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21ST–22ND MARCH 2022

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PROGRAM-AT-A-GLANCE

ADV. CHEMISTRY 2022

DAY 1

MARCH 21, 2022

Scientific Program

BST-British Summer Time

08:45-09:00 Opening Ceremony

Distinguished Speaker Talks

Sessions: Analytical Chemistry | Biochemistry | Chemical Engineering | Electrochemistry | Food Chemistry | Geochemistry | Green Chemistry | Industrial Chemistry | Inorganic Chemistry | Nanotechnology | Materials Science | Medicinal Chemistry | Neurochemistry | Organic Chemistry | Physical Chemistry | Polymer Chemistry | Radiochemistry

09:00-09:20

Title: EVA technology: Chemistry and applications
Pier Giorgio Righetti, *Politecnico di Milano, Italy*

09:20-09:40

Title: Mechanism of gases generation during lithium-ion batteries cycling with standard electrolyte LP57
Nikolay Efimovich Galushkin, *Don State Technical University, Russia*

09:40-10:00

Title: The use of enhanced hydrophobicity of nanofibrillated cellulose derived from oil palm empty fruit bunches as nano-reinforcing agent for poly (lactic acid) nanocomposite films
Dwi Yuni Hastati, *Bogor Agricultural University (IPB University), Indonesia*

10:00-10:20

Title: Savitzky–Golay filtering-Based fusion of multiple exposure images for high dynamic range imaging
Vivek Ramakrishnan, *Datta Meghe College of Engineering, India*

10:20-10:40

Title: Current progress on open tubular ion chromatography
Weixiong Huang, *China University of Geosciences, China*

Refreshment Break 10:40-11:00

11:00-11:20

Title: Radiation-Assisted Green Synthesis and Characterization of Selenium Nanoparticles, and Larvicidal Effects on Culex pipiens complex
A. M. Fadl, *Egyptian Atomic Energy Authority, Egypt*

11:20-11:40	**Title: Meta-interaction physics on the evolution of the universe between dark energy and dark matter** **Li Zongcheng,** *Soochow University, China*
11:40-12:00	**Title: Fabrication of waste-based magnetic activated carbon nanostructures for environmental applications** **Mohamed Abdelaty Habila,** *King Saud University, Saudi Arabia*
12:00-12:20	**Title: Identification and characterization of Prothionamide degradation impurities by MS, NMR, and ultra- performance liquid chromatography method development** **Vijaya Kumar Baksam,** *Micro Labs Ltd, India*
12:20-12:40	**Title: Exfoliation corrosion performance of aeronautical aluminum alloy** **Abdessamad Brahami,** *Université Djilali Liabes, Algeria*
Lunch Break 12:40-13:10	
13:10-13:30	**Title: Electron currents and magnetic pulses in bounded atomic systems** **Shalini Lumb Talwar,** *University of Delhi, India*
13:30-13:50	**Title: Metabolite profile and dynamics during traditional beverages production: Case of palm wines in Côte d'Ivoire** **Theodore N. Djeni,** *Nangui Abrogoua University, Ivory Coast*
13:50-14:10	**Title: Starch-coated magnetic nanoparticles and external electromagnetic field for cancer theranostic** **Veselina Uzunova,** *Institute of Biophysics and Biomedical Engineering, Bulgaria*
14:10-14:30	**Title: Investigation of the potential complexing ability of dissolved organic substances in surface water to Al (III), Fe (III) and Cu (II) ions** **Zhezherya Vladyslav,** *National Academy of Sciences of the Ukraine, Ukraine*
14:30-14:50	**Title: Characterization and anticancer potential of Withania somnifera fruit bioactives (a native species to Pakistan) using GC-MS, NMR and LC-MS-ESI** **Qudsia Tabassam,** *University of Sargodha, Pakistan*

14:50-15:10	**Title: Separation of radioactive Ni from activation products** **Fabiola Monroy-Guzmán,** *Instituto Nacional de Investigaciones Nucleares, Mexico*
15:10-15:30	**Title: Pesticides: Agricultural food products, problems, chemistry** **Lydia Bondareva,** *Federal Scientific Center of Hygiene Maned After F.F. Erisman, Russia*
15:30-15:50	**Title: Possibilities of using biomethane as a low-emission energy carrier in transport in the light of the Green Deal** **Izabela Samson-Bręk,** *National Research Institute, Poland*
15:50-16:10	**Title: Voltammetric study of sulfonated tetra- and octa-substituted cobalt phthalocyanine complexes in aqueous solutions** **Mariia A. Kovanova,** *Ivanovo State University of Chemistry and Technology, Russia*
16:10-16:30	**Title: Experimental study of smart extinguishing material for use in forest and wildland-urban interface fires** **Michail Chalaris,** *International Hellenic University, Greece*

Panel Discussion

End of Day 1

DAY 2

MARCH 22, 2022

Scientific Program

BST-British Summer Time

Distinguished Speaker Talks

08:45-09:00 Introduction

Sessions: Analytical Chemistry | Biochemistry | Chemical Engineering | Electrochemistry | Food Chemistry | Geochemistry | Green Chemistry | Industrial Chemistry | Inorganic Chemistry | Nanotechnology | Materials Science | Medicinal Chemistry | Neurochemistry | Organic Chemistry | Physical Chemistry | Polymer Chemistry | Radiochemistry

09:00-09:20

Title: A novel detection system for fragmented cytokeratin 18 using new antibodies

Minori Yamada, *Bio-Diagnostic Reagent Technology Center, Sysmex Corporation, Japan*

09:20-09:40

Title: Absorbed dose monitoring radiochromic film systems for intense photon and electron radiation processing technologies

Vladimir P Tenishev, *Russian Metrological Institute of Technical Physics and Radio Engineering (VNIIFTRI) Mendeleevo, Russian Federation*

09:40-10:00

Title: A high-performance electrolysis cell promises more cost-competitive renewable hydrogen

Gerhard (Gerry) F. Swiegers, *University of Wollongong, Australia*

10:00-10:20

Title: Spiropyrazolinium salts and O-TOSILATE-β-(BENZIMIDAZOL-1-YL) propioamidoxyme as the products of β-aminopropioamidoximes tosylation

Kayukova Lyudmila Alexandrovna, *JSC A.B. Bekturov Institute of Chemical Sciences, Kazakhstan*

10:20-10:40

Title: Analysis of riverbank erosion – A micro-level approach

Sanchayan Mukherjee, *Kalyani Government Engineering College, India*

Refreshment Break 10:40-11:00

11:00-11:20

Title: More general families of exact solitary wave solutions of nonlinear schro¨dinger equation with their applications in nonlinear optics

Nadia Cheemaa, *Zhejiang Normal University, China*

11:20-11:40	**Title: An introduction to general high-pressure closed acidic decomposition method of rock samples for trace element analysis by ICP-MS** **Xijuan Tan,** *Chang'an University, China*
11:40-12:00	**Title: The effect of Gamma Irradiation on nucleolar activity, the presence of chromosomal abnormalities and the efficiency of energy conversion as indicators for mutation breeding in Triticum turgidum** **Eben von Well,** *Agricultural Research Council – Small Grain, South Africa*
12:00-12:20	**Title: Strip surface defect identification using multiresolution binarized image features** **Zoheir Mentouri,** *University of Guelma, Algeria*
Lunch Break 12:20-12:50	
12:50-13:10	**Title: Selective oxidation of styrene to benzaldehyde over niobium modified phosphomolybdic acid catalyst** **Balaga Viswanadham,** *GMR Institute of Technology, India*
13:10-13:30	**Title: Biodiversity and agricultural heritage: A path to sustainability** **Liane Portuondo Farías,** *Institute of Technologies and Applied Sciences (InSTEC), Cuba*
13:30-13:50	**Title: Hyperbolic tilings and crystallographic structures** **Benedikt Kolbe,** *Hausdorff Center for Mathematics, Germany*
13:50-14:10	**Title: Biochemical reaction networks used in population dynamics and epidemiological modeling** **Svetoslav Marinov Markov,** *Bulgarian Academy of Sciences, Bulgaria* **Milen Borisov,** *Bulgarian Academy of Sciences, Bulgaria*
Refreshment Break 14:10-14:30	
14:30-14:50	**Title: N, S donor acetamide ligand: Silver (I) binding and test silver (I) extraction studies** **Abiodun Daniel Aderibigbe,** *University of Connecticut, USA*
14:50-15:10	**Title: Progressive Sperm Sorting Method using High-throughput Rheotaxis-based device** **Afrouz Ataei,** *Florida Atlantic University, USA*
15:10-15:30	**Title: Combining machine learning and molecular modeling — CASTELO, a 4D submolecular motif identification method for drug discovery** **Leili Zhang,** *IBM Thomas J. Watson Research Center, USA*

15:30-15:50	**Title: Production water analysis by combining Electro Spray on Paper (EPS) and Laser-Induced Breakdown Spectroscopy (LIBS) techniques** **Carlos Albeiro Carreño Barrera,** *Universidad Industrial de Santander, Colombia*
15:50-16:10	**Title: Unknown metabolites identification with high resolution GC-MS and IROA technology** **Yunping Qiu,** *Albert Einstein College of Medicine, USA*
16:10-16:30	**Title: Stability characteristics of nanoparticles in a laminar linear shear flow in presence of DLVO- and non-DLVO forces** **Vivekananda Bal,** *Massachusetts Institute of Technology, USA*
16:30-16:50	**Title: Validation of analytical model and identification of salt effect on wellbore temperature in underbalanced drilling** **Olatunji Olayiwola,** *University of Louisiana at Lafayette, USA*

Panel Discussion

End of Day 2

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4TH ADVANCED CHEMISTRY WORLD CONGRESS

MARCH 2023

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SCIENTIFIC ABSTRACTS

DAY 1

PEERS ALLEY MEDIA

Virtual Event

3rd Advanced Chemistry World Congress

March 21-22, 2022

EVA technology: Chemistry and applications

Pier Giorgio Righetti[1], Gleb Zilberstein[2] and **Svetlana Zilberstein[2]**

[1]Department of Chemistry, Politecnico di Milano, Italy

[2]Spectrophon Ltd, Israel

This novel methodology consists in a hydrophilic polymer of ethylene-vinyl acetate (this is the origin of the acronym EVA) admixed with very fine particles of solid-phase sorbents (strong anion and cation exchangers added with hydrophobic resins such as C8 and C18). These diskettes, when applied to surfaces of items (paper, parchment, canvasses) belonging to the word Cultural Heritage, can capture ultra-minute amounts for proper chemical identification (such as via GC-MS, LC-MS, X-ray). The unique advantage of this probing technique is that it has been proven not to contaminate nor damage any of these precious items stored in museums, libraries, private collections, contrary to other harvesting techniques (e.g. by scraping or rubbing) that are intrinsically damaging. The capture is secured via standard non-covalent bonding (ion-to-ion and hydrophobic interactions as well as hydrogen bonding). EVA is a peculiar chromatographic technique that could be classified as a mixed-bed column. It is based on the use of multiple sorbents mixed together and packed in a single column. Thus EVA diskettes can be assimilated to these mixed-bed packed columns except that they are in a form of a solid state cartridge. In a most recent version, also combinatorial peptide ligand library (CPLL) resins have been admixed to the standard sorbents described above. Thus this novel variant contains several millions of diversified beads able to capture, for instance, also very minor polypeptides in presence of high-abundance proteins. The EVA technique has been applied to the screening of manuscript from famous authors (Bulgakov, Chekhov, Casanova, Jack London, Kepler, Orwell, Stalin) as well as to archaeological items (Egyptian mummies, Dead Sea Scrolls, the Aleppo codex) with extraordinary and quite unexpected results.

