	Moderate–high	Hepatoprotective, lipid-lowering, antioxidant	Lucena et al.,2022
Malay apple (*Syzygiummalaccense*)	Pulp and peel	Anthocyanins, catechin,gallic acid	Moderate	Lipidmetabolism regulation, hepatoprotection	Nunes et al.,2022
Jaboticaba (*Myrciariajaboticaba*)	Peel and seeds	Anthocyanins, flavonoids, tannins	High	Anti- inflammatory, antioxidant;-gut, kidneyand-lung protection	Araújo et al.,2024

Presenter:
Jailane de Souza Aquino
Federal University of Paraíba (UFPB), Brazil

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SPEAKER TALKS

Automated Multimodal Materials Analysis: A Unified Pipeline for Experimental Characterization Data with ML-Based Nanostructure Identification

Kavitha Jayaram[1], Rakshitha G B[1] and **Vishakantaiah Jayaram[2]**

[1]B N M Institute of Technology, India
[2]Managing Partner, Applied Hypersonic Technologies, India

Modern materials research increasingly relies on the interpretation of multimodal characterization data, including X-ray diffraction (XRD), high-resolution transmission electron microscopy (HRTEM), radial distribution function (RDF) analysis, and thickness profiling. However, conventional analysis workflows remain largely manual, time-consuming, and susceptible to user-dependent variability. This work presents an automated multimodal materials analysis framework designed to accelerate, standardize, and enhance the reproducibility of experimental data interpretation.

The proposed system integrates computer vision, signal processing, and machine learning within a unified pipeline as shown in the Fig. 1. A calibrated digitization engine extracts quantitative data from diffractograms, RDF curves, and thickness profiles using color-based curve isolation, Savitzky–Golay smoothing, and adaptive baseline correction. Domain-specific modules perform XRD phase identification, lattice parameter estimation, and crystallite size calculation *via* the Scherrer equation. Image-based analysis includes SAM-assisted HRTEM segmentation, defect mapping, FFT-based periodicity assessment, and fringe-orientation measurements. Thickness profiling modules evaluate waviness, roughness, and dimensional consistency.

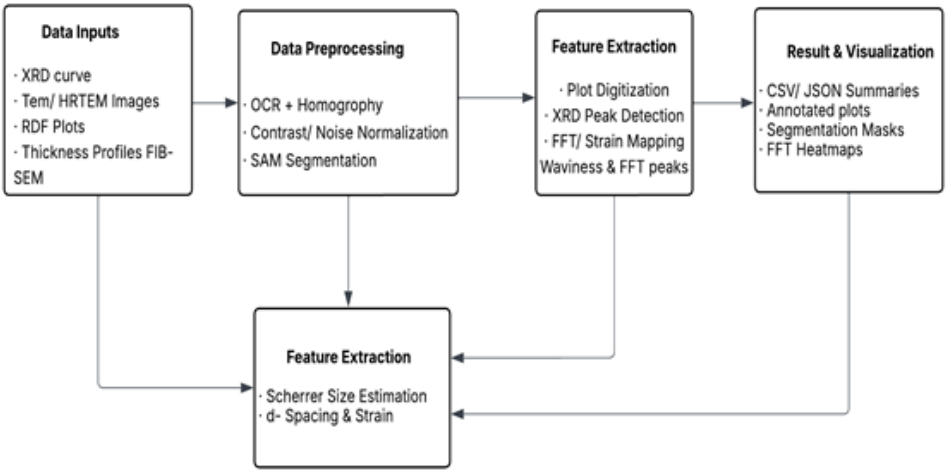


Figure 1: System Architecture and Methodology Workflow

A feature-fusion layer combines descriptors derived from XRD, TEM, RDF, and thickness datasets, enabling robust cross-modal correlation. These integrated features are subsequently employed to train machine learning models, including XGBoost and Random Forest classifiers, for crystalline versus amorphous material discrimination. Batch-processing capabilities and GPU acceleration further support high-throughput analysis.

The framework significantly reduces analysis time while improving consistency, minimizing human bias, and enabling reproducible data outputs. Additionally, the system provides both a Tkinter-based desktop interface for interactive workflows and a Flask-powered web dashboard for end-to-end automated processing. The proposed approach demonstrates the potential of AI-driven multimodal integration in advancing reliable and scalable materials characterization.

The results achieved are: The plot-digitizer reliably reconstructed numerical intensity traces, with OCR-based axis extraction achieving consistent calibration even on low-resolution images as shown in Fig. 2. Peak detection and baseline correction in XRD produced clean peak profiles, and Scherrer estimates closely matched expected crystallite-size ranges for reference quartz and cristobalite SiO_2 compound present in silica tiles is shown in Fig. 3. The software-generated outputs, including tabulated peak parameters and annotated diffraction profiles, enable rapid interpretation and compar-

ison across samples, as illustrated in Fig. 4. The TEM analysis module generates quantitative bright-field metrics, including particle area fraction, void fraction, and equivalent diameter statistics, along with corresponding visual outputs. These results are displayed through a dedicated dashboard interface, as shown in Fig. 5.

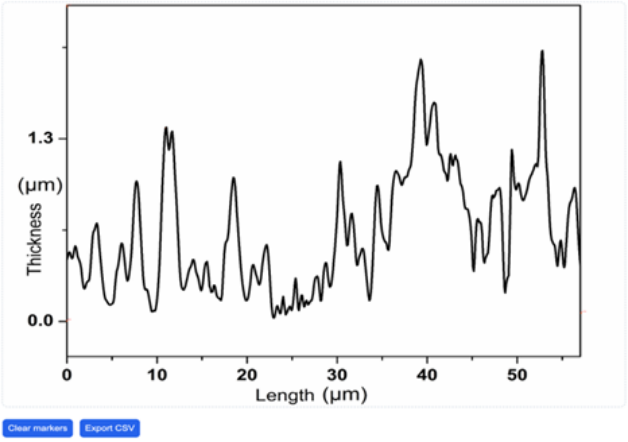


Figure 2: Plot digitization and peak picker

Figure 3: XRD Peak Detection and Scherrer Size Results

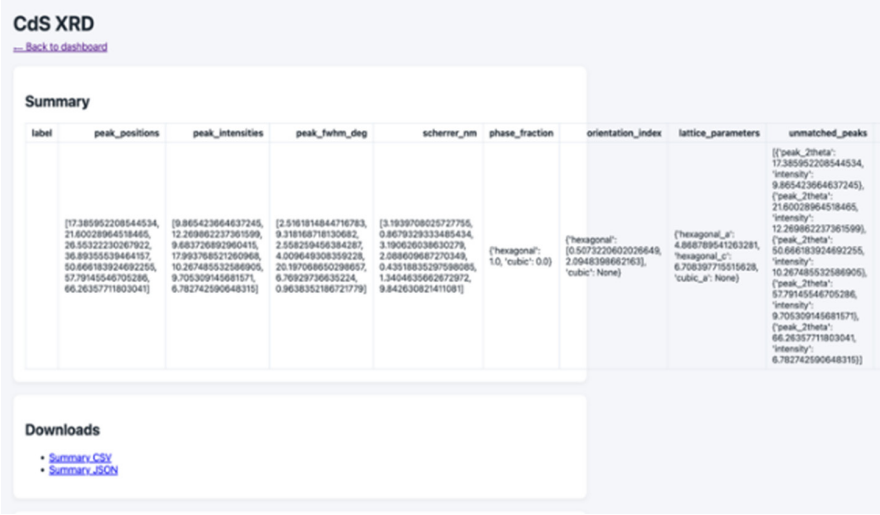


Figure 4: XRD Analysis of CdS with Phase Fraction and Lattice Parameters.

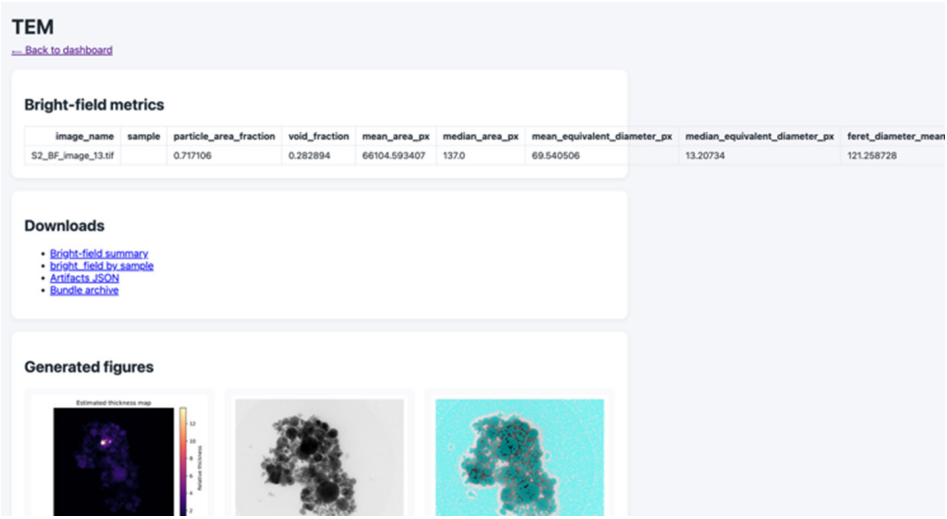


Figure 5: CdS: TEM bright-field segmentation metrics and outputs.

Conclusion

This research work presents a unified and automated workflow for analyzing scientific plots and microscopy data commonly measured using materials characterization techniques. By integrating OCR-based calibration, computer vision techniques, signal-processing pipelines, and AI-driven segmentation, the system eliminates many of the manual, repetitive tasks that traditionally slow down XRD, TEM/HRTEM, RDF, and thickness-profile analysis. The results demonstrate that the framework produces accurate, reproducible, and interpretable outputs across diverse datasets while significantly reducing processing time.

The modular design—supported by both desktop and web interfaces ensures accessibility, scalability, and ease of integration into laboratory and research environments. Overall, the system provides a robust foundation for high-throughput materials analysis and offers a flexible platform that can be extended to additional characterization techniques in future work.

Presenter:
Kavitha Jayaram
B N M Institute of Technology, India

Fluorescent Chemosensors in the Detection of Ultra-Trace Quantity of Toxic Hg^{2+}, Pb^{2+}, Al^{3+}, F^-, AsO_4^{3-}& AsO_{33}-in Water Towards Monitoring Humam Health and Management

Samir Kanti Datta[1], Saugata Konar[1], Shibashis Halder[2] and **Ungwanen John Ahile[3]**

[1]Department of chemistry, The Bhawanipur Education Society College, (Affiliated to the University of Calcutta), India
[2]Department of Chemistry, T.N.B. College, India
[3]Department of Chemistry, Benue State University, Nigeria

Chemosensors have extensive applications in chemical and biological sciences. Fluorescent chemosensors are the most powerful techniques for fast detection of ultra-trace quantity of inorganic ions with high sensitivity. Water is contaminated with various pollutant ions e.g., Cd^{2+}, Cu^{2+}, Hg^{2+}, Pb^{2+}, Mn^{2+}, Zn^{2+}, Al^{3+}, AsO_4^{3-}, AsO_3^{3-} and F^- due to increase industrialisation, usage of fertilizers in agriculture, through food -beverages, water purification instruments and e-wastes. Thus, contaminated drinking water is a potential risk to human health as it transmits various bacterial waterborne disease, so detection of contaminants is essential.

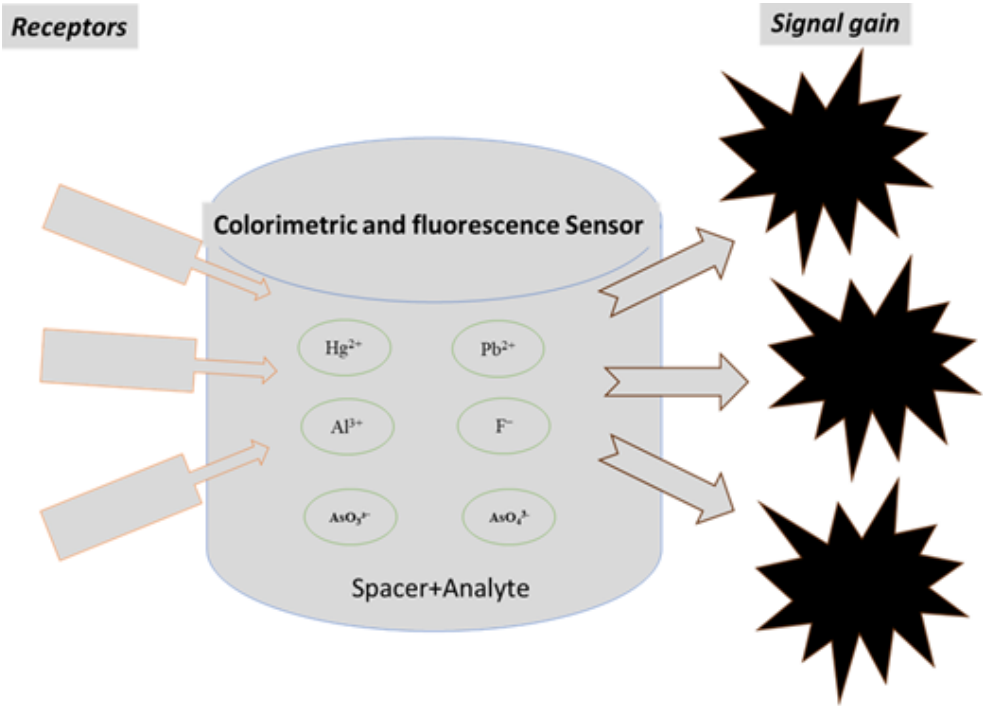
Objective of our work is to detect these trace quantity toxic ions from water bodies, environmental and biological samples thereby protecting and monitoring Humam health.