Biography

P.G. Righetti has developed isoelectric focusing in immobilized pH gradients, multicompartment electrolyzers with isoelectric membranes, membrane-trapped enzyme reactors, temperature-programmed capillary electrophoresis, combinatorial peptide ligand libraries for detection of the low-abundance proteome and the EVA technique for exploration of the Cultural Heritage. In the latter field, his work on manuscripts of famous authors and/or statesmen (Chekhov, Kepler, Bulgakov, Orwell, Casanova, Stalin) has won acclaims also in newspapers, magazines, TV talks and Internet sites around the world. On 560 articles reviewed by the ISI Web of Knowledge and by Mendeley Statistics, Righetti scores 26.680 citations, with an average of 47 citations/article and with a H-index of 76. During the years 2005-2013 he has received citations ranging from 1000 to 1200 per year.

Mechanism of gases generation during lithium-ion batteries cycling with standard electrolyte LP57

N. N. Yazvinskaya, N. E. Galushkin and **D. N. Galushkin**

Don State Technical University, Russia

For the first time, the mechanism of decomposition of the standard electrolyte LP57 during the cycling of lithium-ion batteries has been experimentally proven. This paper studied the gases release of a (graphite//NMC111($LiNi_{1/3}Mn_{1/3}Co_{1/3}O_2$)) cell during cycle in the voltage ranges of 2.6-4.2V and 2.6-4.8V and the temperatures of at 25°C and 60°C. In our experiments, the amount of gases generated using the standard electrolyte LP57 was about the same as when using the electrolyte EC. This experimental result proves that, in a standard electrolyte (LP57), mainly decomposes EC during gases generation. It was proved that the CO_2, CO, and H2 gases are released as a result of electrolyte decomposition. And it shows that the CO and H_2 gases evolution is a direct consequence of the electrochemical reaction of electrolyte decomposition, while the CO2 generation is a consequence of the additional chemical reaction of interaction between the O_2 released from the cathode atomic lattice oxygen and CO released from the same place on the cathode (appearing because of the electrolyte decomposition). That is why at the same electrochemical reaction of electrolyte decomposition, the ratio CO_2/CO varies in the wide range from 0.82 to 2.42 depending on cycling conditions (temperature and cutoff voltage). It was proved that a potential-independent H2 evolution is a consequence of its adsorption in pores of powdered graphite on anode. There was proposed the mechanism of the electrolyte decomposition and the gases evolution in lithium-ion cells at their cycling, which corresponds quantitatively to all obtained experimental results.

Biography

Prof. Dr. Nikolay Galushkin is a professor at Don State Technical University, Russia. He heads a research laboratory "Electrochemical and hydrogen energy". His research interests include: Firstly, the research and development of hydrogen storage systems meeting the criteria for on-board hydrogen storage systems that have been defined by the US Department of Energy. He received experimentally metal-hydrides high capacity. The capacity of the metal-hydrides as a hydrogen absorber was quantified as 20.1 wt% and 400 kg m^{-3}. This value exceed three times the earlier data obtained by traditional methods for any reversible metal hydrides, including magnesium hydride or complex hydrides, also they are far exceed the criteria for hydrogen storage systems established by US DOE.Secondly, the study of the processes of thermal runaway in alkaline, acid and lithium-ion batteries. Third, the modeling of processes in electrochemical batteries to develop battery models suitable for practical use in electric vehicles.

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The use of enhanced hydrophobicity of nanofibrillated cellulose derived from oil palm empty fruit bunches as nano-reinforcing agent for poly (lactic acid) nanocomposite films

DY. Hastati[1], E. Hambali[2,3], K. Syamsu[2], E. Warsiki[2,3] and **NE. Suyatma[4]**

[1]College of Vocational Studies, Bogor Agricultural University (IPB University), Indonesia
[2]Department of Agro-Industrial Engineering, Bogor Agricultural University (IPB University), Indonesia
[3]Surfactant and Bioenergy Research Center (SBRC), Bogor Agricultural University (IPB University), Indonesia
[4]Department of Food Science and Technology, Bogor Agricultural University (IPB University), Indonesia

Nanofibrillated cellulose derived from oil palm empty fruit bunches (NFC-OPEFBs) has a high potential for nano-reinforcement in polymer composites. However, the hydrophilic surface of NFC-OPEFBs limits their usage as nanofiller for the hydrophobic polymers. To overcome the limitation, the enhancement hydrophobicity of NFC-OPEFBs was performed using a sustainable cationic surfactant, i.e., cetyltrimethylammonium chloride derived from palmityl alcohol through surface modification method. In this study, a modified NFC-OPEFBs was reviewed in terms of their effects on mechanical, water vapor permeability, and thermal properties of polylactic acid (PLA) nanocomposite films. The PLA nanocomposite films were prepared with the addition of unmodified NFC-OPEFB (unmodNFC) 0.5 wt%, with the addition of various amounts of modified NFC-OPEFB (modNFC) from 0.5 to 3.0 wt% into PLA matrix by the solvent casting method and neat PLA film as the control. The ultimate tensile strength of PLA films was increased by using 3.0 wt% of the modNFC 87.8 %, while it was decreased by using 0.5 wt% the unmodNFC. This result proved that the hydrophobicity of NFC could improve interfacial adhesion between PLA and NFCs. The water vapor permeability of PLA film was decreased by 36.0 % and 33.3 % with the addition of 2.0 wt% and 3.0 wt% modNFC, respectively. Moreover, the PLA+modNFC films exhibited overall higher crystallinity and higher glass transition temperature than those of neat PLA film. The transparency of PLA nanocomposite films with the incorporation of modNFC was clearer than that of unmodNFC at the same loading level observed with the visual transparency test using background images. This research revealed that the enhanced hydrophobicity of NFC might be used as nanofillers for other hydrophobic matrices such as polypropylene, polyethylene, and other hydrophobic polymers.

Biography

Dr.Dwi Yuni Hastati received her Ph.D degree from Agroindustrial Technology from IPB University-Indonesia in 2020. She joined the Food Quality Assurance Department of College of Vocational Studies, IPB University as a lecturer and a researcher in 2007. She has been an active member of The Indonesian Association of Food Technologist since 2009. Her main research interests are in biomaterial, nanoparticles and their assemblies for applications in food packaging. Her studies were principally published in Journal of the Japan Institute of Energy and Waste and Biomass Valorization.

Savitzky–Golay filtering-Based fusion of multiple exposure images for high dynamic range imaging

Vivek Ramakrishnan and **D. J. Pethe**
Datta Meghe College of Engineering, India

The problem of compositing multiple exposure images has attracted lots of researchers, over the past years. It all began with the problem of High Dynamic Range (HDR) imaging, for capturing scenes with vast differences in their dynamic range. Fine details in all the areas in these scenes cannot be captured with one single exposure setting of the camera aperture. This leads to multiple exposure images with each image containing accurate representation of different regions dimly lit, well lit and brightly lit in the scenes. One can make a combined HDR image out of these multiple exposure shots. This combination of multiple exposure shots leads to an image of a higher dynamic range in a different image format which cannot be represented in the traditional Low Dynamic Range (LDR) formats. Moreover HDR images cannot be displayed in traditional display devices suitable for LDR. So these images have to undergo a process called as tone mapping for further converting them to be suitable enough to be represented on usual LDR displays. An approach based on Savitzky–Golay parametric filtering which preserves edges, is proposed which uses filtered multiple exposure images to generate the alpha matte coefficients required for fusing the input multiple exposure set. The coefficients generated in the proposed approach helps in retaining the weak edges and the fine textures which are lost as a result of the under and over exposures. The proposed approach is similar in nature to the bilateral filter-based compositing approach for multiple exposure images in the literature but it is novel, in exploring the possibility of compositing using a parametric filtering approach. The proposed approach performs the fusion in the LDR domain and the fused output can also be displayed using standard LDR image formats on standard LDR displays. A brief comparison of the results generated by the proposed method and various other approaches, including the traditional exposure fusion, tone mapping-based techniques and bilateral filter-based approach is presented where in the proposed method compares well and fares better in majority of the test cases.

Biography

Prof. Vivek Ramakrishnan, is a research scholar at the department of Electronics Engineering, Datta Meghe College of Engineering, Airoli, Navi-Mumbai, Maharashtra State, India. He has worked in the areas of Computational photography, Computer Vision and Image Processing. He has experience in working in image fusion algorithms for the High Dynamic Range Imaging (HDRI) problem. He specializes in working for the HDRI problem in the filtering and the transform domain.

Current progress on open tubular ion chromatography

Weixiong Huang and **Ge He**

Hubei Key Laboratory of Yangtze River Basin Environmental Aquatic Science, School of Environmental Studies, China University of Geosciences, China

Technical merits of an open tubular (OT) chromatographic system include great permeability, low sample and solvent consumption, etc. The theory of open tubular liquid chromatography (OTLC) was developed more than fifty years ago, however, the practice of OTLC was realized much later due to the difficulties in fabricating OT columns, micro injectors/detectors. As a branch of OTLC, an open tubular ion chromatography (OTIC) system requires to crack all the same issues. The capacitively coupled contactless conductivity detectors, which actually measure the admittance, provide convenient on-column detection capabilities on probing ionic species, and now are commonly used in OTIC systems. In recent years, ion-exchange latex coated cycloolefin polymer (COP) and polyether-ether-ketone (PEEK) based OT columns, along with Nafion-based electrodialytic capillary suppressors, have been developed, and thus paving the way of performing suppressed OTIC using alkali hydroxide eluents. In addition, a moldable strong cation exchange polymer can also be used as a capillary chemical suppressor to match the OTIC columns. Flow-splitting, pneumatic and/or nanopump systems were constructed to run both isocratic and gradient elution. Different approaches, frontal displacement and/or frontal reaction chromatography, are used to characterize the OTIC columns, with column capacities of monolayer latex coated OT columns measured to be on the order of 20 picoequivalent per mm2. The column efficiency of chloride ion can be as high as 1.6×105 plates/m in an anion-exchange latex coated 19 μm i.d. COP column with 4.0 mM sodium salicylate as the eluent. For the capillary electrodialytic suppressor, a suppression length of 1 mm is able to suppress 100 mM hydroxide at 100 nL/min. Very recently, another key component, the nanovolume gas-free hydroxide eluent generator, has been successfully developed for OTIC. The future work of OTIC is to increase the column capacity of separation columns and minimize band broadening caused by extra-column volumes.

Biography

Weixiong Huang was born in Fujian, China. He received all his B.S. degree in Chemistry and M.S. & Ph.D. degree in Analytical Chemistry from Xiamen University (1999-2010). He began his career as a research assistant at State Key Laboratory of Marine Environmental Science (Xiamen University) in 2011. One year later, he became a member of environmental monitoring staff at Guangdong Environmental Monitoring Center. During 2013-2018, he worked as a post-doc research fellow at University of Texas at Arlington, USA. In 2019, he joined China University of Geosciences as a faculty member at School of Environmental Studies. He has been working on ion chromatography (IC) since 2003, focusing on developing some key IC components, including separation columns, suppressors, and detectors, etc., for both regular and capillary IC. His research interest spans IC, instrumentation, environmental analytical chemistry, and electroanalytical chemistry. At present, he has authored or coauthored 20+ scientific peer-reviewed manuscripts.

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Radiation-Assisted green synthesis and characterization of selenium nanoparticles, and Larvicidal effects on *Culex pipiens* complex

A. M. Fadl[1], E. M. S. El-Kholy[1], I. Abulyazid[1], A. A. Shoman[1], H. H. Awad[2] and **H. S. Mohammed[3]**

[1]*Biological Application Department, Nuclear Research Center, Egyptian Atomic Energy Authority, Egypt*
[2]*Entomology Department, Cairo University, Egypt*
[3]*Biophysics Department, Cairo University, Egypt*

Many environmental hazards are due to chemical insecticides and enhance mosquito species' resistance. This problem is solved by using safer nanocides that reduce environmental pollution among integrated pest management (IPM) programs. Selenium nanoparticles (SeNPs) were green synthesized using *Cupressus sempervirens,* microwave (MW), and gamma irradiation (G) methods. Synthesized-SeNPs were characterized using UV–Vis spectroscopy, Fourier transform infrared spectroscopy (FTIR), Dynamic light scattering (DLS), X-ray diffraction (XRD), Zeta potential analysis, and Transmission electron microscopy (TEM). Characterization revealed stable spherical particles with size 11-55 nm for SeNPs-MW (20 min) and 21-75 nm for SeNPs-G (40 KGy). Gamma and microwave irradiations play significant roles in increasing SeNPs yield and decreasing their size. The concentration LC50 of 3rd instar larvae *Culex pipiens* for SeNPs-MW and SeNPs-G were 28.25 mg/L and 31.28 mg/L, respectively. The accumulated selenium concentration was increased in SeNPs-G treated larvae and measured with inductively coupled plasma mass spectrometry (ICP-MS). Ultrastructural study of the integument using TEM and light microscopy examination of midgut showed clear penetration and accumulation of SeNPs in exoskeleton and several deteriorations in epithelial cells. The results highlighted the important role of gamma and microwave irradiation with plant extract in synthesis and stabilization of SeNPs and their insecticidal efficacy against mosquitoes.

Meta-interaction physics on the evolution of the universe between dark energy and dark matter

Li Zongcheng

Research Lab of Interdisciplinary Science, Soochow University, China

The main task of this series of research is to establish a perfect theoretical framework for calculating the interaction between high-dimensional supergravity and dark energy (with strong negative pressure), describing the history of cosmic inflation-expansion and structural growth, so that it can be applied to any dark energy theoretical model and any interaction model. In this research, the pseudo vacuum energy in the inflationary universe model, the Higgs field in the standard physical model and the dark energy in the observational cosmology are reduced to the positive energy system with strong negative pressure, and they are reduced to the repulsion (all the resistance to gravity). In the high-dimensional space-time, corresponding to the introduction of supergravity with the supersymmetry, we put forth the superrepulsion with the supersymmetry, and establish the arche-conjugate relationship between the supergravity and the superrepulsion, so as to extend the holographic principle and the holographic dark energy model, and propose a new mechanism that can be promoted to the super holographic principle of high-dimensional universe. In the super-inflationary universe with rip-rebounding clusters which is studied here, the arche-conjugation is higher than the supersymmetry, so it becomes the core concept. From the basic component point of view, before or after the big bang, the gravitons and repulsons are coupled together, the negative energy contraction and the positive energy expansion work alternately, to form the arche-conjugate pulsator which is neither the point particle nor the linear superstring. In addition, we establish the path integral and its dynamic equation of quantum hedge unified field. For the Tachyon of upheaval in the super-inflating, the quantum theory of the early photons in upheaval is set up, and the analysis on the particles of the ultrahigh energy cosmic ray from the γ ray burst is made.

Biography

Li Zongcheng is a professor who recently retired from Suzhou University in China.

Fabrication of waste-based magnetic activated carbon nanostructures for environmental applications

Mohamed A. Habila

Department of Chemistry, King Saud University, Saudi Arabia

International and local efforts have been paid for the reduction of the hazard from the heavy metals pollution. The spread of heavy metals in the environment is an old issue associated with human mining activities and increased in the last decades due to the spread in the industrialization progress. The heavy metals distributed through the food chain affecting the soil, water systems, plants, animals and human. Much health risk has been recorded form the exposure to heavy metals, for examples when chronic exposure to lead occur, the negative impacts for human health in this case may include damage in nervous system, disturbance in kidney functions as well as raising the blood pressure. On the other hand, the quantity of solid waste is continuously increasing and, if not managed properly, could cause severe harm to the urban environment. The most previous studies for preparing magnetic activated carbon typically start with activated carbon and then introduced magnetic properties via various routes. The novelty trend in this work is to apply solid waste as a starting material for preparing magnetic activated carbon with superior textural properties, magnetic strengths and adsorption capacities. Results showed that the fabricated waste-based magnetic activated carbon nanostructures are promised adsorbents for remediation of metal and dyes pollution by removing Cu(II), Cd(II), Pb(II) and methylene blue from wastewater. The presence of Fe_3O_4 nanoparticle in the prepared adsorbent led to suitable response to the external magnetic field which enables the easy magnetic separation from water medium after adsorption. The modelling of the adsorption data have been applied and the calculated thermodynamic parameters including Gibbs free energy (ΔG^o), enthalpy (ΔH^o) and entropy (ΔS^o) confirm the spontaneous behaviour of the tested pollutants adsorptive-removal by the prepared waste-based magnetic activated carbon nanostructures.

Biography

Dr Mohamed A. Habila works as associate professor of chemistry, King Saud University. He is a board member of Saudi Chemical Society. He is interested in nanotechnology for development of clean methods for separation of environmental pollutants, improvement of solid phase extraction and dispersive micro-extraction, water and wastewater treatments, and synthesis and characterization of nano-porous multifunctional core-shell structures for various applications. Dr Habila is supervising more than 7 MSc and PhD. Students. Dr Habila has published more than 85 scientific article, and has delivered more than 20 public lectures in chemistry in local and international conferences and scientific events.

Awards:

1. Almarai Prize 2014 for the best creative research work (Co researcher). https://www.almarai.com/en/2015/03/04/kacast-announces-winners-of-almarai-prize/
2. Academics World Excellent Paper Award for the category best presentation/best content at the Academics World International Conference held in Athens, Greece on 7th October 2015.
3. Saudi Chemical Society for excellence in Society services, 2019.

Identification and characterization of Prothionamide degradation impurities by MS, NMR, and ultra-performance liquid chromatography method development

Vijaya Kumar Baksam[1,2], N.Saritha[2], Surya Krishna Mohan[1], Sanjeev Shandilya[1] and **Pramod Kumar[1]**

[1]API R&D Centre, Micro Labs Ltd, India
[2]Department of Chemistry, JNTUA College of Engineering, India

Stability-indicating and LC-MS compatible UPLC method was developed for the degradation and drug substances related impurities of Prothionamide. Forced degradation of Prothionamide was carried out under acidic, basic, thermal, oxidative, and photolytic stress conditions. The impurities separation was achieved on Acquity UPLC BEH-C18 (50 mm × 2.1 mm, 1.7 µm) with the mobile phase of 10mm ammonium acetate pH-6.0 and Acetonitrile in a time gradient mode. Related substances by UPLC method was validated according to ICH tripartite guidelines. Degradation products were isolated by Column chromatography and characterized by LC-MS, 1H, and 13C NMR spectroscopy. The developed related substances method showed adequate specificity, sensitivity, accuracy, linearity (0.4-1.5 µg ml-1), precision, and robustness in line with ICH tripartite guidelines for validation of analytical procedures. LOD and LOQ were 0.1 µg ml-1 and 0.4 µg ml-1 respectively for Prothionamide and all the impurities. The method was found to be linear with a correlation coefficient >0.99, precise (% RSD < 5.0), robust and accurate (% recovery 85-115%).

Biography

- Having 15 yrs experience in pharmaceutical industries
- Dealing analytical method development , method validations, regulatory activities
- Working as senior manager at Microlabs ltd.

Exfoliation corrosion performance of aeronautical aluminum alloy

A. Brahami[1] and **J. Fajoui**[2]

[1]*Laboratoire de Matériau et des Systèmes Réactifs, Université Djilali Liabes, Algeria*

[2]*Institut de Recherche En Génie Civil et Mécanique, IUT de Saint-Nazaire GeM, France*

Quantitative examination of localized corrosion, namely exfoliating corrosion (EXCO), of aluminum alloys 2024 T3 and 7075 T6 is carried out in this paper. The EXCO mechanism was also considered, with an emphasis on the consequences of a combination of materials, environment, and mechanical stress. Microstructures of different alloys were examined using an optical microscope (MO) and a scanning electron microscope (SEM) with an energy-dispersive spectroscope (EDX). To correlate the influence of corrosion/microstructure coupling on the fatigue behavior of different aluminum alloys, fatigue tests were done on compact tension specimens CT. The crack growth rate of the different materials for pre-corroded specimens was affected according to the microstructure of these two alloys.

Biography

PhD in mechanical engineering, option:damaging and reliability of structures, Abdessamad BRAHAMI particularly interested in material fatigue, FSW process and numerical modeling.

He's graduated with a bachelor's degree in Productics and then a Master's degree in optimization of production systems at the University of DjilaliLiabes of SidiBel Abbes.