Regarding methodology we have highlighted here recently developed single, dual and multi-analyte fluorescent chemosensors ligands for the detection through selective binding of trace quantity of critically toxic ions e.g., Hg^{2+}, Pb^{2+}, Al^{3+}, F^-, AsO_3^{3-} and AsO_4^{3-} in water and food samples. Binding of ions through different Sensing mechanism: Intramolecular Charge transfer (ICT), Foster Resonance energy transfer (FRET), Photo induced electron transfer (PET) etc. have also discussed. We have used easily synthesizable chemosensor ligands i) derivatives of rhodamine dyes and phenanthroline ii) Schiff base with rhodamine B thiohydrazide and quinoline moiety iii) a chromone-quinolinyl hydrazide Schiff base as dual sensors iv) Nitro-furaldehyde based Schiff base as multy-analyte sensors for the detection of the concerned toxic ions.

Results: The detection of toxic ions characterized by FTIR, UV-Vis, Fluorescencespectroscopic studies and also by various signalling mechanisms.

Scope: This work will help future researchers to design unknown organic fluorescent Schiff's bases from non-fluorescence Schiff's bases by incorporating specific chromophores like different organic functional groups.

The creation of single, double and multi-ion chemosensors has been vibrant research in recent years due to its biological significance.



Presenter:
Samir Kanti Datta
The Bhawanipur Education Society College, India

A Comparative Analysis of Deep Learning and Machine Learning Models for Fruit and Fruit Disease Recognition: Applications to Citrus, Guava, and Mango

Zarif Wasif Bhuiyan, Rana Rakib, Monayem Hossain Limon, Sayeda Rahnuma Akthar, Tarek Habib and **Mahady Hasan**

Department of Computer Science and Engineering, School of Engineering, Technology and Sciences, Independent University Bangladesh, Bangladesh

Advancements in deep learning (DL) and machine learning (ML) have significantly improved the ability to recognize and classify fruit diseases, offering valuable tools for modern agriculture. This research presents a comprehensive framework for recognizing and classifying diseases in economically important fruits—citrus, guava, and mango—by comparing both DL and ML models. A diverse dataset of 13,700 images was curated, covering multiple fruit disease classes, including citrus black spot, citrus canker, guava phytophthora, guava scab, guava styler and root, mango anthracnose, healthy mango, and mango stem-end rot.

The evaluated models include Convolutional Neural Networks (CNNs) and Shallow Neural Networks (SNNs) as DL models, as well as K-Nearest Neighbors (KNN) and Support Vector Machines (SVM) as ML models, with a focus on assessing their effectiveness in fruit disease recognition. The findings highlight the superiority of DL models, particularly CNN and SNN, in handling complex image classification tasks due to their ability to learn hierarchical feature representations. Meanwhile, ML models such as KNN and SVM provide practical solutions for simpler classification scenarios, especially in resource-constrained environments.

This research supports sustainable farming by offering accessible and efficient tools for early disease detection, benefiting both commercial farmers and small-scale agriculturalists in maintaining crop health and preventing economic losses. Additionally, the comparative analysis provides insights into selecting appropriate models based on accuracy requirements and

computational constraints. analysis offers valuable insights into selecting the most appropriate model based on specific agricultural needs, advancing efforts in precision agriculture and food security.

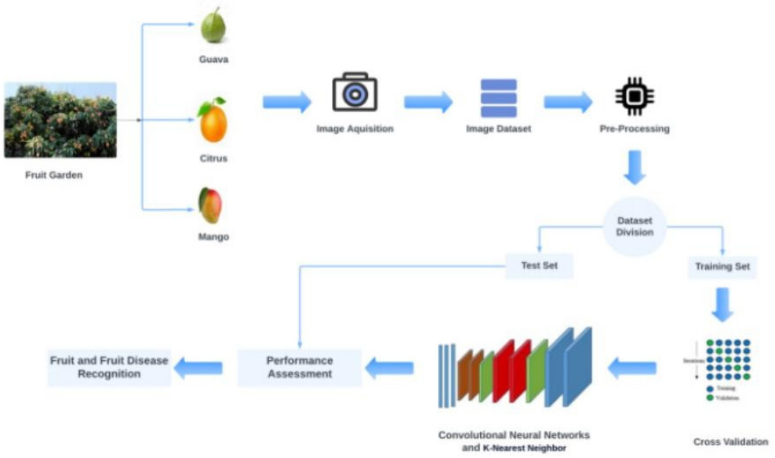


Fig. Conceptualframeworkofthepproposedmethodinthisresearch.

Presenter:
Sayeda Rahnuma Akthar
Independent University Bangladesh, Bangladesh

Uncertainty-Based Efficient Neutrosophic Imputation Methods for Population Mean

Vishal Kumar and **Anoop Kumar**
Central University of Haryana, India

In survey sampling, imputation methods are essential for handling missing data, which can have a large impact on statistical analysis and inference. Neutrosophic logic is an extension of classical logic that provides a robust framework for tackling indeterminate, inconsistent, and incomplete information. In this article, some uncertainty-based efficient neutrosophic imputation methods (ENIMs) and the resulting efficient neutrosophic estimators are developed to estimate the population mean under simple random sampling (SRS). The mean square error (MSE) of the resulting neutrosophic estimators is obtained to the first-order approximation. The proposed ENIMs are evaluated through extensive simulations and real data applications, demonstrating superior performance in terms of reduced MSE and increased percent relative efficiency (PRE). The findings of this study suggest that neutrosophic imputation methods (NIMs) offer a significant advancement in survey sampling methodologies, enhancing the accuracy of statistical inferences in the presence of incomplete data.

Presenter:
Vishal Kumar
Central University of Haryana, India

Integration of Technologies to Study the Interference Effect of Coexisting Ions through Algorithmic Analysis

Parul Taneja[1], Santosha Kumar Dwivedy[1, 2] and **Raj Kumar Gupta[2]**

[1]Technology Innovation Development & Foundation, Indian Institute of Technology Guwahati, India
[2]Department of Mechanical Engineering, Indian Institute of Technology Guwahati, India
[3]Department of Physics, Birla Institute of Technology and Science (BITS), India

The study implements the integration of acoustic mass sensor-based quartz crystal microbalance (QCM) device with electrochemical cell based potentiostat. The idea was taken from the manual of QCM device and implemented with eagerness that how to make QCM device efficient for the real sample monitoring. The quartz wafer clamped between two O-rings and fixed inside the quartz holder, where front face of crystal interacts with aqueous medium. The octadecyl amine carbon nanotubes (ODA-CNTs) Langmuir-Schafer (LS) film functionalized quartz crystal plays the dual role as part of oscillator circuit of QCM and working electrode of potentiostat. From where, EQCM technique has emerged, which complements electrochemical and QCM experiments and gives insights by providing both the results simultaneously. The effect of potential controlled redox reaction is highlighted in the piezo response, which gives a strong intuition between the coordination of these two techniques. The EQCM setup employed for the sensing of divalent metal ions *viz*. Pb (II), Cd (II), and Hg (II). The mildly acidic medium with a scan rate of 0.1 V/s for the cyclic voltammetry (CV) method, these were evaluated as key input features for reliable device performance. Furthermore, the clustering method was applied as a potential unsupervised machine learning algorithm onto mass and voltammogram outcomes. All metal ions are clustered individually and widely spread across the principal components (PCs) plot.

Presenter:
Parul Taneja
Indian Institute of Technology Guwahati, India

Synergistic *Artemisia Monosperma* with Royal Jelly: Antibacterial, Antioxidant, Antibiofilm, and Anti-Alzheimer Potential

Sally Said Ehmedan[1], Naglaa Elshafey[1], Nashwa Hagagy[2,3], Shereen M. Elbanna[4] and **Reham Z. Sadek[4]**

[1]Faculty of Science, Department of Botany & Microbiology, Arish University, Egypt
[2]Department of Biology, College of Science & Arts at Khulis, University of Jeddah, Saudi Arabia
[3]Faculty of Science, Botany & Microbiology Department, Suez Canal University, Egypt
[4]Faculty of Science, Zoology Department, Suez Canal University, Egypt

The increasing prevalence of multidrug-resistant pathogens and neurodegenerative disorders highlights the urgent need for effective, natural therapeutics. This study investigates the synergistic effects of *Artemisia monosperma* leaf extract and fresh royal jelly, focusing on their antibacterial, antioxidant, antibiofilm, and anti-Alzheimer activities.

Gas chromatography–mass spectrometry (GC–MS) revealed 16 compounds in A. monosperma and 13 compounds in royal jelly, including fatty acids, alcohols, and bioactive esters. Both extracts exhibited strong antioxidant potential in the DPPH assay, with IC_{50} values of 5.48 ± 0.002 µg/mL (A. monosperma) and 14.56 ± 0.004 µg/mL (royal jelly). Their 1:1 synergistic mixture significantly enhanced antibacterial efficacy against multidrug-resistant strains (*Bacillus subtilis, Enterococcus faecalis, Staphylococcus aureus, Klebsiella pneumoniae, Salmonella typhi*, and *Pseudomonas aeruginosa*), producing inhibition zones comparable or superior to gentamycin. The combination also markedly reduced bacterial bio film formation.

Furthermore, the extracts inhibited butyrylcholinesterase (BChE), a key enzyme in Alzheimer's disease. IC_{50} values were 4.35 ± 0.002 µg/mL (A. monosperma), 4.9 ± 0.002 µg/mL (royal jelly), and 3.55 ± 0.002 µg/mL (combination), closely aligning with rivastigmine (3.9 ± 0.002 µg/mL). In silico docking confirmed high binding affinities (–6.6 to –10.3 kcal/mol) of major compounds with the human acetylcholinesterase protein, alongside favorable ADMET profiles.

Collectively, the findings highlight that the synergistic bioactive compounds of A. monosperma and royal jelly exert potent antibacterial, antioxidant, an-

tibiofilm, and anti-Alzheimer effects. These results suggest promising applications in phytotherapeutics and drug development targeting multi-drug-resistant infections and neurodegenerative diseases.

Presenter:
Sally Said Ibrahim Ehmedan
Arish University, Egypt

Exploring the Functional Food Potential of *Grand Naine* Banana Flour (GBF) as a Prospective Weaning Formulation by Developing GBF-Based Composite Flour Mixes

Das Mamoni, Hazarika Udipta, Saikia Prapt, Choudhury Manisha and Gohain Donee

Faculty of Community Science, Department of Food Science and Nutrition, Assam Agricultural University, India

This study was focused on investigating a viable and efficient approach for the utilization and valorization of green banana flour (grand naine cultivar, AAA) (GBF). A series of composite mixes were formulated and tested as a source of affordable, energy-rich weaning food with high market acceptance. The complementary mixes included the following additional ingredients, *viz*., rice flour, roasted yellow lentil f lour, pumpkin seed flour, and sesame seed flour, which afforded four composite mixes (MIX-1 to MIX-4) with saliently increasing concentrations of GBF. Further characterizations revealed that the MIX-4 composite mix had the most favourable characteristics in terms of proximate composition, including protein (15%), moisture (4.48%), and total energy values (401.44 kcal). MIX-4 also showed the highest water-absorption capacity (2.57%) and low solubility (8%), akin to complementary mixes. The high total phenolic content (1.03 mg CE per g) and inhibition capacity (47.94%) of MIX-4 suggest that it has a strong antioxidative capacity as well, which was confirmed by the peroxide and free fatty acid studies done over a period of 60 days. Rheological characteristics further confirmed that the resistant starch in GBF played a significant role in lowering the solubility and enhancing the starch gelatinization of MIX-4. Overall, these results corroborated the functional food potential of GBF-based composite flour mixes for the development of prospective weaning food formulations and for reducing post-harvest economic losses.

Presenter:
Mamoni Das
Assam Agricultural University, India

Development of Herbal Toothpaste against Tooth-Associated Ailments

Sakthi Priyadarsini S, Srilakshmi S, Bhujithra M, Srikanth P and **Kabilan G**

Faculty of Medicine and Health Sciences, Department of Pharmacognosy, SRM College of Pharmacy, SRM Institute of Science & Technology, India

Oral health is vital for overall well-being, as numerous dental illnesses affect communities worldwide. Traditional and contemporary dentistry have advanced considerably, emphasizing herbal formulations for effective and safe oral care. This study seeks to develop and assess a new herbal toothpaste that includes medicinal herbs recognized for their antibacterial, anti-inflammatory, and antioxidant characteristics. Four different formulations with varying concentrations of herbal extracts were developed to determine the optimal composition. The formulated toothpastes underwent various physicochemical and antimicrobial assessments to ensure its efficacy and stability. Evaluation parameters included colour, odour, taste, smoothness, homogeneity, tube inertness, abrasiveness, pH, viscosity, spreadability, foaming power, and moisture content. Additionally, Fourier-transform infrared (FT-IR) spectroscopy, thin-layer chromatography (TLC), and fluorescence analysis were employed to characterize the formulations.

The antimicrobial activity of the formulations was assessed using agar-well diffusion tests against key oral pathogens, including *Fusobacterium nucleatum* and *Streptococcus mutans,* which are primarily associated with periodontitis, gingivitis, and dental caries. The results demonstrated significant antibacterial efficacy, indicating the potential of the herbal toothpaste to combat oral infections effectively. Overall, the findings suggest that the developed herbal toothpaste formulations exhibit promising antimicrobial properties, making them a natural and effective alternative to conventional toothpastes.

Presenter:

Sakthi Priyadarsini. S

SRM Institute of Science & Technology, India

The Role of Supply Chain Agility and Resilience in Enhancing Firm Performance

Esra Nur GOKHAN
Beykoz University, Turkey

In today's turbulent and highly competitive business environment, agility and resilience have become indispensable capabilities for supply chains. Firms that can swiftly adapt to changing customer needs and volatile market conditions are more likely to sustain their competitive advantage and improve overall performance. This study investigates how supply chain agility and supply chain resilience influence firm performance, with a particular focus on the mediating role of customer satisfaction. Furthermore, the study explores the moderating effect of digital transformation, emphasizing how digital technologies enhance the relationship between agility and customer responsiveness.

Findings highlight that agile firms, strengthened by resilience, are better positioned to manage risks and uncertainties while maintaining high levels of operational efficiency. Integrating digital technologies into supply chain operations enables companies to respond more rapidly to evolving customer expectations, ultimately driving satisfaction and loyalty. The results contribute to the growing body of literature on supply chain management by bridging perspectives from operations and marketing, while also offering practical insights for managers seeking to align agility, resilience, and digital transformation in their strategies.

This research underlines that in an era defined by uncertainty, firms that invest in both agility and resilience—supported by digital initiatives—are not only more adaptable but also more customer-oriented, which directly translates into superior performance outcomes.

Presenter:
Esra Nur Gokhan
Beykoz University, Turkey

Global Market Trends in Biomedical Sensors: Materials, Device Engineering, and Healthcare Applications

V. R. Palanivelu[1] and **K. Mahalakshmi**[2]

[1]Professor, Department of Management Studies. Periyar University, India
[2]Research scholar, Department of Management Studies, Periyar University, India

This study explores the expanding global market for sensor technologies, with a specific focus on their applications within biomedical materials and devices. It highlights key trends, opportunities and challenges associated with sensor exports, particularly in the context of advancing healthcare technologies. Recent innovations in smart, wireless, and multifunctional sensors have significantly enhanced the capabilities of biomedical devices, supporting more accurate diagnostics, real-time monitoring and therapeutic interventions. These technological developments, combined with the integration of Internet of Things (IoT) platforms, are reshaping performance requirements for implantable devices, with a focus on bio-compatibility, durability, and long-term functionality. Biomedical devices, which play a critical role in restoring and maintaining physiological functions, are witnessing increased demand across healthcare, assistive technologies and industrial biomedical applications. A regional analysis reveals strong market growth in North America, Europe, and Asia–Pacific, with emerging opportunities in Latin America and Africa. Additionally, the rise of smart healthcare systems, remote patient monitoring, and automation in medical and pharmaceutical sectors is further driving the need for advanced sensor integration. This research underscores the potential for exporters and developers of biomedical sensors to diversify into high-impact areas such as wearable health technologies, environmental bio-sensing, and smart agriculture. However, successful participation in global markets requires careful navigation of regulatory frameworks, intellectual property rights and supply chain logistics. Over-all, the biomedical sensor market represents a significant area of growth, particularly for companies capable of innovating in materials, device engineering and adaptive sensor platforms to meet the evolving needs of modern healthcare systems.

Presenter:
V. R. Palanivelu
Periyar University, India

Evaluation of Testicular Protective Effects of *Prunus Amygdalusand* Zinc Against Cadmium Induced Toxicity in Rats

Faiza Zubair, Naila Riaz and **Ayesha Tehreem Shahbaz**
Department of Zoology, University of Sargodha, Pakistan

Cadmium (Cd) and other dense metals are highly toxic and reported to induce infertility through testicular apoptosis and free radicals production. Cd is a widespread pollutant in the atmosphere due to the combustion of automobiles and industries. *Cd→ROS↑→*Damage. This study assessed the harmful impacts of Cd on the reproductive health of humans and all other animals. Combined and individual ameliorative influence of Zinc (Zn) and *Prunus amygdalus* (almonds) on Cd-administered testicular toxicity in male albino Wistar rats was also reported in this research. Rats were divided into five groups: standard, Cd, Cd+Zn+*P. amygdalus*, Cd+Zn, and Cd+*P. amygdalus* groups. Rats were treated with 50 mg/kg of $CdCl_2$ once in a week for 28 days; 17 mg/kg/day $ZnCl_2$ and 400 mg/kg/day *P. amygdalus* were given as a protective measure after 2 h of Cd dosage. Cd toxicity caused a considerable decrease ($P<0.001$) in body weight, testicular weight, level of testosterone, sperm count, sperm motility, count of testicular germ cells, Leydig's cells, and average cross-sectional area (ACSA) of germinal tubules and lumen of germinal tubules. On the other hand, Cd+Zn+*P. amygdalus* rats significantly improved ($P<0.001$) the testicular parameters. Cd+Zn partially improved ($P<0.001$) the fertility of rats, and Cd+*P*. amygdalus slightly improved ($P<0.05$) the gonadal health of male rats. Zn and *P*. amygdalus have a synergistic effect over Cd-intoxication of testes. Out of Zn and *P*. amygdalus, Zn is more effective in mitigating the toxicity of Cd, while combined supplementation is much more effective than individual dosages of protective measures. *Zn+Almond→Antioxidants↑→Repair.*

Presenter:
Faiza Zubair
University of Sargodha, Pakistan

Biochemical Profiling of Freshwater Fish Species from the North-Western Himalayas

Rakesh Kumar, Hishani Kumari and **Kushal Thakur**

Department of Animal Sciences, School of Life Sciences, Central University of Himachal Pradesh, India

The present study evaluated the proximate composition, vitamin content, mineral concentration, and fatty acid profile of three fish species (i.e., Schizothorax richardsonii, Systomus sarana, and Oreochromis niloticus) to assess their nutritional quality and potential health benefits. Moisture content ranged from 78.34% in *S. sarana* to 80.07% in O. *niloticus*, while crude protein was highest in *O.niloticus* (18.91%), followed by *S.sarana*(18.03%) and

S. richardsonii(17.35%). Lipid content varied between 1.04% (O. niloticus) and 3.22% (S. sarana), and carbohydrates ranged from 0.65% (S. richardsonii) to 1.14% (O. niloticus). Among vitamins, S.sarana exhibited higher concentrations of vitaminA (108.07µg/100g) and vitamin D (123.29 µg/100g), where as O.niloticus recorded moderate vitamin D (55.37 µg/100 g) and vitamin K (5.33 µg/100 g) levels. Mineral analysis indicated potassium as the most abundant element across all species, followed by sodium, phosphorus, and iron. Fatty acid profiling revealed species-specific variations among omega-3 fatty acids; *S. richardsonii* showed a higher proportion of eicosapentaenoic acid (EPA-5.69%), and *O. niloticus* showed the highest α-linolenic acid (7.82%). Among MUFA, the *S. sarana* showed higher palmitoleic acid(11.61%). These findings highlight the nutritional significance of the sespecies as valuable sources of essential nutrients supporting human health and dietary diversification.

Presenter:
Rakesh Kumar
Central University of Himachal Pradesh, India

Hydrochemical Assessment and Environmental Value of Karst Springs in Vlore County, Albania

Marinela Muço[1], Fatlinda Shkurti[2] and **Anila Haxhiraj[3]**

[1]Faculty of Technical and Natural Sciences, "Ismail Qemali" University, Albania
[2]Faculty of Human Sciences, "Ismail Qemali" University, Albania
[3]Faculty of Technical and Natural Sciences, "Ismail Qemali" University, Albania

The purpose of this study is the identification, analysis, evaluation and management of karst springs in the geospace of the Vlora region in Albania. Karst springs constitute assets with scientific, hydrological, aesthetic, didactic and touristic values. The Vlora region has a considerable number of karst springs, some of which have the status of Hydromonuments (seven hydromonuments). To achieve the purpose of this work, we first focus on collecting data to identify the springs offered by the area, data that we have from previous publications, statistical data from local and central government, field trips and data presented for the first time in this study. The methodology used to achieve the purpose lies in the use of literature from the fields of geology, chemistry, hydrology, physical geography, tourism geography, scientific studies and articles for this purpose, tourist guides, field expeditions, legislation on protected areas, etc. From the study, we will present the results achieved regarding karst springs, their typification, the characteristics that identify them, since they represent valuable assets for the population living in these areas, but not only, they also must be managed and protected. The conclusions of the paper based on quantitative data show the importance of karst springs and the increasing trend in the number of local and foreign tourists who explore, trespass and visit these hydromonuments with numerous values. Finally, starting from the importance and values of karst springs, their preservation and management helps in the sustainable development of the communities of the Vlora region. With the analysis of the changes that have occurred in the trend of tourist demands, the article also provides some suggestions for updating plans and strategies for the sustainable development and management of karst springs, in the context of nature-based tourism.

Presenter:
Marinela Muco and Fatlinda Shkurti
"Ismail Qemali" University, Albania

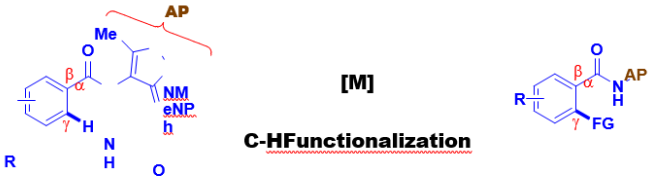
Recent Developments in Directed Metal-Catalyzed C-H Bond Functionalization

Hamad H. Al Mamari

Department of Chemistry, College of Science, Sultan Qaboos University, Sultanate of Oman

C-H Bond functionalization has emerged as a powerful strategy for constructing C-X bonds. Given the ubiquity of C-H bonds in natural products and numerous organic molecules, functionalizing these inert bonds is a vital approach to rapidly access functional molecules and materials. This strategy will enable there cycling of otherwise wasted hydrocarbons and their reuse in an efficient, environmentally benign manner. Therefore, functionalization of C-H bonds is considered a green approach. Recent research as focused on developing strategies to improve the efficiency of C-H bond functionalization. One strategy used to address regioselectivity is the use of directing groups. The use of monodentate and bidentatedirectinggroupsallowsdeliveryofthe transition metal catalyst to a proximal C-H bond and, accordingly,-functionalization of such a bond. Thus, chelation-assistance allows cleavage of an ortho C-H bond with respect to the directing group. Directing groups have allowed a wide range of C-H bond functionalization reactions catalyzed by various second and the more earth- abundant, first row-transition metals.

The presentation will report on developments in metal-catalyzed C-H bond functionalization reactions using a novel directing group recently discovered by our research group. Emphasis will be placed on the use of the cheap and commercially available 4-aminoantipyrine (**AAP**) as a bidentate directing group in metal-catalyzed C-H bond functionalization reactions.



Presenter:

Hamad H. Al Mamari

Sultan Qaboos University, Sultanate of Oman

Analyzing Twitter and Youtube Posts for Identifying Influencers of Apple Products in the Bangalore Region: A Comprehensive Study with Sentiment Analysis

Purushottam Bung[1], Noor Firdoos Jahan[2], Jahnavi M[3], N. Nagasubba Reddy[4] and **Shubha R[5]**

[1]Professor and Director, RV Institute of Management, India
[2]Professor, Department of Marketing,RV Institute of Management, India
[3]Associate Professor, Department of Finance and Business Analytics, RV Institute of Management, India
[4]Research scholar, Assistant Professor, Department of IT and Business Analytics, R V Institute of Management, GITAM (Deemed to be University), India
[5]Executive Content Writer, Infovision, India

The contemporary landscape of marketing strategies navigates through a complex interplay of influencer effectiveness, website analytics, and social media sentiments. This research investigates the multifaceted factors influencing the efficacy of influencers in contemporary marketing, researching into authenticity, relevance, and audience sentiments. Through a rigorous SimilarWeb audit, the study scrutinizes critical insights into website traffic sources, demographic patterns, and user engagement metrics, particularly focusing on Apple's online ecosystem.

Social sentiment analysis on platforms like Twitter and YouTube unveils nuanced insights into audience perceptions and content resonances, emphasizing the prominence of positive sentiments surrounding flagship Apple products. Identifying potential influencers within the Bangalore region becomes pivotal, where a weighted criteria analysis isolates top performers across Twitter and YouTube, shedding light on their impact, engagement metrics, and content sentiments.

Key conclusions highlight the significance of authenticity-driven marketing collaborations, tailored content strategies aligned with platform preferences, and strategic partnerships to amplify reach. The study underscores the need for continuous adaptation based on evolving trends, sentiments, and platform dynamics. In synthesizing these findings, this research not only illuminates the factors shaping influencer marketing effectiveness but also provides actionable insights for refining marketing strategies within the Bangalore market for Apple products. The strategic conclusions drawn from

comprehensive data analysis serve as a guidepost for enhancing brand resonance, user engagement, and audience connection in an ever-evolving digital landscape.