He worked as a technology engineer in an Algerian-Finnish company. Currently, he is working on an international project on the topic of bioengineering.

He has participated in several international conferences around the world. He supervised 8 students in bachelor's degree and 5 in Master's degree.

He worked as Postdoc position at the University of Zaragoza –Spain-, working on colon motility and diseases experimental investigation and numerical modelization

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Electron currents and magnetic pulses in bounded atomic systems

S. L. Talwar[1], S. Lumb[2] and **V. Prasad[3]**

[1]Department of Physics, Maitreyi College, University of Delhi, India
[2]Department of Physics and Electronics, Rajdhani College, University of Delhi, India
[3]Department of Physics, Swami Shraddhanand College, University of Delhi, India

The current study aims at exploring the persistent electron currents and hence induced magnetic fields at the centre of hydrogenic atoms. A Hulthén screened spherically confined hydrogenic atom in a non-central ring potential is considered. The time-independent Schrödinger Equation (TISE) is solved using the finite difference approach. This yields the energy levels and corresponding wave functions and thus the probability current density, charge current and induced magnetic field at the nucleus are calculated.

The charge currents and induced magnetic fields vary as Z2 and Z3, respectively, for the simple case of Coulomb potential. This fact remains valid even in the presence of the ring potential but is not followed when the Hulthén potential is taken into account. It is found that the magnitude of current and induced magnetic field decreases due to screening as well as ring potential for an unbounded hydrogen atom.

When the system is subjected to an ultrafast Right Circularly Polarized Laser (RCPL) pulse, current and induced magnetic field are collectively controlled by the extent of spherical confinement, parameters characterizing the strengths of Hulthén and ring potentials as well as the laser parameters. For appropriately fixed parameters, femtosecond current and magnetic pulses are produced in the off-resonant case. Due to the availability of tunable lasers, such a situation may be experimentally realizable.

Further, the tightening of spherical confinement is found to enhance the magnitudes of such pulses even in the presence of Hulthén screening or non-sphericity. The augmented induced magnetic field as well as magnetic pulses of larger magnitude may prove to be beneficial in biomedical research.

Biography

Shalini Lumb Talwar is an Associate Professor in the Department of Physics at Maitreyi College, University of Delhi, where she has been involved in teaching undergraduate courses as a faculty member since 2008. Shalini completed her Ph.D., Masters and undergraduate studies from University of Delhi. She has been consistently engaged as a researcher in Theoretical Physics along with teaching. Her research interests include the study of confined atomic and molecular systems, laser-atom interaction and nanoscience. Shalini has published more than twenty research papers in international journals in addition to publishing in conference proceedings. She has participated in many national and international conferences. She believes that there is no age bar for learning new things which inspires her to constantly enhance her knowledge and aim towards achieving greater heights.

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Metabolite profile and dynamics during traditional beverages production: Case of palm wines in Côte d'Ivoire

T.N. Djeni[1,2], K.H. Kouame[1], F.D.M. Ake[1], L.S.T. Amoikon[1] and K. Jeyaram[2]

[1]Laboratoire de Biotechnologie et Microbiologie des Aliments, Unité de Formation et de Recherche en Sciences et Technologie des Aliments (UFR-STA), Université Nangui Abrogoua, Côte d'Ivoire
[2]Microbial Resources Division, Institute of Bioresources and Sustainable Development (IBSD), India

Palm wine, the most commonly consumed traditional alcoholic beverage in Western Africa, harbours a complex microbiota and metabolites, which plays a crucial role in the overall quality and value of the product. In the present study, a combined metagenomic and metabolomic approach was applied to describe the microbial community structure and metabolites profile of fermented saps from three palm species (Elaeis guineensis, Raphia hookeri, Borassus aethiopum) in Côte d'Ivoire. Lactobacillaceae (47 %), Leuconostocaceae (16 %) and Acetobacteriaceae (28 %) were the most abundant bacteria and Saccharomyces cerevisiae (87 %) the predominant yeasts in these beverages. The microbial community structure of raphia wine was distinctly different from the others. Multivariate analysis based on the metabolites profile clearly separated the three palm wine types. The main differentiating metabolites were putatively identified as gevotroline hydrochloride, sesartemin and methylisocitrate in Elaeis wine; derivative of homoserine, mitoxantrone in Raphia wine; pyrimidine nucleotide sugars (UDP-D-galacturonate) and myo-Inositol derivatives in Borassus wine. The enriched presence of gevotroline (an antipsychotic agent) and mitoxantrone (an anticancer drug) in palm wine supports its therapeutic potential. In addition, the decline in the relative abundance of gevotroline and essential amino acids during the later stages of palm wine tapping (15-25 days) supports the difference in the health benefits of the palm wine obtained from different days of tapping, indicating that early stages of tapping is more nutritional and healthy than the later stages. The microbial dynamics may be a potential indicator of metabolite changes during palm sap fermentation, thus contributing to establish particular features of palm wines in different stages of tapping. This understanding of microbial ecology and chemical composition changes during palm wine tapping can be used as biomarkers to assess palm wine's quality and help to design an optimum starter culture consortium.

Biography

Theodore N. DJENI, Ph. D., is Professor of Microbiology and Permanent Secretary of the Food Security Research Center at the University Nangui Abrogoua of Abidjan in Côte d'Ivoire. His current research interest is in the area of selection of performing indigenous microorganisms that can be used in processes for foods value adding and biobased products production from low cost materials. In addition, he investigates the application of specific enzymes producing microorganisms in the biotratment of industrial wastewaters.

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Starch-coated magnetic nanoparticles and external electromagnetic field for cancer theranostic

V. Uzunova[1], A-R. Tsiapla[2], Ts. Dimitrova[3], I. Georgieva[1], S. Apostolova[1], B. Borisova[1], O. Kalogirou[2], T. Samaras[2], M. Angelakeris[2], J. Tchekalarova[3] and **R. Tzoneva[1]**

[1]Laboratory of Transmembrane Signaling, Institute of Biophysics and Biomedical Engineering, Bulgaria
[2]Department of Physics, Aristotle University of Thessaloniki, Greece
[3]Department of Neurobiology, Institute of Neurobiology, Bulgaria

In recent years, magnetic nanoparticles (MNPs) have demonstrated progress in the field of medical industry and therapies. Internalization of MNPs in target cells may cause changes in cytoskeleton network, which in turn would lead to various functional alterations, including the inductions of apoptosis and oxidative stress. For that reason, the purpose of the study was to discuss the effects of MNPs and pulsed electromagnetic field (PEMF) on the actin cytoskeleton network and nucleus morphology in MDA-MB-231 and MCF-10A cell lines as well as the induction of oxidative stress and hepatic toxicity by intracerebroventricular (icv) injection of MNPs in ICR mice.

Initially, 100 µg/mL MNPs were added to the test cell lines and effects on cytoskeleton network and nucleus morphology were observed with fluorescent microscope (JenaLumar with camera Zeiss and objective HI100x/1,30). Oxidative stress after injection of MNPs in doses of 10-200 µg/kg in mice was evaluated by ELISA assay for malondialdehyde (MDA) and superoxide dismutase (SOD) production. Hepatic toxicity of combined treatment of mice of magnetic field and MNPs was examined by blood test for different serum markers.

Our results demonstrate biocompatibility and safety of nanoparticles for biological systems. In contrast, PEMF and 100 µg/mL MNPs appear to be toxic to cancer MDA-MB-231 cells and exert effects on the cytoskeleton, related to the cell migration. Morphological changes in the nuclei were also observed. Unlike cancer cells, in the non-cancerous MCF-10A the effects were slight and temporary. In vivo results suggest low oxidative stress and lack of hepatic toxicity in ICR mice with application of the combination PEMF/MNPs.

These studies showed that the MNPs could be used in various methods for influencing cancer as hyperthermia or magneto-mechanical stress.

Acknowledgements: This work was supported by National Research Program "Young scientists and postdoctoral students (DCM#577/17.08.2018)" - Bulgarian Ministry of Education and Science.

Biography

Veselina Uzunova, has completed her PhD at the age of 30 years from Institute of Biophysics and Biomedical Engineering (IBphBME), Sofia, Bulgaria. She is working as post-doc in Laboratory of Transmembrane Signaling, IBphBME. She has published 2 papers in reputed journals, and her publication h-index is 8. She has research interests in the field of anti-tumor therapy and regenerative medicine. Holds the Innovative Product Award in 2011, and she has also two awards from scientific conferences (2014, 2017).

Investigation of the potential complexing ability of dissolved organic substances in surface water to Al (III), Fe (III) and Cu (II) ions

V.A. Zhezherya[1], P.M. Linnik[1], R.P. Linnik[2] and V.P. Osipenko[1]

[1]Institute of Hydrobiology, National Academy of Sciences of the Ukraine, Ukraine

[2]Taras Shevchenko Kyiv National University, Ukraine

The potential complexing ability (PCA) of dissolved organic substances (DOS) is expressed in terms of metals concentration that can be bound into complexes by DOS upon reaching equilibrium conditions.

Our research concerned the study of the total PCA of DOS to metals, as well as their individual groups.

We used water filtrates from the Kaniv Reservoir and Verbnoye Lake (Kyiv City), which differ in DOS concentration and the ratio of humic substances (HS), carbohydrates and protein-like substances (PLS). The water was filtered through membrane filter with a pore diameter of 0.45 μm. The concentration of HS, carbohydrates, PLS and dissolved Al(III), Fe(III) and Cu(II) in water filtrates and concentration of metals in complexes with DOS were determined before and during the 1, 7, 14, and 28 days of the experiment. At the beginning of the experiment, 500 μg/L of each metal was added to water filtrates and purified tap water (control).

The total PCA of DOS in the water filtrates of the Kaniv Reservoir and Verbnoye Lake was 11.0–15.5 and 14.9–15.8 μmol/L and changes insignificantly seasonally. PCA of DOS in the water in the studied water bodies for each metal averaged 4.7, 3.9, and 4.6 μmol/L and 5.6, 6.0, and 3.7 μmol/L for Al(III), Fe(III), and Cu(II), respectively. The metals were bound into complexes during the first days, reaching an equilibrium state on the 7th day of the experiment. The complexes with DOS already contained 36.8–49.6% of added metals concentration. In the water filtrates of the Kaniv Reservoir and Verbnoye Lake, the share of Al(III), Fe(III), Cu(II) in the complexes with DOS averaged 20.5%, 32.7, 46.8% and 20.8%, 46.4, 32.8% of their total concentration in these complexes. This indicates the competition of metals for binding sites in DOS. HS were bound into complexes mainly by Fe(III) and Cu(II), the share of which was 27.5–81.5% of Febound and 48.0–77.5% of Cubound. The share of aluminum did not exceed 32% of Albound. The studied metals were predominantly bound into HS complexes with a molecular weight of <5 kDa. The share of metals in the complexes with carbohydrates increased in summer and autumn, when concentration of these ligands also increased. According to the research results, the detoxification of water from metals in case of rapid discharge of wastewater will occur due to adsorption and sedimentation, and then complexation.