Presenter:
Purushottam Bung
RV Institute of Management, India

Unlocking the Energy Potential of Moroccan Bentonite Clay: Structural, Optical, and Thermal Insights for Advanced Applications

NouraElGhoubali[1,2], AbdelkrimMaaroufi[1], Adnane El Hamidi[2] and **Aumeur El Amarani[3]**

[1]Laboratory of Composite Materials, Polymers and Environment, Faculty of Sciences, Mohammed V University in Rabat, Morocco
[2]Materials, Nanotechnologies and Environment Laboratory, Faculty of Sciences, Mohammed V University in Rabat, Morocco
[3]MIN Research Group, Electrical Engineering Department, ESTM, LASMAR Laboratory, Moulay Ismail University of Meknès, Morocco

This study focuses on exploring Moroccan bentonite clay for its potential applications in the energy sector, particularly by examining its behavior and properties under various conditions.

The main objective is to assess its viability as a material for energy systems, particularly for energy storage, insulation, and advanced energy harvesting technologies.

Bentonite clay solution sat various concentrations were prepared.Monitoringchemical stability over time is essential to understand the clay's behavior under various environmental conditions. Parameters such as pH and electrical conductivity were continuously measured to ensure the stability of the solutions and assess any changes that could affect the clay's performance.

Several key factors were optimized during this process, such as clay concentration, annealing temperature, and stirring time. Opticalmicros copy was usedtovisualizeand refine these factors to produce high-quality films with the desired characteristics. Structural characterizations, including SEM, XRD, and ATR-FTIR, confirmed the presence of a montmorillonite structure, a key mineral component of bentonite, and revealed a homogeneous surface. Thermal analyses, performed by thermo gravimetry (TGA), differential thermogravimetry (DTG), and differential thermal analysis (DTA), were used to study thematerial's responseto temperature variations.Theresults showed significant endothermic effects, indicating dehydration of the water absorbed in the montmorillonite, followed by structural transformation at higher temperatures. Electrical conductivity showed that the clay film sex

hibited excellent insulating properties, suggesting potential applications in fields requiring electrical insulation. In terms of optical properties, thef ilms demonstrated good transparency, which could be useful for applications requiring light transmission. Optical properties, including film thickness, optical band gap, and Ur bach energy, were also determined, highlighting the promising potential of bentonite clay in the energy sector.

The results indicate that bentonite clay could be used as a new, sustainable material for energy applications. This research not only paves the way for more practical uses of this natural resource, but also highlights the importance of understanding its behavior under different environmental conditions in order to tailor it to specific energy applications.

Presenter:
Noura El Ghoubali
Mohammed V University in Rabat, Morocco

Effects of Novel Fulvic Acid Amendments on Soil Structural Stability and Organic Carbon–Nitrogen Pools in Three Agro-Ecological Soils

Mahendar Kumar Soothar[1], Hafeezullah Babar[1] and Xibai Zeng[2]

[1] Agriculture Research Centre, Soil Fertility Research Institute, Pakistan

[2] Institute of Environment and Sustainable Development in Agriculture, Chinese Academy of Agriculture Sciences, China

Organic manures such as Humic and Fulvic acids can enhanced various soil properties such as water holding capacity, increases aggregation and also can directly alter soil structure and influences soil organic carbon (SOC) and Total nitrogen (TN), soil aggregate stability and Mean weight Diameter in soil. In this regard a pot experiment was conducted to evaluate the effect of three organically derived fulvic acids (FA), fulvic acid powder (0.25% S), Natural liquid (0.50% NL) and plant-derived liquid (.50% P) compare with an untreated control (CK) on mean weight diameter (MWD), water-aggregate stability, SOC and TN content in aggregate size distribution (>250 mm, 250–53 mm and <53 mm sizes) in three obstacle soils: Shahjiang Black (SH), Irrigated Desert (IR) and Albic Black (AL). The results demonstrated that FA application markedly improved soil aggregation and nutrient retention, with responses varying among soil types and FA forms. Water-stable aggregates increased by 39.6% in AL soil following the 0.25% S treatment relative to CK, while the highest MWD (1.51) was achieved with the 0.50% P treatment in the same soil. In IR soil, SOC and TN contents in macroaggregates (>2 mm) increased significantly by 35–40% and 60–80%, respectively. The 2–0.25 mm aggregate fraction exhibited higher SOC and TN concentrations in AL soil than in IR and SH soils. Additionally, SOC and TN in the 0.25–0.053 mm fraction increased by 12–40% and 12–16%, respectively, in SH soil. Microaggregates (<0.053 mm) contained the highest TN in AL soil and the highest SOC in SH soil. Overall, these findings indicate that both liquid and solid fulvic acid amendments substantially enhance soil aggregation, promote SOC and N sequestration within different aggregate fractions, and improve overall soil quality. Fulvic acids therefore represent an effective and sustainable strategy for restoring soil structure and supporting long-term agricultural productivity.give clear indication of the objectives, scope, results, methods used, and conclusion of your work. One figure and one table can be included in your results and discussions.

Presenter:

Dr. Hafeezullah Babar

Agriculture Research Centre, Soil Fertility Research Institute, Pakistan

SPH Framework for Solid–Fluid Interaction

Elías Santacruz-Yunga and **Diana Águila Chavez**
Facultad de Ciencias Naturales y Matemáticas, Escuela Superior Politécnica del Litoral (ESPOL), ESPOL Polytechnic University, Ecuador

Accurate modeling of solid–fluid interactions remains a critical challenge in particle-based methods, particularly for applications involving wetting, adhesion, and confined microfluidic flows. In previous work, we introduced a physically motivated pairwise potential formulation for fluid–fluid interactions within a Smoothed Particle Hydrodynamics (SPH) framework, enabling stable representation of cohesive forces and interfacial dynamics. While this approach successfully captured the fluid behavior, extending it consistently to solid boundaries requires additional considerations.

In this study, we present a three-dimensional SPH framework for solid–fluid interaction that explicitly separates impenetrability enforcement from wettability control. Solid surfaces are discretized using fixed boundary particles, and their interaction with the fluid phase is modeled through a distance-dependent normal force composed of two distinct contributions: (i) a short-range repulsive term ensuring non-penetration and numerical stability, and (ii) a smoothly decaying attractive term governing adhesion and effective wettability. This decoupled formulation avoids force discontinuities at the wall, allows independent tuning of contact behavior, and preserves compatibility with the previously developed fluid–fluid pair potential.

The Results demonstrate improved stability near solid boundaries, physically consistent equilibrium shapes, and controlled transition between hydrophilic and hydrophobic regimes without altering bulk fluid properties. The framework provides a robust and extensible basis for modeling complex solid–fluid interactions in microfluidic and multiphase applications, while maintaining physical interpretability and numerical robustness.

Presenter:
Elías Jeffersson Santacruz Yunga
ESPOL Polytechnic University, Ecuador

The Chemistry of Stradivari and Guarneri—The Defining Aspect of their Excellence

Joseph Nagyvary

Professor Emeritus, Department of Biochemistry and Biophysics, Texas A&M University, USA

The mystery of the Stradivarius has for centuries fascinated both violin experts and physicists. This author proposed in 1978 that the tonal differences between Stradivaris and new violins were due to chemical differences of their wood and varnish materials. Initiating our inquiry along these lines, the composite nature of the old Italian varnish was discovered in 1988. For the sound of the instrument, the wood was deemed more important. During the past 40 years, the wood of 10 instruments made during the golden age of Cremona was analyzed in collaboration with many scientists, and all wood samples revealed the presence of preservative minerals and accelerated aging of their wood. This author has proposed that the wood of Stradivari was "green" wood soaked in a mixture of salts and then dried in a suitable hot and smokey chimney space of his roof-top *seccador*. With respect to the underlying chemical mechanisms, two original propositions have been made: 1. the H+ required for the partial hydrolysis of hemicellulose was released from its uronic acids (-COOH) *via* ion-exchange by cations of salts, and 2. atmospheric and chimney CO_2 could play an important role in splitting of the glycosidic linkage by forming a neighboring carbonic ester intermediate. It could then be shown that fresh spruce from Val di Fiemme and Transylvania, having been treated by modeling the above scenario of mineralization and repeated chimney exposure, could be fashioned into new violins which possess the characteristic features of the fine Stradivari or Guarneri sound. Beginning with 1980, an increasing number of luthiers have embraced either the above-mentioned principles or related thermochemical methods, and this has led to the current renaissance of violin making. But luthiers still have their secrets, and so did Stradivari.

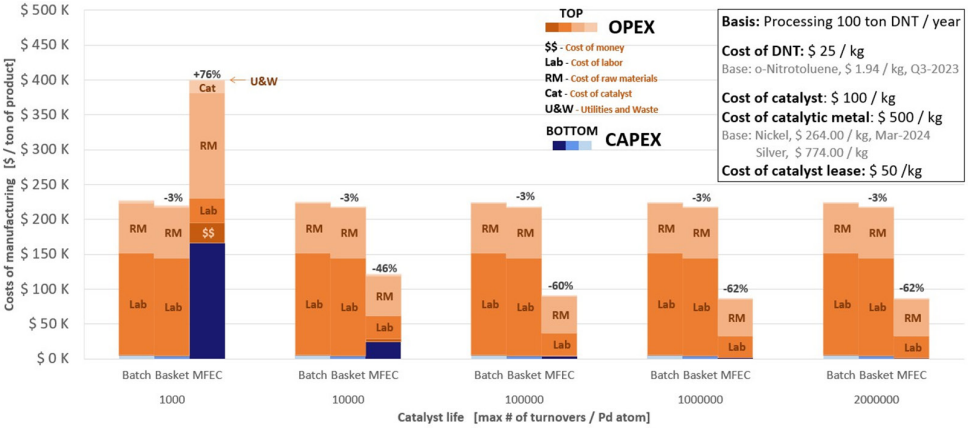
Presenter:
Joseph Nagyvary
Texas A&M University, USA

Comparative Economic Analysis of Batch vs. Continuous Manufacturing in Catalytic Heterogeneous Processes: Impact of Catalyst Activity Maintenance and Materials Costs on Total Costs of Manufacturing in the Production of Fine Chemicals and Pharmaceuticals

Felix Mendoza Suarez and **Bruce Tatarchuk**

Center for Microfibrous Materials Manufacturing (CM3), Auburn University, United States

To evaluate the feasibility of transforming batch manufacturing processes in the fine chemicals and pharmaceutical industries to continuous synthesis, Capex, Opex and the total cost of manufacturing are estimated for production facilities for the hydrogenation of a nitro compound to its final amino counterpart. Two cases are evaluated: First, a high annual production dedicated plant, designed on the basis of processing 100,000 kg of the principal raw material per year, where raw materials cost, catalyst cost, and catalyst activity maintenance are varied over a broad range for typical industrial cases. Second, a “short campaign” model for a small volume production trial setup designed for the manufacture of only 100 kg of the final product, as a way to evaluate relevant industrial scenarios of scale-up and process development. A comparison is made between slurry batch, catalyst basket batch reactor and fixed bed continuous reactor manufacturing facilities. The hydrogenation of 2,4-dinitrotoluene was chosen as a probe reaction for the development of the manufacturing processes, with costs of the key raw material varying between $5 and $100 per kilogram, costs of catalyst varying between $100 and $1,500 per kilogram, and catalyst activity maintenances varying between 1,000 and 2,000,000 total turnovers before a change in catalyst load is necessary. For low catalyst activity maintenance, the total manufacturing costs for the fixed bed reactor process were always found to be higher than those of the two other alternatives. As catalyst activity maintenance increases, the manufacturing costs for the continuous alternative rapidly fall, reaching savings between 37 and 75% compared to the base batch reactor case, depending on the combination of costs of the key raw material and catalyst used.



Presenter:
Felix Mendoza Suarez
Auburn University, United States

Carbazole Derivatives as Platforms for Luminescent Organic and Hybrid Crystalline Materials

Alonso Acosta-Vera[1], Jade Cisneros[2], Erick Hernández Santiago[2], Armando Navarro-Huerta[2] and **Braulio Rodríguez Molina[2]**

[1]Department of Chemistry, University of Rochester, USA
[2]Department of Organic Chemistry, Institute of Chemistry, National Autonomous University of Mexico (UNAM), Mexico

In recent years, there has been a remarkable surge of interest in developing smart luminescent crystalline materials to create efficient optoelectronic devices. Carbazole (*Cz*) has emerged as a promising core thanks to its exceptional photophysical properties and structural accessibility, making it an ideal component for designing chromophores with novel optical responses when integrated into solid materials. In this work,the luminescent properties of *Cz* and its functionalized derivatives in the solid state, followed by several instances of *Cz*-based photoresponsive crystalline materials, including organic crystals, cocrystals, and porous frameworks are summarized. Furthermore, examples of *Cz*-derivatives incorporated as emitting layers in *OLEDs* and *OFETs* are provided, highlighting the state-of-the-art in this field and the myriad of diverseapplications that these molecular building blocks exhibit in the crystalline state such as sensing, photoprinting, encryption photothermal conversion, and lasers.

Presenter:
Alonso Acosta Vera
University of Rochester, USA

Fate of Micro- Nanoplastics in Treatment Wetlands

Amado E. Navarro-Frómeta, Paula M. Crespo Barrera and **Guillermo M. Horta Valerdi**
Universidad Tecnológica de Izúcar de Matamoros, México

More than 430 million tons of plastic are produced annually, two-thirds of which are short-lived products that quickly become waste. The fragmentation of plastics in ecosystems leads to the formation of micro- (< 5 mm, MP) and nanoplastics (< 1 µm, NP), considered as pollutants of emerging concern. It is of interest to evaluate their behavior in treatment constructed wetlands, one of the nature-based systems capable of being applied on a small to medium scale as primary, secondary or tertiary treatment of domestic and municipal wastewater.