Biography

Education: Dnipropetrovsk National University, Faculty of Biology and Ecology, diploma of a specialist in "Biology" (2001–2006).

Institute of Hydrobiology of the National Academy of Sciences of Ukraine, postgraduate study in the field of 11.00.07 "Land hydrology, water resources, hydrochemistry" (2008–2011).

Candidate of Geographical Sciences in the field of 11.00.07 "Land hydrology, water resources, hydrochemistry" (2012).

Work experience: I work as a senior researcher at the Freshwater Hydrochemistry Department of the Institute of Hydrobiology of the NAS of Ukraine.

Research experience: My research concerns the study of coexisting forms of metals in surface waters. Particular attention is paid to the study of the metal concentration in the labile fraction, which belongs to the potentially bioavailable form. I investigate the complexing ability of dissolved organic substances in relation to metals in surface water.

Characterization and anticancer potential of Withania somnifera fruit bioactives (a native species to Pakistan) using GC-MS, NMR and LC-MS-ESI

Qudsia Tabassam[1], Tahir Mehmood[1,2], Farooq Anwar[1] and **Abdul Rauf Raza[1]**

[1]Institute of Chemistry, University of Sargodha, Pakistan
[2]Institute of Biochemistry and Biotechnology, University of Veterinary and Animal Sciences-UVAS, Pakistan

Introduction: *Withania somnifera* is a plant with remarkable pharmacological properties. The plant has an impressive profile of medicinal uses in the folk medicine system of several civilizations.

Aim: This comprehensive study is aimed to characterize phytochemicals in fruit of *W. somnifera* and tested for in vitro anticancer potential to find out active candidate in disease prevention and treatment

Method: The bioactive components from *W. somnifera* fruit were extracted with polar and non-polar solvents. Anticancer potential of the isolated bioactive was assessed against different cancer cell lines through MTT assay and Incucytes imaging analysis. The extracts were characterized for secondary metabolites using GC-MS, LCMS-ESI and 1H-NMR techniques.

Results: Both freeze-dried and rotary evaporator condensed extracts exhibited anticancer potential against MDA-MB-231, MCF7- SKOV3 and SKBR3 cell lines. The tested extracts have cell growth inhibition potential against mammalian cancer cell line. Hexacosanedioic acid purified from n-hexane extract through HPLC was investigated for its cytotoxicity against breast cancer cell line SKBR3 by using Incucytes imaging analysis

Conclusion: We found that a variety of bioactive compounds existed in this plant. One identified compound that was not investigated for cytotoxicity in previous studies was purified and its application showed cytotoxicity on breast cancer cell lines. A number of bioactive identified from *Withania somnifera* fruit may have an effective potential for development into chemotherapy drugs.

Biography

Dr. Qudsia Tabassam research background is in Natural Products Chemistry. Her research interests focus on the isolation and structure elucidation of novel metabolites and nanocarrier with diverse chemical structures and potential as anticancer, antimicrobial including antiviral, or antifungal agents. The overall goal of her research is to identify biologically active molecules that can act as templates for the development of new therapeutic agents having eco-friendly (green nature) for the treatment of diseases especially cancer. She have published 18 research articles in my field with 30 impact factor and published two thesis and 1 book chapter. Currently, working as visiting lecturer in two public sector Universities in Pakistan.

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Separation of radioactive Ni from activation products

F. Monroy-Guzmán

Instituto Nacional de Investigaciones Nucleares, Mexico

Ni-63 is generated by oxide activation produced in components that are in contact with the primary coolant of light-water reactors. Ni-63 has a half-life of 101.2 years and is a pure beta emitter with a maximum energy of 67 keV, so that its isotopic characterization, necessary for decommissioning and radioactive waste management activities, involves separation processes to isolate and analyze it. Therefore, the goal of the present work was to develop a separation method for Ni-63 from activation products such as Fe-55 (2.7 y), Fe-59 (44.49 d), Zr-93 (1.61×10^6 y), Co-58 (70.86 d), Co-60 (5.27 y), Nb-94 (20,300 y). Two separation methods were applied, first ion exchange chromatography, using DOWEX 1X8 anionic resin packed in chromatographic columns and HCl solutions as eluent. Separation tests were performed as a function of HCl concentrations, based on the adsorption properties of these elements on anionic resins, reported in the literature. Finally, Ni was purified by precipitation with dimethylglyoxime which is deposited on an inert support. The precipitate is washed with ammonium citrate solutions and Ni is recovered by dissolving the nickel dimethylglyoxime chelate [$Ni(DMG)_2$] with

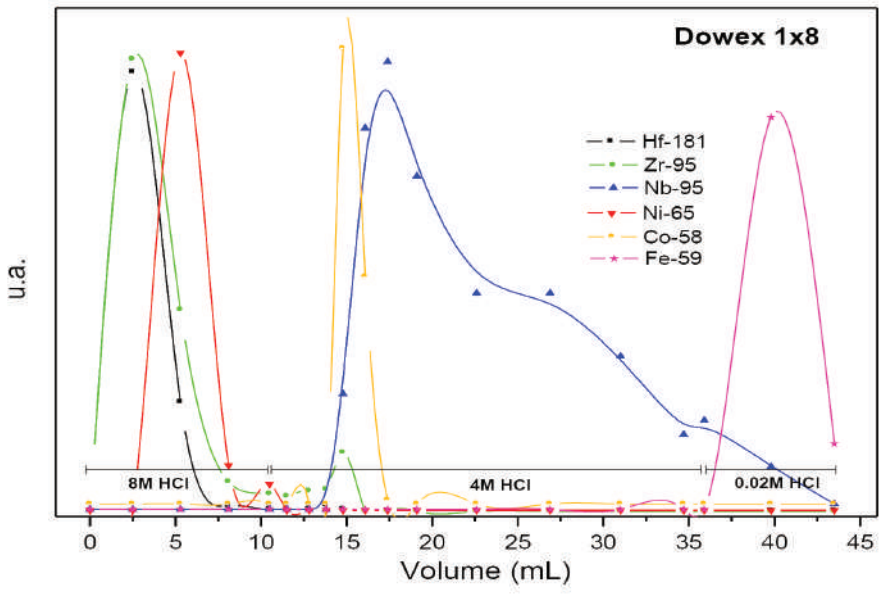

Figure 1. Separation of nickel by anion exchange.

HNO_3. Several inert supports (Amberlite®XAD4, PTFE and Silica Gel) and ammonium citrate concentrations were tested in order to define the best Ni recovery conditions. The short half-life radioactive tracers and gamma emitters Ni-65 (2.52 h), Co-58, Fe-59, Zr-95 (64.03 d), Nb-95 (34.99 d), and Hf-181(42.39 d) were used to facilitate the monitoring of the separation process, which were produced by irradiation of Ni, Zr and Fe nitrates in the Triga Mark III reactor at ININ. Ni, Zr and Hf are eluted from the anionic resin with 8 M HCl as shown in Figure 1 and finally Ni is separated from Zr and Hf by precipitation with dimethylglyoxime.

Biography

Fabiola Monroy-Guzmán: Chemical Engineer and Master in Nuclear Sciences from Faculty of Chemistry at the National Autonomous University of Mexico. PhD. from University of Paris XI, France; 20 years of experience in radiochemical separation processes. Founder and leader of the ININ's Radioactive Waste Laboratory. Leader of projects funded by CONACYT (National Council for Science and Technology, Mexico), IAEA (International Atomic Energy Agency) and UNESCO (United Nations Educational, Scientific and Cultural Organization), focused on the production of radioisotopes for medical purposes, archaeometry and management of radioactive waste. ININ full-time researcher.

Pesticides: Agricultural food products, problems, chemistry

L. Bondareva and **N. Fedorova**

Federal Scientific Center of Hygiene Maned After F.F. Erisman, Russia

On the global scale the damage of agricultural crops is caused by approximately 50 000 species of plant pathogens, 9 000 species of insects and mites and 8 000 species of pest plants. This damage of crops is estimated as the crop loss due to plant pathogens - 13%, due to pest insects - 14% and due to pest plants - 13%. Furthermore, pesticides are indispensable for growing plants, especially for growing economically important crops. The present our research we considers potential approaches to the solution of an important problem, i.e. the impact of pesticides of various classes and applications on living organisms, mainly, on food crops Special attention is paid to the validation of the multi-residual method for determining 40 items of pesticides in agricultural food products, with the following practical application of the method to determine pesticides in real food products, as well as in components of model experiments. The distribution of pesticides between the components of the system soil-plant was studied at an example of rimsulfuron, a pesticide belonging to the class of sulfonylureas. Moreover, grain crops were shown to be less susceptible to the impact of such pesticides as acetamiprid, flumetsulam and florasulam while the shoot development in bean plants was hindered, with the subsequent death of the plants.

Biography

- Lydia Bondareva, PhD of Analytical Chemistry, Full Professor of Ecology
- Leader research in Analytical laboratory.
- **Education:** Lomonosov's Moscow State University, Analytical chemistry.
- **Field:** Analytical chemistry, radioecology, chemistry of pesticides, aquatic plants
- I have more than 200 scientific articles in top-rated scientific journals and am the author and co-author of monographs.

Possibilities of using biomethane as a low-emission energy carrier in transport in the light of the Green Deal

I.samson-Bręk[1] and **K.Biernat**[2]

[1]*Environmental Protection Institute, National Research Institute, Poland*

[2]*Łukasiewicz Research Network, Automotive Industry Institute, Poland*

The current effects of global warming are undisputed and increasingly felt in all regions of the world. One of the main causes of global warming is anthropogenic emissions of greenhouse gases (GHG), mainly carbon dioxide (CO_2), caused by the burning of fossil fuels. Together with diffuse emissions other than CO_2 in the energy system, they are responsible for over 75% of the total greenhouse gas emissions in the European Union countries. One of the most emitting sectors in the EU is transport, which is responsible for as much as 27% of EU carbon dioxide emissions. This sector requires urgent and intensive measures to reduce GHG emissions. This is particularly important in the context of the European Green Deal goals, which assume the reduction of GHG emissions by 55% in 2030 compared to the base year (1990), as well as achieving climate neutrality in 2050. One of the most promising energy carriers in transport, the greatest potential for a significant reduction in heat gas emissions is biomethane. However, its widespread use as an energy carrier in transport is associated with a number of technical, quality and cost problems.

The aim of this publication is to present the possibilities and perspectives of using biomethane as an energy carrier in transport, taking into account the current technological and quality requirements and their impact on GHG emissions in the life cycle of biomethane. In addition, the publication also indicates the main barriers to the development of the biomethane market, based on the example of Poland.

Biography

Izabela Samson-Bręk, Ph.D. graduated from the Cardinal Stefan Wyszyński University in Warsaw (Master in environmental protection, specialization: technologies used in environmental protection). In 2019, she obtained a Ph.D. in technical sciences at the Faculty of Automotive and Construction Machinery Engineering of the Warsaw University of Technology. The subject of the Ph.D. dissertation included issues related to the assessment of the environmental effects of using biogas as an energy carrier to power a stationary internal combustion engine. She is the author or co-author of numerous scientific publications. She also participated in many R&D projects concerning the biofuels and alternative fuels production technologies, as well as environmental protection. He is a co-founder of the Polish Scientific Recycling Association and an ordinary member of the Association of the Polish Chamber of Biofuels. Researcher at the Institute of Environmental Protection-National Research Institute in Warsaw and the Polish Chamber of Biofuels. He specializes in environmental life cycle assessment (LCA) and carbon footprint calculation, as well as sustainable production of transport fuels and biofuels, in particular biogas and biomethane.

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Voltammetric study of sulfonated tetra- and octa-substituted cobalt phthalocyanine complexes in aqueous solutions

M. Kovanova, P. Derbeneva and **A. Vashurin**

Ivanovo State University of Chemistry and Technology, Russia

In this study, we synthetized six different cobalt phthalocyanines (CoPc, Figure 1). All the complexes were characterised by IR spectroscopy, 1H and 13C NMR spectroscopies, and mass spectrometry. The effect of the nature of peripheral substituents on the electrochemical behaviour of series of cobalt phthalocyanines peripherally substituted with consistently changing sulfonated fragments has been studied by cyclic voltammetry. The aqueous cyclic voltammetry of CoPcI-CoPcVI has been examined in alkaline solution (KOH, pH 12) at a platinum (Pt) disk electrode. Commercial cobalt tetra-4-(4-sulfo)phthalocyanine was used as a reference. It was found that all considered metal complexes exhibit the irreversible redox behaviour. We concluded that in alkaline media, the catalytic activity of metal phthalocyanines of cobalt is manifested in the form of a hydroxide oxidation reaction with the formation of molecular oxygen. It was found that the electrocatalytic properties of the Pt electrode with respect to hydroxide are generally independent of the nature of the substituent in the phthalocyanine macroring. It has been established that the processes of oxidation (reduction) of the central metal ion and the stage of electroreduction of the organic ligand are one-electron. Based on studies concerning the catalytic activity of, on the one side, cobalt macrocycles towards small adducts other than hydroxide and, on the other hand, the electrocatalytic activity of cobalt oxides towards the oxygen evolution, a possible mechanism of increased reactivity of macrocycles of cobalt ions with respect to oxygen evolution is suggested.

The authors are grateful for the financial support of this work by the Russian Science Foundation, 17-73-20017.

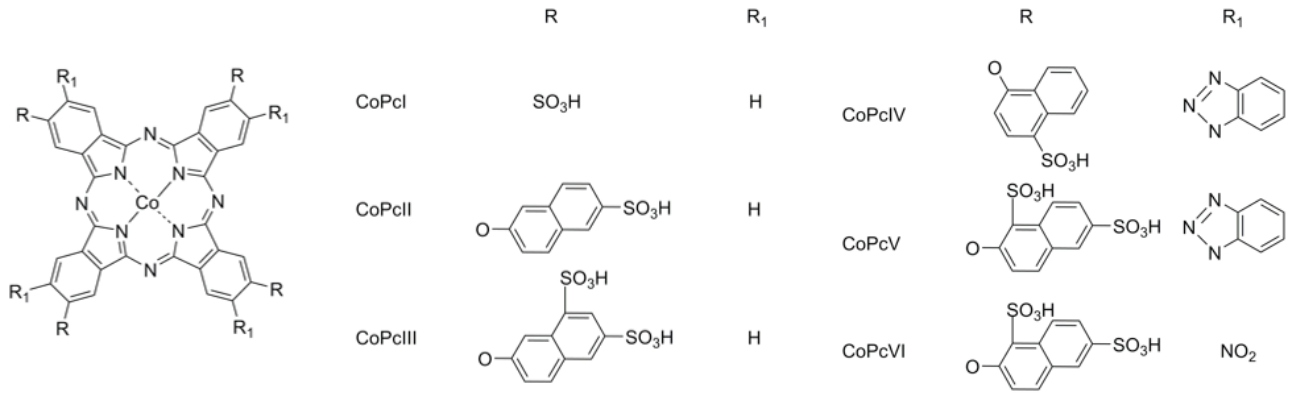

Figure 1. The scheme of the study objects.

Biography

Dr. Mariia A. Kovanova is a Senior Lecturer at the Department of Inorganic Chemistry of the Ivanovo State University of Chemistry and Technology. She received her Ph.D. in the area of Inorganic and Physical chemistry. She routinely teaches Inorganic chemistry, Medical and pharmaceutical chemistry, Modern information technologies in chemistry. Dr. Kovanova's research interests are related to the study of solvation effects and solvent dynamics in electron transfer reactions involving macroheterocyclic compounds.

Experimental study of smart extinguishing material for use in forest and wildland-urban interface fires

M. Chalaris

Hephaestus Advanced Laboratory, Department of Chemistry, International Hellenic University, Greece

The aim of the study is to compare the effectiveness of Water and Bonpet liquid for suppression of forest fires and WUI Fires.

Water is suitable for fire class A and Bonpet liquid is suitable for fire class A, B in F and the consequences from the fire class C. Bonpet liquid is a water solution of inorganic salts and organic compounds: Ammonium carbonate $CH_2O_{3-x}H_3N$, Ammonium hydrogen carbonate $CH_2O_{3-}H_3N$, Towalex AFFF 3% UL. BONPET liquid absorbs at least 10 times more energy from the burning surface than water would.

We will present tests that have proven that mixing only 6% of BONPET Liquid with water will increase fire extinguishing performance. This means that 20 times less consumption of water is needed, and the collateral damage caused by a fire is smaller when extinguishing with BONPET liquid. Furthermore, non-decomposed components of BONPET liquid that remain on the surface after the fire has been extinguished, have the ability to disintegrate and cool the surface if there is a slight increase in temperature

The most significant benefit of using BONPET liquid is that it will greatly reduce extinguishing times due the enhanced extinguishing capabilities. This also means far less CO_2 emissions from the fire and less burned area to restore back to its original state.

The second benefit is cost-effectiveness. The liquid can be premixed with water to the optimal ratio for many types of fires including larger ones. This means that the cost can be greatly reduced, and the extinguishing effect still obtained.

The third benefit is regarding the environment. The liquid is designed to not produce any harm when extinguishing and after. It is not harmful to any wildlife or plant life, therefore being environment friendly

Biography

Michail Chalaris is an Assistant Professor at the Department of Chemistry, International Hellenic University(IHU) and Professor in MSc "Analysis and Management of Manmade and Natural Disasters" in the course Technological disaster and environmental emergencies since 2015 and in MSc Oil and Gas Technology in the course Hazard Identification & Risk Management since 2018. He is Research Director on Risk, Hazards, Crises, and Safety of Hephaestus Advanced research Laboratory of School of Science, IHU. He has been an adjunct professor at the Hellenic Fire Academy (1999 – 2021) and at Military Nursing Academy(SAN) (2017 – 2021).

Prof. Chalaris is a Retd Major General with 25-year at the fire service. He is a program committee member of several international conferences. He has organized/coordinated or participated as a keynote and invited lecturer on several advanced training courses and advanced research workshops. He also managed/participated in several multi-year projects related to the area of his expertise.


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SCIENTIFIC ABSTRACTS

DAY 2

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A novel detection system for fragmented cytokeratin 18 using new antibodies

Minori Yamada[1], Koji Okuno[2], Koji Sakaguchi[1] and Tetsuji Yamaguchi[3]

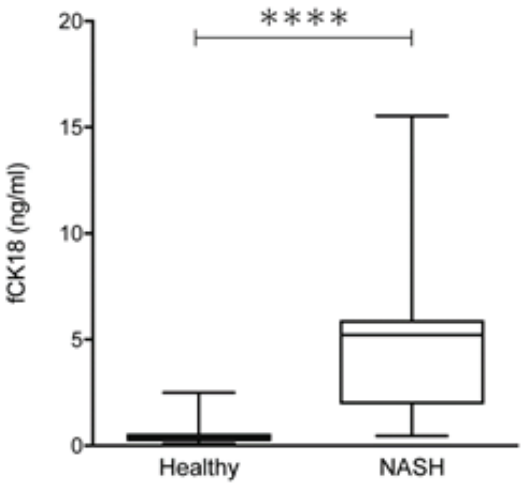
[1]Bio-Reagent Material Development, Bio-Diagnostic Reagent Technology Center, Sysmex Corporation, Japan
[2]Scientific Affairs, Sysmex Corporation, Japan
[3]Manufacturing Technology Development 2, Sysmex Corporation, Japan

Background: Fragmented cytokeratin 18 (fCK18) released from epithelial cells undergoing apoptosis is widely studied in various diseases. However, fCK18 measurement is not utilized in clinical practice due to imprecise disease-state cutoff values. Therefore, we generated new monoclonal antibodies (mAbs) and developed a highly sensitive chemiluminescent enzyme immunoassay (CLEIA).

Methods: Capture (K18-624) and detection (K18-328) mAbs were generated from mice immunized by either a synthetic peptide or a commercial recombinant protein. The mAb characterization was performed using immunoblotting, immunoprecipitation and reactivity with synthesized peptides. A recombinant fCK18 (rfCK18) produced in Escherichia coli was purified by affinity column chromatography. Analysis of performance and measurement of human fCK18 were evaluated using K18-624 and K18-328 in a highly sensitive CLEIA.

Results: K18-624 had a high binding ability compared to the current commercial antibody. K18-328 recognized 323S-340G of CK18. A rfCK18 was expressed in the soluble fraction of E. coli when the N-terminal region (260 amino acid residues) of CK18 was truncated. Based on the fCK18 CLEIA performance, the coefficients of variation (CV) for within-run and between-day repeatability were below 10% and the recoveries were in the range of 15%. The detection sensitivity was 0.056 ng/mL. Serum fCK18 levels were significantly increased in NASH patients when compared to healthy individuals.

Conclusions: Our new fCK18 mAbs showed high affinity and sensitivity. CLEIA using our new antibodies will be useful in measuring fCK18 in human blood thereby generating accurate clinical diagnoses of human liver diseases.