Treatment wetlands (TW) have different configurations, so it is expected that they have diverse mechanisms for retaining MPs and NPs, resulting in different levels of performance and removal. The review of recent literature presented in this work shows that removal levels of 40 to 100% are generally achieved, and that this is influenced not only by particle size but also by the polymers that make up the MPs and NPs.

The primary retention mechanism is filtration, although there is evidence, especially when using novel materials such as biochar as the granular component of the TW, of a significant role for absorption in the removal process. Biodegradation is, of course, another mechanism involved in the removal of MP and NP in TW, with the type of polymer present in the particles having a significant influence, leading to different biodegradation rates for different polymers. Bacterial degradation of MP and NP begins with the adhesion of microorganisms, followed by biofilm formation, enzymatic oxidation, depolymerization, monomer absorption, and mineralization. The macrophytes used in TW also contribute, through phytoremediation, to the removal of these contaminants, as they can trap, adsorb and accumulate them in their roots, although adsorption can be reversed by changes in the root´s environment.

Presenter:
Amado Enrique Navarro Frómeta
Universidad Tecnológica de Izúcar de Matamoros, México

Direct Determination of 2, 4-D in Natural Water Samples by Solid Surface Fluorescence

Talio Maria Carolina[1,3] and **Fernández, Liliana Patricia**[1,2]

[1]INQUISAL-CONICET., Argentina
[2]Facultad de Química, Área de Química Analítica, Bioquímica y Farmacia. Universidad Nacional de San Luis, Argentina
[3]Facultad de Química, Área de Química General e Inorgánica., Bioquímica y Farmacia. Universidad Nacional de San Luis, Argentina

2,4-Dichlorophenoxyacetic acid (2,4-D) is a selective, low-volatility systemic herbicide. It is used to control broadleaf weeds in certain crops, such as rice and wheat. It belongs to the group of hormonal herbicides known as auxins. The use of 2,4-D has become widespread in both the agricultural and industrial sectors, with the serious drawback that its residues can contaminate food, soil, and groundwater. Furthermore, occupational exposure can cause eye and skin irritation, nausea, weakness, and, in some cases, neurotoxic effects such as inflammation of nerve endings. The International Agency for Research on Cancer has classified it as a Group 2B carcinogen. Molecular fluorescence is a valuable instrumental technique in various fields due to its ability to detect and quantify compounds that meet specific chemical requirements. Therefore, its specificity is a significant advantage, as are its sensitivity and wide linearity range. These characteristics can be further enhanced by combining other preconcentration/sensitization techniques that eliminate potential interferences and matrix effects, in addition to preconcentrating the desired analyte. In this work, we were proposed the development of a new methodology, an alternative to traditional techniques, for the control and monitoring of 2,4-D in natural water samples, using instruments readily available in control laboratories. The herbicide was quantified directly at pH 7.0 in the presence of the anionic surfactant SDS. Samples were filtered through blue ribbon filter paper as a solid support before determination by solid surface fluorescence. The proposed methodology represents an alternative to conventional methods for monitoring 2,4-D and has been successfully applied to natural water samples from agricultural areas near the Quinto River in the province of San Luis. Furthermore, among its advantages is the generation of low volumes of waste, which contributes to the preservation of the environment and compliance with the principles of green chemistry.

Presenter:
Maria Carolina Talio
Universidad Nacional de San Luis, Argentina

ESG Challenges in the Social Context of the Animal Protein-Based Food Sector: The Brazilian Case

Juliana Damaris Candido de Lima, Renan Carriço Payer Samuel Martins Drei, Lizzie Bessa Risicato, Ruben Huamanchumo Gutierrez, Lidia Angulo-Meza, Gilson Brito Alves Lima, Lincoln Campelo Dias and **Pâmela de Carvalho Marques Silva**

Universidade Federal Fluminense, Brazil

This study aims to develop and apply a structured sustainability assessment model for companies in the Brazilian animal protein industry by integrating the Triple Bottom Line (TBL) approach with the Technique for Order Preference by Similarity to Ideal Solution (TOPSIS). Scope: The research focuses on evaluating corporate sustainability performance from economic, environmental, and social perspectives within the animal protein sector, considering issues such as environmental impacts of livestock production, animal welfare, productivity, and stakeholder expectations in a complex production chain. Methods: The methodological approach is quantitative and applied. Sustainability indicators aligned with the Triple Bottom Line were selected based on internationally recognized frameworks, particularly the Global Reporting Initiative (GRI). The indicators were normalized and weighted, and the TOPSIS multicriteria decision-making method was applied to rank companies according to their proximity to the ideal and negative ideal sustainability solutions. Results: The results demonstrate that the proposed model effectively differentiates sustainability performance among companies in the animal protein industry. Organizations with higher levels of environmental management, social responsibility practices, and governance structures achieved superior rankings. The findings also indicate that investments in sustainability are associated with productivity improvements, enhanced product quality, and stronger corporate reputation. Conclusion: The study concludes that the integration of the Triple Bottom Line framework with the TOPSIS method provides a transparent, systematic, and reliable tool for sustainability assessment and managerial decision-making. The proposed approach supports the identification of strengths and weaknesses in corporate sustainability strategies and contributes to the development of competitive advantages aligned with the principles of sustainable development.

Presenter:

Juliana Damaris Candido de Lima

Universidade Federal Fluminense, Brazil

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SPEAKER TALKS

Chapter-Wise Question Generation from Academic Book Pdfs using Generative AI

Dhiraj Karwatkar[1], Arvind Bhave[2] and **Rupali Gomase[3]**

[1]TGPCET, India
[2]IICC, R T M Nagpur University, India
[3]TGPCET, India

Objective: To generate chapter-wise questions from the academic book pdf's using generative AI.

Generative Artificial Intelligence (AI) is significantly transforming educational content development by automating cognitively demanding tasks, such as chapter-wise question generation. This paper introduces an intelligent system that extracts chapter-level content from academic textbooks in PDF format and generates domain-relevant questions using advanced Large Language Models (LLMs) including T5, GPT-3.5, and GPT-4. It integrates Natural Language Processing (NLP) pipelines for PDF parsing, rule-based chapter segmentation, OCR-based text extraction, and Bloom's taxonomy-driven prompt engineering. Performance evaluations using BLEU, ROUGE, METEOR, and grammar validation tools confirm high linguistic accuracy and pedagogical relevance. This framework supports scalable assessment systems, LMS integration, and AI-assisted curriculum development.

Scope:

- Educational Coverage:
- Chapter-Wise Segmentation & Targeted Generation:
- Multiple Question Formats & Difficulty Levels:
- LMS Compatibility:

Result:

The AI-driven question generation framework demonstrated strong performance across multiple evaluation metrics:

- Grammar Accuracy: Over 90%, indicating highly correct and polished question text.

- Relevance to Chapter: Above 80%, showing generated questions closely align with chapter content.

- Pedagogical Alignment: Approximately 75%, reflecting good coherence between questions and educational goals.
- BLEU Score: Ranged between 0.35 and 0.50, consistent with acceptable n-gram overlap for diverse valid questions.
- METEOR Score: Between 0.52 and 0.60, indicating reasonable linguistic alignment with reference questions.
- Manual Validation: Domain experts reviewed samples and found that over 80% of the questions required minimal revision, underscoring practical usability.

Conclusion and Future Work

This study demonstrates an AI-driven framework for automating chapter-wise question generation from academic PDFs. Its modular, scalable design supports a wide range of educational applications and LMS platforms. Future work will target: - LMS plugin development

- Adaptive question difficulty modeling
- Integration of multimodal inputs (diagrams, tables)
- Subject-specific model fine-tuning and multilingual support

Presenter:
Dhiraj Ghanshyam Karwatkar
TGPCET, India

Promising Materials for Optoelectronics $CdIn_2s_4$: Experimental Studies of Electronic Properties

Zafar Kadiroglu

İnstitute of Physics, Ministry of Science and Education,
Republic of Azerbaijan

$CdIn_2S_4$ is one of the photosensitive semiconductors with potential applications for optoelectronics. $CdIn_2S_4$ has two kind atoms in cationic sublattice. It is possible formation of antistructural defects, due to substitution of cations (Cd_{In} and In_{Cd}), apart from cation and anion vacancies. As results, in the forbidden band of $CdIn_2S_4$ exists a lot of local levels. However, the role of various centers in the recombination process, energy spectra of local levels and nature of local centers has not been sufficiently studied.

We presented investigation results thermal and optical quenching of the photoconductivity at the different illumination intensities, the temperature dependence of dark electrical current and thermally stimulated currents (TSC) in the $CdIn_2S_4$ crystals in the temperature range 110÷450. It was found activation energies different levels located at 0.03, 0.15, 0.22, 0.5 and 1.0 eV in the band gap below the conduction band bottom.

Possible experimental manifestations of repulsive barriers for electrons in CdIn2S4 are discussed. An analysis of the long-term relaxation of non-equilibrium positive (σ+) and negative (σ-) residual conductivities, the effects of changes in the spectrum of TSC under the influence of light depending on the illumination temperature and the jumply transition from the state of increased conductivity (in the relation to the dark conductivity) to that below the dark conductivity allowed us to conclude that in the $CdIn_2S_4$ there are repulsive potential barriers for electrons, which cause the above mentioned effects.

The temperature dependence of the specific electrical conductivity in the dark (σ_{dark}) of $CdIn_2S_4$ single crystals obtained by the gas transport method was studied in the temperature range of 290÷430 K and information about the phase transition at 403 K was confirmed

Presenter:
Zafar Kadiroglu
Ministry of Science and Education, Republic of Azerbaijan

Application of Liquid Biofertilizers Derived from Industrial Effluents for Legumes: An Option of Sustainable Waste Management

Chauhan. S.[1*], Satyanarayana[1,2], Poonam, C. S.[3], Mishra, R.[1, 4] and **Rajesh, M.[2]**

[1]Kumarappa National Handmade Paper Institute (KNHPI), India
[2]Department of Chemical Engineering, School of Bioengineering, SRM Institute of Science and Technology, India
[3]National Botanical Research Institute (NBRI), India
[4]Khadi & Village Industries Commission, India

In the present scenario of sustainable development, waste recycling and management is the need of the hour. Although a green and clean industry, handmade paper industry (HMPI) also requires a sustainable waste management to further improve its ecofriendly credentials and also to improve profitability of the sector. The present study aims to develop and evaluate liquid biofertilizers derived from waste effluents of the HMPI especially when cow dung is used as a raw material. Application of such biofertilzer samples (prepared with and without adding specific microorganisms) was studied on the leguminous crops of chick pea and pea.

To meet out the main objective of the study, experiments were conducted under both *in vitro* and field conditions using Randomized Block Design (RBD) for evaluating the effects of the effluent referred here to be Raw Liquor (RL) as such and also combined with certain Plant Growth Promoting Rhizobacterial strains (PGPRs) on chickpea and pea plants. RL was used in combination with Chickpea rhizobium (CP), *Bacillus* species isolated from garden soil (B.st (s)), *Bacillus* species isolated from textile industry effluent (B.st (w)), *Bacillus megaterium* (BM), Phosphate solubilizing bacteria (PSB), Pea rhizobium (Pea R), and *Enterobacter Kobei* (ECM). During *in vitro* seed germination studies, both the autoclaved and un-autoclaved RL was used however only the un-autoclaved RL was used in subsequent field studies.

In vitro, autoclaved RL and CP treatments achieved 100% germination in chickpea, with shoot and root lengths of 4.625±2.0cm and 10±1.96cm. Pea seeds treated with RL and PSB showed 100% germination, with shoot and root lengths of 2.5±0.58cm and 6.12±0.63cm for autoclaved seeds. Chickpea seeds treated with un-autoclaved RL, CP in combination with BM achieved 100% germination and the highest number of branches. Pea seeds treated

with un-autoclaved RL, PSB, and Pea R showed 100% germination, with the longest shoots. Field studies showed 100% germination for chickpea with RL and CP treatment while for pea with RL (as such). Chickpea root and shoot lengths were maximized in the case of RL and CP combined with B.st (s), while pea plants showed the longest root and shoot lengths with RL combined with PSB. Yield analysis revealed the highest number of chickpea fruits with RL and CP combined with BM (33.6±15.67fruits), and the highest number of pea fruits with RL and PSB (14±33 fruits).

Thus the present study establishes the recyclability and biofertilization potential of waste liquor, RL leading to sustainable agricultural practices.

Presenter:
Sunita Chauhan
Kumarappa National Handmade Paper Institute, India

Persistence of information in the quantum measurement problem

Shantena Augusto Sabbadini
Pari Center, Italy

The quantum measurement problem has to do with the compatibility of two different prescriptions for the end state of a quantum measurement process:

(1) *a superposition representing an entangled state of object system and apparatus;*

(2) *a mixture of correlated states of object system and apparatus.*

The first prescription is a consequence of the linearity of time evolution in quantum mechanics; the second one (corresponding to what is usually called the 'collapse of the wave function') is a basic feature of the axiomatic structure of the theory.

This paper proves that the two prescriptions are *exactly* equivalent whenever information about the results of the measurement persists, i.e. whenever there is some kind of record or trace of the results (all the measurements we are ordinarily concerned with fulfill this requirement). Experimental evidence is cited suggesting that indeed we should expect the equivalence of prescriptions (1) and (2) *to* hold *when and only when* information about measurement results persists.

Presenter:
Shantena Augusto Sabbadini
Pari Center, Italy

cfDNA Liquid Biopsy: Revolutionizing Breast Cancer Diagnostic, Prognostic & Precision Oncology

Heba Kamel Mahmoud Badawy
Sinai University, Egypt

Cell-free DNA (cfDNA), particularly circulating tumor DNA (ctDNA), has emerged as a transformative liquid biopsy biomarker for breast cancer diagnosis, prognosis, and monitoring. Recent studies (2024-2025) highlight ctDNA's analytical validity and clinical utility in early and metastatic settings. Huebner et al. (2025) analyzed ctDNA in 49 advanced breast cancer patients using Guardant360 CDx, detecting somatic alterations in 67%, including TP53 (29%), PIK3CA(24%), and ESR1 (12%), influencing treatment decisions in 35%of patients. Van et al.(2025) demonstrated multimodal cfDNA analysis (methylation&fragmentomics) enhancing breast cancer detection in 273 patients, outperforming single modalities for early screening.

Our recent publication, ''Plasma cell-free DNA as novel diagnostic and prognostic tools in breast cancer'' (Abd El-Fatah et al., Cancer Genet 2025), validated plasma cfDNA's(KLK10, SOX17, WNT5A, MSH2) superior sensitivity (92%) and specificity (88%) versus CA15-3 for detection (AUC = 0.95), correlating cfDNA levels/integrity with tumor stage, lymph node metastasis, and poor prognosis (HT=2.8 for relapse). Elevated cfDNA distinguished triple-negative from HR+ subtypes ($p<0.001$).

cfDNA enables non-invasive genomic profiling(PIK3CA, ESR1, BRCA1/2), minimal residual disease tracking, and therapy response prediction, as in PADA-1 trial where ESR1 monitoring doubled PFS. Challenges include low ctDNA shedding in early disease and standardization, but FDA/CE-marked assays like, Guardant360 address these.Integrating cfDNA into routine practice promises precision oncology, reducing biopsies and enabling dynamic monitoring for breast cancer management.

Presenter:
Heba Kamel Mahmoud Badawy
Sinai University, Egypt

AI Driven Algorithms for Predictive Compound Design and Optimization in Drug Discovery

Subhranil Das
School of Computer Science UPES, India

The application of Artificial Intelligence (AI) and advanced algorithm development is significantly transforming the landscape of drug discovery and design. This work presents a novel AI-integrated framework that synergizes deep generative models with reinforcement learning-based optimization for the de novo design of drug-like molecules. The proposed system utilizes a variational autoencoder to generate chemically valid molecular structures, which are then optimized using reinforcement learning agents guided by multi-objective fitness functions. These functions are tailored to enhance pharmacological properties such as binding affinity, bioavailability, and target specificity while minimizing off-target interactions and toxicity risks.

Our approach is trained and validated using extensive datasets from ChEMBL and ZINC databases, ensuring robust generalization across a wide range of biological targets. Comparative studies demonstrate that our hybrid AI model consistently outperforms traditional QSAR models and docking-based approaches in terms of hit generation speed, novelty of scaffolds, and prediction accuracy.

In retrospective case studies, the model successfully identified analogs of FDA-approved drugs with improved predicted ADMET properties. Furthermore, prospective simulation results showcase its potential to discover first-in-class molecules against underexplored therapeutic targets. The framework is designed to be modular and scalable, allowing easy integration of target-specific data, pathway information, and emerging constraints such as green chemistry metrics.

This AI-powered platform not only accelerates early-phase drug discovery but also improves the likelihood of clinical success by embedding intelligence in each stage of compound generation and evaluation. Our results underscore the paradigm-shifting role of AI in predictive, efficient, and intelligent drug development pipelines.

Presenter:
Subhranil Das
School of Computer Science UPES, India

River and Groundwater used for Irrigation of Agricultural Crops

Smailov Eltar Ablametovich[1] and **Sydykbaeva Telegey Israyilovna**[2]

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Global threats such as climate change are exacerbating the challenges facing Kyrgyzstan's agricultural sector.

The most dangerous consequence of climate change is the reduction of the flow of numerous rivers, which are the basis of irrigated agriculture and, consequently, the country's entire rural economy. There is an urgent need to reduce irrigation losses by constructing new water supply systems and using groundwater for irrigation. One of Kyrgyzstan's main crops is the world-famous Uzgen rice, grown in the floodplains of the rivers of the Osh, Batken, and Jalal-Abad regions. Its production directly depends on the composition and quality of the water used for irrigation. Vegetable growing for export also contributes to the widespread cultivation and production of sweet peppers (Capsicum annuum L). In the Batken region, irrigation water supply is paramount for agriculture, where many regions exclusively use artesian groundwater for irrigation. The purpose of this study is to analyze the composition of river water in southern Kyrgyzstan, groundwater from wells in the Batkenand Osh regions, and groundwater from springs in mountainous areas used for agricultural irrigation, and to assess their effectiveness. In terms of calcium and magnesium content, water from the Kara-Darya, Zhazy, and Zarger rivers and the Makarenko well meets these standards, indicating that the water promotes normal plant growth and development. Water from the Dosmat well, however, exceeds these standards by more than three times. This significant excess can cause soil salinization, block the absorption of other elements such as magnesium and potassium, and form solid deposits in irrigation systems, reducing irrigation efficiency. Water from the Kara-Darya, Zhazy, and Zarger rivers and the Makarenko well meets these standards. The Makarenko well is considered moderately hard, while the Dosmat well is considered hard. According to US regulations, the waters of the Kara-Darya, Zhazy, and Zarger rivers and the Dosmat well are considered very hard, while the water at the Makarenko well is considered hard. In general, using artisanal water for irrigating sweet peppers requires

pre-treatment and ongoing soil monitoring to avoid negative impacts on yield and product quality.

Table 1. Results of the study of the composition of irrigation water from rivers and wells for the cultivation of agricultural crops

Хозяйство	Образец	Лаб. № образца	pH, ед	EC, µS/cm	TDS, мг/л (ppm)
рекаКара-Дарья	№ 1	1	6,59	547	350
рекаЖазы	№ 2	2	7,20	531	340
рекаЗаргер	№ 3	3	7,77	607	388
Досмат (скважина)	№ 4	4	7,38	2355	1507
Макаренко (скважина)	№5	5	7,50	276	176
Вода подземная (артизанская) Баткенская обл. продолжение табл.3	№6	6	7,54		

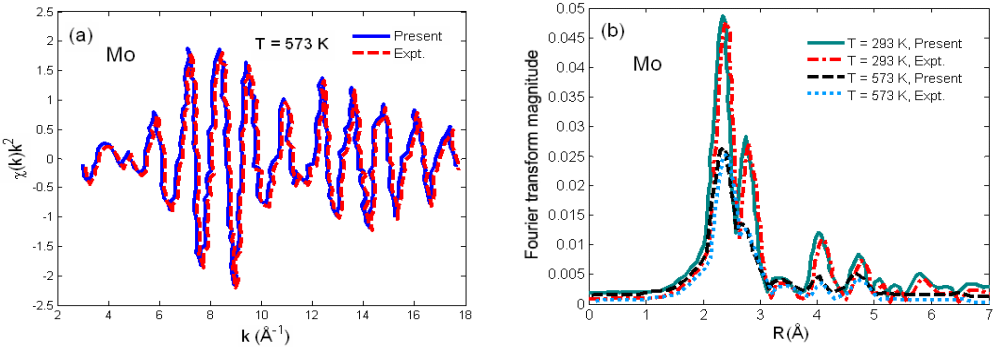
Ca, мг/л	Mg, мг/л	Ca, мг-экв/л	Mg, мг-экв/л	Ca+Mg мг-экв/л	$CaCO_3$, мг/л (ppm)	°dH	Жесткостьводы по нормам США	Жесткость воды по нормам России
32	13	1,6	1,1	2,7	133	7,5	Оченьжесткаявода	Водасредне йжесткости
30	12	1,5	1,0	2,5	124	7,0	Оченьжесткаявода	Водасредне йжесткости
32	15	1,6	1,2	2,8	142	7,9	Оченьжесткаявода	Водасредн ейжесткости
490	86	24,5	7,1	31,5	1578	88,3	Оченьжесткаявода	Жесткаявода
16	3	0,8	0,2	1,0	52	2,9	Жесткаявода	Водасредне йжесткости
						12,74	Оченьжесткаявода	Жесткаявода

Presenter:
Smailov Eltar Ablametovich and **Sydykbaeva Telegey Israyilovna**
International Kyrgyz-Uzbek University named after B. Sydykov, Kyrgyzstan
National Academy of Sciences of the Kyrgyz Republic, Kyrgyzstan

Contributions of Debye-Waller Factors and EXAFS to Materials Chemistry Based on Advanced Anharmonic Correlated Einstein Model

Nguyen Van Hung
University of Economics - Technology for Industries, Vietnam

This work presents the contributions of Debye-Waller factors (DWF) and extended X-ray absorption fine structure (EXAFS) to studying the thermodynamic properties, many-body and anharmonic effects, as well as the structural determination in materials chemistry based on the advanced anharmonic correlated Einstein model (AACEM). The advances in this model lead to avoiding the limitations of the previous ones, to creating a method for the accurate structural determination of materials by EXAFS, and to good agreement of the numerical results of Mo (Molybdenium) with the experimental values.



Figures: (a) EXAFS spectrum at 573 K and (b) Fourier transform magnitudes of EXAFS spectra at 293 K and 573 K of Mo calculated using the FEFF-code [7] modified into the anharmonic one based on the present theory compared to the experimental values (Expt.) [9].

Presenter:

Nguyen Van Hung
University of Economics - Technology for Industries, Vietnam

Spatial Mapping of Soil Salinity in a Semiarid Region using a Machine Learning Model Based on Spectral Indices and Ground Data

Khalid El Bahjaouy[1], Ahmed Barakat[1], Abdessamad Hilali[2], Hassan Mosaid[1] and **Amine Oussilkane[1]**

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[2]Regional Centre of Agricultural Research of Tadla, National Institute of Agricultural Research (INRA), Morocco

The expansion of intensive agriculture has led to increasing soil salinity worldwide. highlighting the critical need for accu rate soil salinity measurements is essential to address this situation. In this context, digital soil salinity mapping becomes necessary to properly manage soil resources in limited data regions. Therefore, this study aimed to map soil salinity using a Random Forest (RF) model that incorporated several spectral indices and physicochemical properties in the Tadla Plain. 149 samples were used to investigate the physical and chemical characteristics of soils in the study area. the dataset was divided into 70% of the ground data for model training and 30% for validation. The results show that 81.1% of the studied soil is non-saline, 15,5% is slightly saline, and 3,4% is moderately saline. However, statistical metrics showed that the RF model performed well with a salinity index (SI6), achieving a correlation coefficient (R2) of 0.80 and Root Mean Square Error (RMSE) of 0.084. Salinity indices SI1, SI2, SI3, SI4, SI5, and SI7 yielded results with low precision, with R2 values below − 0.2. These findings provide valuable insights for developing strategies to mitigate soil salinity in semi-arid areas.

Presenter:
khalid EL BAHJAOUY
University Sultan Moulay Slimane, Morocco

An Innovative Way to use an Extract of the Viticulture By-Products

Zulfiya Shakiryanova and **Almira Saparbekova**
M. Auezov South Kazakhstan Research University, Kazakhstan

Nowadays using of the viticulture by-products can play key role as natural additive with antioxidant effect for favourable influence of phenols on human health. Also as an agent to stabilize the color of meat products; however, usage of these additives at high levels could lead to toxicity and cancer originating from the formation of nitrosamines. Currently, application of natural preservatives in order to reduce the nitrite content in meat products is increasing.

Presenter:
Zulfiya Shakiryanova
M. Auezov South Kazakhstan Research University, Kazakhstan

Minority Power: Driving Change Through Social Influence

Imane MARGOM[1] and **Zainab BERRADA**[2]

[1]Sidi Mohamed Ben Abdellah University (USMBA), Morocco
[2]Laboratory for Innovation in Management and Engineering for Enterprise (LIMIE), Morocco

This communication explores the dynamics of social influence through the lens of relationships between majority and minority groups, drawing on the foundational works of Asch and Moscovici. Social influence has long been perceived primarily as a manifestation of conformity and the power of the majority. However, studies in social psychology have shown that minority groups can exert significant influence by challenging prevailing norms and introducing new perspectives, thus acting as drivers of social change and innovation.

By revisiting key contributions, this study examines how majority influence often operates through normative and informational pressures, promoting-conformity, while minority influence relies on consistency, innovation, and the ability to persuade through novel arguments. Minoritynon-conformism, when expressed strategically, canserve as a catalyst for progress, creativity, and collective problem-solving within groups and organizations.

From a managerial perspective, the study emphasizes the importance of recognizing and valuing minority voices as a strategic resource. Organizations that foster cognitive diversity and encourage constructive dissent are better positioned to innovate, adapt, and make informed collective decisions.