Biography

Minori Yamada is a researcher who studies the biomarkers for liver diseases including nonalcoholic steatohepatitis (NASH). She has a master of Human Science by the studies of fat cells mechanisms of metabolic syndrome measuring adipocytokines (Biochem Eng J 2009 and J Biomed Sci Eng 2007). In Oriental Yeast Corporation, she was a leader and achieved the developing enzymes and proteins. Now, she found a biomarker candidate of NASH diagnosis and has been moving the project in Syemex corporation.

Absorbed dose monitoring radiochromic film systems for intense photon and electron radiation processing technologies

V.P. Tenishev

Russian Metrological Institute of Technical Physics and Radio Engineering (VNIIFTRI) Mendeleevo, Russian Federation

Radiochromic films dosimetry tools are presented developed at the Russian Federal State Unitary Enterprise "VNIIFTRI" for metrological control of the absorbed dose in the medical devices sterilization, food and agricultural products treatment by ionizing radiation, industrial processing of polymer products for the modifying their properties, establishing the radiation resistance of packaging materials and etc.

Biography

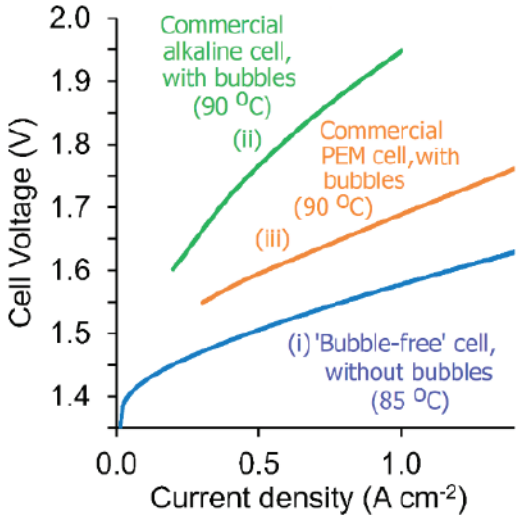
Born in 1954; Education – MPHTI, 1980; PhD – 1987; Senior Researcher-CERN, Switzerland 1998; Invited Researcher at Atom Physics division at Lund University, Sweden 2002-2004; since 2004 – Senior Scientist at VNIIFTRI, Russia.

A high-performance electrolysis cell promises more cost-competitive renewable hydrogen

G. F. Swiegers, A. Hodges, A. L. Hoang, G. Tsekouras, K. Wagner, C.-Y. Lee, P. Tiwari and **G. G. Wallace**

Intelligent Polymer Research Institute and Australian Research Council's Centre of Excellence for Electromaterials Science, University of Wollongong, Australia

Renewable, or green, hydrogen will play a critical role in the decarbonization of hard-to-abate sectors and will therefore be important in limiting global warming. However, renewable hydrogen is not cost-competitive with fossil fuels, due to the moderate energy efficiency and high capital costs of traditional water electrolysers. Here a unique concept of water electrolysis is introduced, wherein water is converted directly to hydrogen and oxygen gas, leading to inherently bubble-free operation at the electrodes. A bubble-free alkaline water electrolysis cell of this type demonstrates performance exceeding commercial cells, with a cell voltage at 0.5 A cm-2 and 85 °C of only 1.51 V, equating to an energy consumption of 40.4 kWh/kg hydrogen (vs. ~47.5 kWh/kg in commercial electrolysis cells) (Fig. 1). This is within the IRENA target of 42 kWh/kg by the year 2050. High energy efficiency, combined with the promise of a simplified balance-of-plant, brings cost-competitive renewable hydrogen closer to reality.



Biography

Gerhard (Gerry) F. Swiegers is a professor at the University of Wollongong, Australia. He leads an active research group focussing on electrochemical catalysis and production of hydrogen from water using renewable electricity. He also works in the fields of electrocatalytic process engineering and industrial electrochemistry. He has published 2 book, 135 peer-reviewed papers/chapters and 55 patent families. He has founded 7 spin-off companies and licensed out 3 new technologies in the last 20 years.

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Spiropyrazolinium salts and O-TOSILATE-β-(BENZIMIDAZOL-1-YL) propioamidoxyme as the products of β-aminopropioamidoximes tosylation

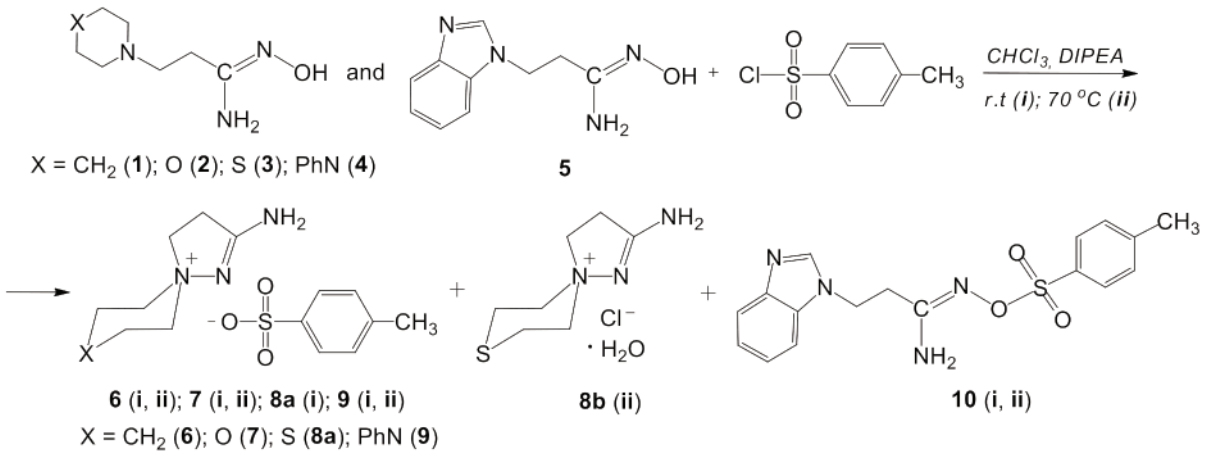
L.A. Kayukova[1], A.V. Vologzhanina[2], G.P. Baitursynova[1], E.M. Yergaliyeva[1], A.B. Uzakova[1], G.T. Dyusembayeva[1] and S.B. Zhambyrbai[2]

[1]JSC A.B. Bekturov Institute of Chemical Sciences, Kazakhstan
[2]X-Ray Structural Centre, A.N. Nesmeyanov Institute of Organoelement Compounds, Russian Federation

Pyrazolines structures have practically valuable biological properties. Their methods of synthesis mainly consist in the reactions of cyclization of steroid compounds containing an enone fragment with a variety of hydrazines. We have previously obtained new spiropyrazolinium compounds by hydrolysis of 3-(β-heteroamino)ethyl-5-aryl-1,2,4-oxadiazoles and by arylsulfochlorination of β-aminopropioamidoximes. Here we were interested in the dependence of the structure of β-aminopropioamidoximes tosylation products from the structure of the initial substrates.

The tosylation of β-aminopropioamidoximes (β-amino group: piperidin-1-yl, morpholine-1-yl, thiomorpholin-1-yl, 4-phenylpiperazin-1-yl, benzimidazol-1-yl) (1–5) was carried out in chloroform using diisopropylethylamine as a base. The synthesis was carried out at r.t. (i) for 15–20 h and at 70 ☐ (ii) for 8 h. The progress of the reaction was monitored by TLC. After completion of the reaction product precipitation was recrystallized from isopropanol.

The tosylation products of β-aminopropioamidoximes were identified



using physicochemical, spectral [IR, NMR (1H and 13C)] and X-ray diffraction characteristics. Tosylation of β-aminopropioamidoximes 1–4 at r.t. proceeds with the formation of spirocyclic compounds – arylsulfonates of 2-amino-1,5-diazaspiro[4.5]-dec-1-ene-5-ammonium (6, 7, 8a, 9) in 45–65%. Carrying out this reaction at 70°C for amidoximes 1, 2, 4 increases the yield of spirocompounds 6, 7, 9 to 53–70%; while the tosylation of β-(thiomorpholin-1-yl) propioamidoxime 3 gives only 2-amino-8-thia-1,5-diazaspiro[4.5]dec-1-ene-5-ammonium chloride hydrate 8b in 84% amount. Tosylation of β-(benzimidazol-1-yl)propioamidoxime (5) at r.t. and at 70°C gives the product on the oxygen atom of the amidoxime group 10 in 45% and 53%, respectively.

Thus, it is obvious that during the tosylation of amidoximes 1, 2, 4, 5 the tosylates of spiropyrazolinium compounds 6, 7, 9 and the O-tosylation product of β-(benzimidazol-1-yl)propioamidoxime 10 are the products of kinetic control; while tosylate 8a is a product of kinetic control, and chloride hydrate 8b is a product of thermodynamic control.

Biography

Lyudmila Kayukova – Chief Researcher of the Laboratory of Chemistry of Synthetic and Natural Drug Substanses of the JSC «A.B. Bekturov Institute of Chemical Sciences» (Almaty, Kazakhstan), Doctor of Chemical Sciences, Professor. Education: Leningrad State University, Chemical Faculty, Department of Physical Organic Chemistry. She is the first author of about 200 papers in the journals from the Web of Science and Scopus list and in the scientific journals of the RK; of 40 patent documents of the RK and Russia; the head and executor of grants from the SC ME&S RK, CRDF, Innovation Fund of the RK. She is a scientific head of 8 candidate and PhD dissertations.

Analysis of riverbank erosion – A micro-level approach

Sanchayan Mukherjee

Kalyani Government Engineering College, India

Riverbank erosion is a phenomenon that has been a matter of interest to many researchers till date. A riverbank may be considered a cluster of grains in micro-level. There are forces that bind them together. The complexity of the entire scenario increases to a great extent as the water level of the river varies. On the other hand, for an unsaturated soil matrix, the small amount of water between a pair of grains plays a significant role. The distance between a pair is important and so is the size of the grains. A river has always its own unique features and, this is why, a general and theoretical approach is a challenge. A thorough analysis of the forces may lead to a model that helps estimation of erosion to a great extent. Here, an effort is made in this direction with an existing model called "Truncated Pyramid Model". In this model, the particles are assumed to be spherical in shape and arranged in a typical configuration for the stability of the bank as a whole. Fundamental principles of mechanics are used to arrive at a solution. This model is applicable to different riverbanks and it helps to understand the behaviour of the bank. The model can be modified to suit different conditions and validated against experimental results.