Overall, this communication demonstrates that the interaction between majority and minority groups constitutes a strategic lever for fostering creativity, social cohesion, and innovation, both at the organizational and societal levels.Understanding these dynamics provides critical insights into how social influence can be leveraged to encourage inclusive decision-making, support change initiatives, and drive long-term progress.

Presenter:
Imane MARGOM
Sidi Mohamed Ben Abdellah University (USMBA), Morocco

FasalNirog: A Multimodal AI-Driven Web Platform for Crop Disease Diagnosis and Expert-Guided Support

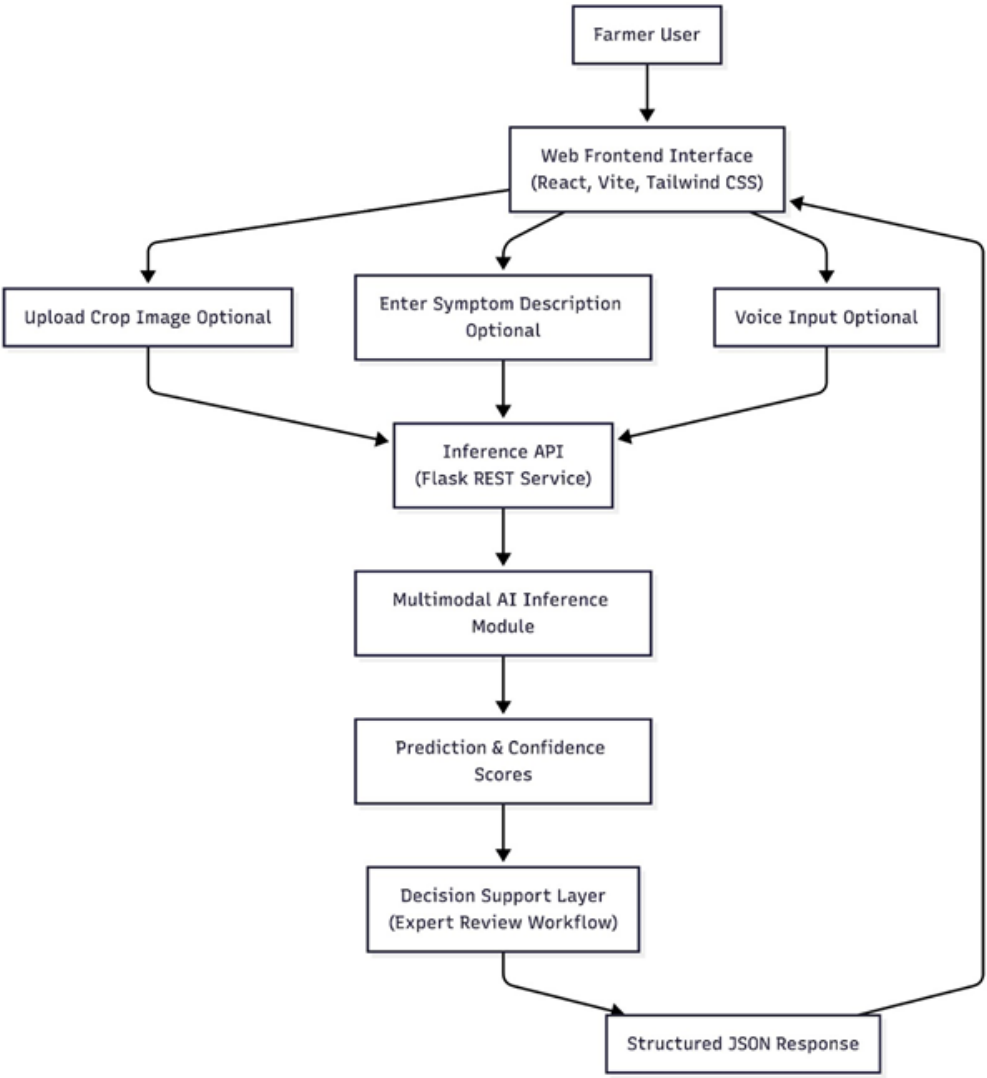
Sujata Kulkarni, Sanika Gadkari, Sarvesh Deshpande and **Shubh Gupta**

Bhartiya Vidya Bhavans Sardar Patel Institute of Technology, Mumbai, India

Timely identification of crop diseases is essential for ensuring agricultural productivity and reducing economic losses among smallholder farmers. However, limited access to expert guidance and digital agricultural tools continues to pose challenges in rural and resource- constrained environments. This paper presents FasalNirog, an AI-enabled web-based decision support system designed to assist farmers in diagnosing crop diseases and obtaining guided recommendations through an accessible and human-centered interface.

The platform integrates multimodal inputs, including crop images, textual symptom descriptions, and optional voice-based queries, to improve robustness in real-world scenarios where image-only diagnosis may be insufficient. A vision–language model fine-tuned on agricultural datasets is deployed as part of a modular inference pipeline, enabling flexible processing of image-only, text-only, or combined inputs. The backend is implemented as a stateless REST-based service to support scalability and ease of deployment, while the frontend is optimized for mobile accessibility and multilingual usability. In addition to automated predictions, the system incorporates an expert-in-the-loop workflow that allows agricultural specialists to review cases and provide personalized recommendations when required.

The proposed architecture emphasizes practical integration of existing AI technologies within a scalable web system rather than model-level innovation. The system demonstrates the practical feasibility of integrating multimodal AI within a scalable web-based agricultural decision support platform. FasalNirog provides a replicable framework for integrating multimodal AI into precision agriculture platforms, contributing toward scalable and accessible digital farmer support systems.



Presenter:
Sujata Kulkarni
Bhartiya Vidya Bhavans Sardar Patel Institute of Technology, India

Effects of Electron Beam Irradiation on the Physicochemical, Functional, Nutritional Properties, and Microstructure of Millet Flour (*Pennisetum Glaucum* L.R.Br.)

Dely Maissa[1], Zaouak Amira[2], Essafi Wafa[3], Mnasser Hassouna[1] and **Mankai Melika[1]**

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[2]Research Laboratory on Energy and Matter for Nuclear Science Development (LR16-CNSTN02), National Center for Nuclear Science and Technology, Tunisia
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The study investigates the impact of electron beam irradiation at doses rangingfrom 1 to 4 kGy on the physicochemical, functional, proximate, and microstructural characteristics of pearl millet flours.The findings revealed that with increasing irradiation dose, therewas a significant reduction in severalparameters, includings welling index, pH, lipid content, fiber content, total tannins, and lightness (L* value). Conversely, solubility index, total flavonoid content, polyphenol content, antioxidant activity, and color parameters (redness a* and blueness b*) exhibited a significant increase compared to control samples. However, E-Beam irradiation did not significantly affect water and oil absorption capacity, moisture content, carbohydrate content, or grossenergy value of millet flour.Additionally, irradiation at different doses (1 to 4 kGy) significantlyimproved the microbiologicalquality of the flours by reducing total aerobicmesophilic flora, yeasts and molds, total coliforms, and fecalcoli forms compared to non-irradiated samples. Fourier Transform Infrared (FTIR) spectroscopy analyses indicated changes in the molecular structure of millet flour following irradiation. Furthermore, irradiated flour sex hibited lower crystallinity compared to non-irradiated samples. Overall, the reduction in anti nutritional factors and the enhancement of functional properties suggest that electron beam irradiation could serve as an effective pretreatment for the development of value-added millet-based food products.

Presenter:
Dely Maissa
University of Carthage, Tunisia

Assessment of Oropharyngeal Dysphagia in Patients with Rheumatoid Arthritis

Dina Ibrahim, Ahmed Abdelmonem, Ramez Reda, Enas Abdelaleem and Rabie Youssef

Faculty of Medicine, Beni-suef University, Egypt

Objectives: Patients with rheumatoid arthritis (RA) frequently experience dysphagia but limited studies analyzed it. This study aimed to assess swallowing in RA patients by Fiber optic Endoscopic Evaluation of Swallowing (FEES). Methods It was a cross-sectional study that included 30 patients diagnosed with RA and complaining of dysphagia. All patients were subjected to patient interviews bedside swallowing screening and examined by FEES using different food consistencies: thin fluids, 5 mL and 10 mL, semisolids, and solids. The Mansoura Fiberoptic Endoscopic Evaluation of Swallowing Residue Rating Scale (MFRRS) and the 8-point penetration-aspiration scales were used to interpret FEES findings and assess swallowing efficiency and swallowing safety.

Results: The most reported symptoms were foreign body sensation (90.0%), xerostomia (80.0%), chewing problems (76.7%), teeth problems (70.0%), and self-feeding difficulty (53.3%). Most of these patients reported changing eating habits like using fluids with solids (73.3%) and increasing their meal time (60%). All patients had negative bedside swallowing screening. FEES revealed that the anatomy and the physiology of swallowing were normal, the larynx was normal, and MFRRS revealed that most of the patients had no residue for different food consistencies. No penetration or aspiration was detected in the thirty patients.

Conclusion: Data obtained from the study not only provided compelling evidence regarding the high prevalence of current swallowing disorders among individuals diagnosed with rheumatoid arthritis but also confirmed the importance of direct assessment and the need of more concern regarding dysphagia related to RA.

Presenter:
Dina Wael Ibrahim
Beni-suef University, Egypt

Spatial Access Differentials to Healthcare Facilities: A Secondary Analysis of the Democratic Republic of Congo

Elizabeth Avosuahi Dania
The University of the Western Cape, South Africa

Healthcare services are widely recognised as a crucial and necessary component in achieving Sustainable Development Goal 3, which underscores the importance of healthy lives and the promotion of well-being for individuals of all ages. The availability of transportation to healthcare facilities constitutes a fundamental milestone in societal development. Nonetheless, access to healthcare varies considerably across nations, accentuating disparities, especially in Africa. These disparities can be analysed by examining individual responses to socio-economic factors within healthcare systems. In the Democratic Republic of the Congo, ongoing conflicts and political instability have continually undermined and challenged the country's healthcare infrastructure. This paper, therefore, explores the challenges and implications faced by the healthcare system in the Democratic Republic of Congo. It emphasises socioeconomic factors, such as age groups, educational status, occupational status, and wealth index, which disproportionately impact women and young girls. The population under investigation consists of women aged 15-49 who are the household heads. The study utilised nationally representative data from the Demographic and Health Surveys conducted in the Democratic Republic of the Congo in 2023-2024. The data was analysed at two levels. The univariate analysis involves descriptive analysis of variables, and the bivariate analysis, which entails cross-tabulation and the Chi-square test to demonstrate disparities in healthcare access. The study revealed that the overall proportion of individuals walking to healthcare facilities was 94%, whereas 5.9% utilised transportation means to access healthcare services. This underscores the disparities in healthcare access. These findings will inform policymakers and program developers about the necessity of addressing these challenges in healthcare access and decision-making processes aimed at enhancing women's healthcare services in the Democratic Republic of Congo, with the objective of effectively bridging gender and socioeconomic disparities.

Presenter:
Elizabeth Avosuahi Dania
The University of the Western Cape, South Africa

Comprehensive Physicochemical Characterisation of Bovine Bone as a Sustainable Biomaterial for High-Value Applications

Ziningi Rosebud Myeni, Sani Gumede and **Teboho Serobanyane**
Technology Innovation Agency, South Africa

The valorisation of agro-industrial waste into high value functional materials is a critical component of sustainable chemistry and circular bioeconomy strategies. This study presents a comprehensive physicochemical characterisation of bovine bone as a renewable and sustainable biomaterial with potential applications in biomedicine, environmental remediation, catalysis and advanced material development. Bovine bone, an abundant waste product of the meat industry, is composed of an inorganic hydroxyapatite phase integrated within an organic collagen matrix, making it an attractive candidate for multifunctional material platforms. Raw bovine bone samples Structural, compositional, and morphological properties are being evaluated using X-ray diffraction (XRD) to determine crystallinity and phase composition, Fourier transform infrared spectroscopy (FTIR) to identify functional groups, scanning electron microscopy (SEM) to assess surface morphology, and thermogravimetric analysis (TGA) to examine thermal stability and organic content. Elemental composition is being analysed using energy-dispersive X-ray spectroscopy (EDS) to determine calcium-to-phosphorus ratios and trace mineral content. The outcomes of this study are expected to provide insight into the structural integrity, purity and application potential of bovine bone derived materials. This work contributes to advancing green material innovation through the upcycling of biological waste into functional advanced materials within a circular bioeconomy framework.

Presenter:
Ziningi Rosebud Myeni
Technology Innovation Agency, South Africa

Livelihood Transformation of Tribals through SHG and Water Hyacinth Product Entrepreneurship: A Case in West Bengal

Dipanwita Chakraborty and **Parmod Kumar**
Giri Institute of Development Studies, India

The tribes comprise nearly 3 percent of the entire population of West Bengal. They are, in general, confined to the rural belt of the state. Bauls, Bhuyiya, Santhal, Oraon, Paharia, Munas, Lephcas, Bhutiyas, Chero, Khariya, Garo, Magh, Mahli, Mru, Munda, Lohara and Mal Pahariya are amongst the popular tribes in West Bengal. However, Scheduled Tribes of Bengal record very high levels of poverty, and the pace of poverty reduction among them has been conspicuously slow. Self-help Groups are the most prominent channels for empowering rural communities, particularly women, and enable them to move from subsistence to sustainability. Numerous of such groups are outstanding producers/creators of local arts and craft of great aesthetic value. However, development of household decours and hasndicrafts from natural fiber sources such as water hyacinth can be ecologically sustainable and economically remunerative entrepreneurial option for these rural poor. However, it is still an innovation operating at a small-scale prevailing at in experimental stage. Cost of raw material is negligible as the water hyacinth grows in any water body left stagnated for long without any cost of maintenance involved. In fact, they are hazardous in nature because this aquatic plant is a prolific vegetable matter-producer and has the ability to choke out any closed waterbody at an astonishing rate by cutting off sunlight as well as reduce oxygen level in the water, making it unfit for commercial use. So making commercial use of them can help managing them rationally and making use of the features of water hyacinth to the maximum advantage in an environmentally sustainable manner. Producing natural fiber handicrafts can be an important commercial use of the water hyacinth that can be easily adopted by SHGs given the high labour intensive and low investment nature of enterprise. In view of the fact that Eco-friendly product market has grown geometrically over the last 7 years globally owing to rising awareness about climate change and its alarming ramifications on the environment-man kind, with India no exception, a research study by TerraChoice, a global marketing company revealed a 73 percent growth in the eco-friendly product market over the above reference period and more new companies and products are making new entry into this space with each passing day. Given this,

water hyacinth natural fiber-based handicraft development can prove to be a sustainable lucrative enterprise solution for the poor mass of tribals of Bengal in near future through thorough and sincere involvement. With this as the backdrop, a primary survey is carried out in the FY of 2023 in Birbhum, one of the major tribal belt of West Bengal where the water hyacinth based artifact entrepreneurship was incepted on an experimental basis in Bengal, a new initiative for transforming the livelihood of the tribals. 14 SHGs, primarily comprising women belonging to ST category had been trained by NABARD/local NGOs on an experimental basis to recycle widely available water hyacinth in the water bodies around and develop natural fiber-based handicrafts as an pioneering initiative to improve the livelihood of these cohort of impoverished women. Each of the 14 SHGs comprised 12 members on an average. Therefore, for the purpose of primary data collection, 3 members each from the 34 SHGs were selected through Random Sampling Method' and the total sample came to be 42 (3 members each from the sample SHGs, selected randomly). A small sample of control group was also selected for comparative analysis as to the economic empowerment of the female entrepreneurs which included SHG non-participant women working in household industries available in the study area (30) and in the farm against wages (30). Findings show the major natural fiber-based merchandise produced by the surveyed women belonging to SHGs of the study area Birbhum, included purse, table mats, ladies hand bags, official folders, laundry baskets, laptop bags, tiffin bags, bottle carrier and like. To the complacency, the surveyed women entrepreneurs experienced a 7 percent more household income than the control group engaged in household sector and a perceptible 16 percent more than the female counterparts working as farm labourers by virtue of water hyacinth fiber handicraft works. The share of natural fiber handicraft-based earning claimed a significant 48 percent of total household income during reference period of study.

Presenter:
Dipanwita Chakraborty
Giri Institute of Development Studies, India

AI Meets Reality: Detecting Rice Diseases in Benin — A Bibliometric and Field Perspective

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Institut de Mathématiques et de Sciences Physiques,
Universitéd'Abomey-Calavi – IMS, Bénin

This study aims to assess the gap between global research on Artificial Intelligence (AI) for rice disease detection and the operational realities of Benin's rice sector. Its objectives are twofold: first, to map the scientific literature on AI-based rice disease detection through bibliometric analysis; second, to investigate how local stakeholders perceive and anticipate AI diagnostic tools. The scope covers both the global research landscape (2019–2024) and a local field study in Benin's Ouémé and Collines departments. The methodology combines a quantitative bibliometric analysis of 543 documents extracted from the Scopus database using Biblioshiny software, and a qualitative survey based on 25 semi-structured interviews with farmers, extension agents, agronomists, and researchers. The bibliometric results reveal a 46.14% annual growth rate, dominated by India and China (58% of publications, 23% of citations). Convolutional Neural Networks (CNNs) are the predominant approach, frequently reporting over 95% accuracy in controlled environments. However, African contributions remain marginal, and no existing model addresses Benin's specific rice varieties, disease strains, or field conditions. The field survey shows that 80% of farmers cannot visually identify diseases before an extension agent intervenes, diagnostic delays often exceed one week, and no AI-based tool is currently deployed—despite strong farmer interest in smartphone-based solutions. We conclude that a profound gap exists between technological readiness and field deployment in Benin. This study advocates for a context-driven research agenda prioritizing local datasets, frugal architectures, and participatory design to support digital sovereignty and food security in West Africa.

Presenter:
HOUNGUE Y. Pélagie Elyse
Universitéd'Abomey-Calavi – IMS, Bénin

Catalytic Functions for Hydrogen Production and Storage

Ernest Ilisca[1,2]

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Unlike current hydrogen storage methods aiming for permanent storage, themethod presentedis a transient process that transforms liquid hydrogen into gas during a period of time that can be adjusted to suit the desired end-up application. The porous materials used in the suggested storage are similar to those acting as catalysts in industrial liquefiers, but they combine a larger variety of functions: transient adsorption, flow regulation, heat exchange, catalytic conversion of hydrogen.The material compound of the microporous plugs introduced in the vessels will be related to necessary temporal functions. Three material parameters of the catalysts: surface electronic structure, porosity, thermal conductivity ensurethese main functions.Among the porous adsorbents under consideration, metal–organic frameworks present a configuration ofmetal ions connected *via* organic linkers promising materials for H_2 storage due to their high surface area and their high chemical and structural tunability.Their ability to bind hydrogen at open metal coordination sites,characterized also by sharp electromagnetic gradients,allowsalso fast catalytic rates.While the hydrogen conversion energy emittedis a harmful inconvenience in the cooling process,it is advantageous in storage because it absorbs the environmental heat. Similarly, the inconvenience of thepressure drops produced by the catalyst porosity in the liquefiers are advantageous in the storage by producing necessary expansions that regulate the hydrogen capillary flow. Along the hydrogen current, each of successive microporous plugs retains some molecules and opens the door to a cascade, producing a JT expansion that reduces the pressure of the following compartment.The presented transient hydrogen storage using the complementary, although inverse, liquefaction and storage processespromotes a rational way in the delivery of future storage tanks and thusin the use of the hydrogen energy by integrating the production, storage and dispensing processes.

Presenter:
Ernest Ilisca
Université de Paris-Cité, France

Discovery of a Novel Small Molecule Degrader of Mutant Estrogen Receptors using DNA Encoded Libraries

Murugesan Palaniappan[1,2]

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Somatic ESR1 mutations Y537S and D538G occur frequently in endocrine therapy-resistant metastatic breast cancer. Estrogen receptor α (ERα) variants with these ligand binding domain (LBD) mutations are activated independently of estradiol and are less sensitive to standard-of-care drugs that bind ERα directly. The identification of drugs targeting ERα mutants is challenging. Here, we use our multibillion compound DNA-encoded libraries (DELs) to identify small molecules that bind to purified wild-type and mutant ERα LBDs. Our DELs screen discovered small molecule hits that were enriched strongly with all three LBDs and some that discriminated between the LBD variants. We selected the hit compound, CDD-1274 that was most enriched with all three LBDs for further characterization. CDD-1274 acted as an antagonist in the LBD binding assays and blocked estradiol-independent binding of the coactivator peptide to Y537S and D538G LBDs. CDD-1274 treatment decreased WT and mutant ERα protein levels and inhibited ERα-mediated gene expression. Furthermore, CDD-1274 diminished estradiol-driven proliferative markers in several ER-positive breast cancer cell lines including single mutant CRISPR Y537S and D538G but, not in normal mammary epithelial cells or ER-negative breast cancer cells. We demonstrated that CDD-1274-induced proteasomal degradation of wild-type and mutant ERα in breast cancer cell lines, and induced Y537S ERα degradation more effectively than elacestrant in a palbociclib-resistant cell line. Together, these findings establish that CDD-1274 potently blocks ligand-dependent and independent ER signaling in endocrine-resistant breast cancer cells and could be further optimized for developing a new class of ERα degraders for endocrine therapy-resistant breast cancer.

Presenter:
Murugesan Palaniappan
Baylor College of Medicine, USA

Effective Preparation for STEM Learning in Early Childhood

Jabari Mahiri
Universidad Surcolombiana, Colombia

This qualitative study explored how four and five-year-olds were effectively prepared to engage in STEM learning through a project and play based pedagogy anchored in a social-emotional learning approach. All three of these aspects of the two focal teachers' approaches – project-based learning, play-based learning, and social-emotional learning – were critical to how these early learners showed significant development regarding preparatory concepts STEM as well as initial developments of "engineering mindsets." The teachers' focus was around using LEGO materials designed for this age group to build model objects, structures, and robotic devices. Eight of 11 students were in transitional kindergarten (TK) and three were in kindergarten while also participating in this free afterschool program. Researchers observed, video recorded, wrote field notes and video content logs, reviewed curricular materials, and conducted semi- structured and informal interviews with the teachers and a school administrator during Fall and Spring semesters of one academic year. Results were that the program's multi-layered approaches to learning activities facilitated these students developing of computational thinking skills and enabled them to individually and collaboratively build LEGO constructions that reflected and integrated key elements of foundational STEM learning. In this process, the four-and-five-year -lds ultimately were able to build robots with two motors (or brains) that allowed the students to program them to follow the lines of a variety of geometric shapes. These findings are significant for informing the current movement for expanding Transitional Kindergarten about viable pedagogical approaches to stimulate, guide, and connect STEM, SEL, and project and play-based learning for young children.

Presenter:
Jabari Mahiri
Universidad Surcolombiana, Colombia

Multiphysics Simulation and Machine Learning for Intelligent Optimization of Coffee Roasting Processes

Jaime Daniel Bustos-Vanegas[1], Gentil Andrés Collazos-Escobar[2], Nelson Gutiérrez-Guzmán[1] and **Tatiana Campo[1]**

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Coffee roasting is a complex thermo-physical process in which heat and mass transfer, particle dynamics, and chemical transformations interact under highly variable operating conditions. This work presents an integrated framework combining multiphysics simulation (CFD–DEM) and machine learning techniques to improve process understanding, control, and optimization in rotary drum coffee roasters. A coupled CFD–DEM model was implemented to simulate the interaction between the gas phase (air, water vapor, CO_2, volatiles) and the granular phase (coffee beans). The fluid domain was solved through the conservation equations of mass, momentum, and energy using the finite volume method, while individual bean motion and rotation were resolved *via* the discrete element method. Convective heat transfer between phases was modeled using empirical Nusselt correlations, and drag forces were calculated from Reynolds-dependent expressions. The model was validated against experimental roasting profiles, showing agreement between simulated and measured temperatures. Simulation results revealed that air recirculation significantly reduces temperature dispersion within the bean mass, improving roast homogeneity and decreasing the fraction of underdeveloped or over-roasted beans. Complementarily, supervised machine learning models (Support Vector Machines and Artificial Neural Networks) were trained to predict the area under the roasting curve (AUC), used as an indicator of process energy input. Based on a multifactor experimental design varying burner pressure and valve opening time, optimized SVM and ANN models achieved high predictive performance ($R^2 > 80\%$, MRE < 3%). The flexibility of these algorithms enables incorporation of additional inputs such as bean properties and operational parameters, supporting adaptive and data-driven process optimization. The combined use of multiphysics modeling and machine learning provides a robust strategy toward intelligent, self-optimizing roasting systems aligned with Industry 4.0 principles.

Presenter:
Jaime Daniel Bustos Vanegas
Universidad Surcolombiana, Colombia

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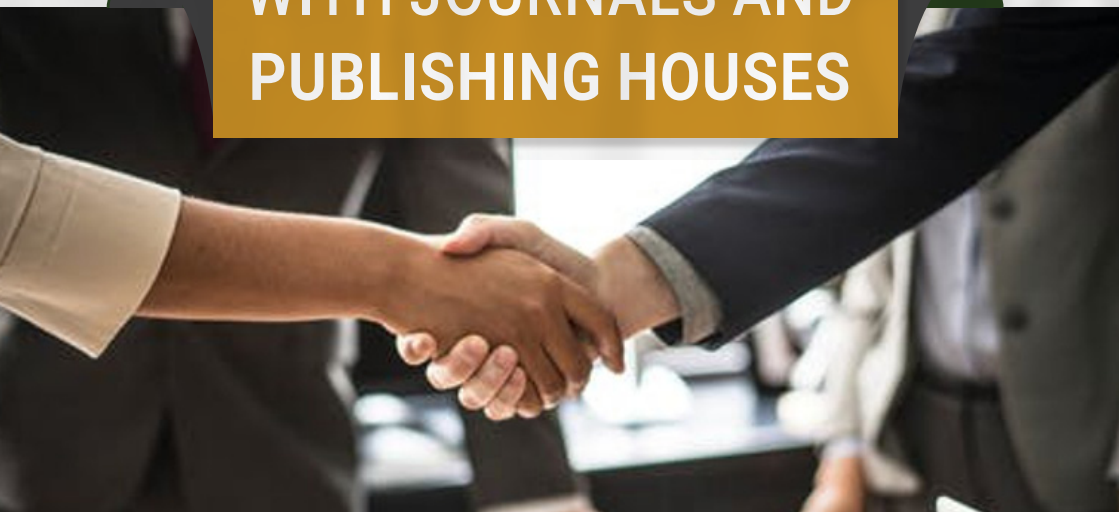

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