Biography

Dr.Sanchayan Mukherjee, Ph.D. (Engineering), served four years in industry before joining academics in July 2000. He authored five text books and edited two conference proceedings. He wrote thirty journal papers, presented papers at about thirty national/international conferences. He won three best research paper awards in three different conferences till date. He acted as a session chair and delivered invited talks in many conferences. A member of the Editorial Board of six journals, he is a regular reviewer of many reputed journals of high impact factor, e.g., Journal of Hydro-environment Research (Elsevier), Journal of Hydraulic Engineering (ASCE), Journal of Applied Mathematical Modelling (Elsevier), KSCE Journal of Civil Engineering (Springer), Engineering Applications of Computational Fluid Mechanics (Taylor & Francis), International Journal of Energy Research (Wiley), International Journal of Fluid Mechanics Research (Begell House), Groundwater for Sustainable Development (Elsevier) etc.. He reviewed three books. He is a member/fellow of many professional societies.

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More general families of exact solitary wave solutions of nonlinear schro¨dinger equation with their applications in nonlinear optics

Nadia Cheemaa[1], Aly R.Seadawy[2,3] and **Wen-Xiu Ma[1,4,5,6]**

[1]*Department of Mathematics, Zhejiang Normal University, China*
[2]*Department of Mathematics, Faculty of Science, Taibah University, Al-Madinah Al-Munawarah, Saudi Arabia*
[3]*Mathematics Department, Faculty of Science, Beni-Suef University, Egypt*
[4]*Department of Mathematics, King Abdulaziz University, Saudi Arabia*
[5]*Department of Mathematics and Statistics, University of South Florida, USA*
[6]*International Institute for Symmetry Analysis and Mathematical Modelling, Department of Mathematical Sciences, North-West University, South Africa*

In this article we studied analytically complex nonlinear schro¨dinger equation with kerr law nonlinearity using auxiliary equation mapping method, as a result, we found a series of more general and new families of exact solutions, which are more powerful in the development of soliton dynamics, quantum plasma, adiabatic parameter dynamics, biomedical problems, fluid dynamics, industrial studies, nonlinear optics and many other fields. The calculation- s demonstrates that this method is more reliable, straight forward, and effective to study analytically other nonlinear complicated physical problems modeled by complex nonlinear partial differential equations arising in mathematical physics, hydrodynamics, fluid mechan- ics, mathematical biology, plasma physics, engineering disciplines, chemistry and many other natural sciences. We also have expressed our solutions graphically with the help of Mathe- matica 10.4 to understand physically the behavior of different shapes of solutions including kink-type, anti kink type, half bright and dark soliton.

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An introduction to general high-pressure closed acidic decomposition method of rock samples for trace element analysis by ICP-MS

Xijuan Tan

College of Earth Sciences and Land Resources, Chang'an University, China

Objective: Trace elements in geological samples provide important information on understanding the rock formation, the mantle and crustal evolution and the magmatism of planetary bodies. Undoubtedly, the quality of analytical data is an essential index in geochemical process quantification. To accurately determine trace elements in geological samples, complete sample decomposition is critical and fundamental. This work aimed to propose a general digestion approach for rock samples by ICP-MS.

Method: Considering the complex property of geological samples and drawbacks of the reported digestion methods (alkali fusion, open vessel acid digestion, and microwave dissolution), a high-pressure closed acidic method was thus studied for the decomposition of rock samples ranging from basic to acidic materials. Here, by using the HNO3-HF mixed system, different geological reference materials (including W-2a, BCR-2, GSP-2, AGV-2, and GSR-1) were investigated for trace element determination by ICP-MS, with acid ratio, decomposition time, digestion temperature,

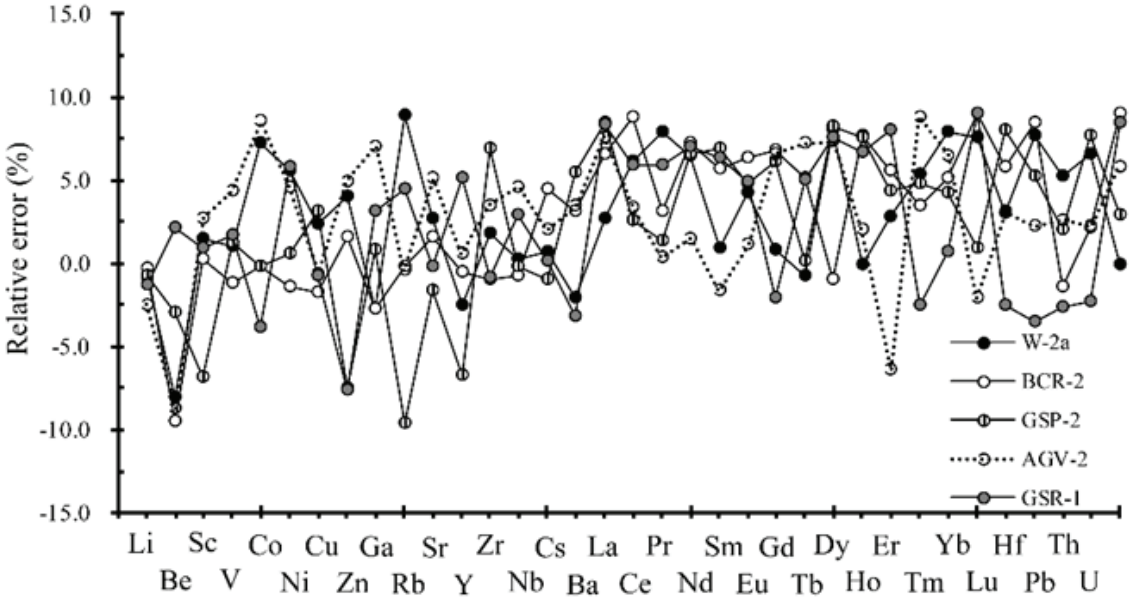

Figure 1 REs for trace element analysis for Geological Standard Materials by ICP-MS

sample mass and reagent amount assessed in detail. In brief, 2.0 mL of HNO3-HF with a ratio of 1:1, and a digestion time of 12 hr at 185 °C in high-pressure sealed bomb were optimal for 50 mg rock sample decomposition.

Results: The determined trace elements of the studied standard materials agreed well with certified values showing relative errors (REs) less than 10% (see Figure 1), which confirmed the robustness and reliability of this proposed high-pressure closed acidic digestion method of rock samples for trace element analysis.

Conclusion: This proposed high-pressure sealed digestion method was characterized with less acid consummation, complete digestion and less damage for digestion process, well meeting the requirements for large sample throughput in geological laboratory.

Biography

Dr. Xijuan Tan is a lecturer in Chang'an University, China since April 2014. Dr. Tan did her Ph. D in Chemibiology on protein-small molecule interaction characterization at College of Chemistry & Materials Science, Northwest University, China. In September 2018, she joined the group of Prof. Dr. Detlef Günther at ETH Zurich and started her one-year post-doc on element composition and lithium isotope study of spodumene by LA-(MC)-ICP-MS. Her research interests are trace element characterizations of different samples from geological science (rocks, sediments, minerals, clays, etc.) to biological materials (human hair, garlic bulbs, etc.) by ICP-MS and LA-ICP-MS. She is also interested in figuring out the potential factors (such as signal beat) affecting quantification accuracy of LA-ICP-MS analysis.

The effect of Gamma Irradiation on nucleolar activity, the presence of chromosomal abnormalities and the efficiency of energy conversion as indicators for mutation breeding in *Triticum turgidum*

E. Von Well[1], A. Fossey[2] and **M. Booyse[3]**

[1]*Agricultural Research Council – Small Grain, South Africa*

[2]*Retired Professor, South Africa*

[3]*ARC – Biometry, South Africa*

Introduction: The effect of gamma irradiation of kernels on nucleolar activity, mitotic index, as well as the number of bridges, ring chromosomes, micronuclei and incomplete mitosis as indicators of metabolic activity and growth retardation, was investigated in root tip cells of tetraploid wheat T. turgidum. The efficiency of energy conversion into growth was used as an indicator for the optimal dosage for mutation breeding.

Material and Methods: Seeds of Triticum turgidum ssp. durum L. cv. Orania (AABB) were given gamma irradiation dosages of 50, 150, 250 and 350 Gy. Root tips were fixated in La Cour's 2BD from 17.5 to 47.5 h after the onset of imbibition to study the first mitotic division and its consequences on the cells that were in G2 and G1 phases at the time of gamma irradiation.

Results: Untreated material produced a maximum of four nucleoli formed by the nucleolar organizing regions (NORs) on chromosomes 1B and 6B. In irradiated material additional nucleoli were noted in the nuclei and nucleoli were also noted in the micronuclei. Highly significant increases in the number of bridges, micronuclei, ring chromosomes and interphase cells with incomplete mitosis occurred at different irradiation intervals. The efficiency of energy conversion into growth retarded accordingly with an increase in gamma irradiation dosages.

Discussion: The increase in number of nucleoli in the nucleus was due to incomplete mitosis and the overall increase in nucleoli in cells was due to activation of the NORs on chromosome 1A in micronuclei. The efficiency of energy conversion into growth decreased due to cell death and energy used for repairing of damaged cells. The efficiency of energy conversion into growth predicted a dosage that is in line with what is prescribed by the IAEA for the gamma irradiation of seeds of Triticum turgidum ssp. durum L.

Biography

I am presently working for the Agricultural Research Council – Small Grain as a wheat and mutation breeder as well as being the Curator of the Small Grain Germplasm Collection (for 15 years now). I also have experience in human cytogenetics karyotyping. As mutation breeder, I have been involved in two projects collaborating with the IAEA. I am investigating methods to determine the optimal dosage for mutation breeding in seed propagated plants. I am making use of Triticum as my model plants, because of the fact that it is a polyploid complex. The efficiency of energy conversion into growth is promising as an indicator for the prediction of the optimal dosage for mutation breeding. The efficiency of energy conversion into growth is therefore compared with nucleolar activity, appearance of chromosomal abnormalities, mitotic index, fertility, appearance of branched ears and disease resistance mutations. I am also a reviewer for five journals.

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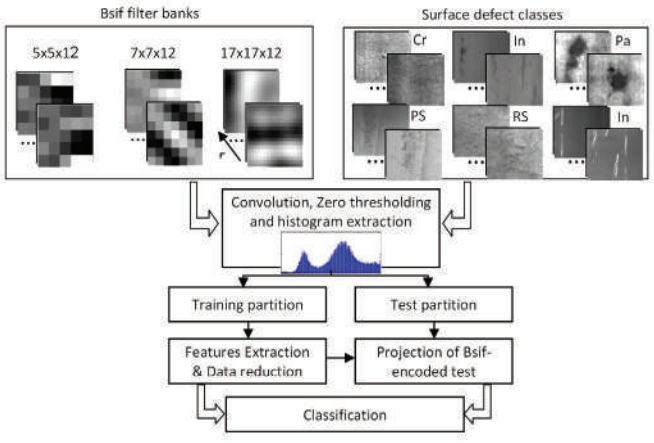
Strip surface defect identification using multiresolution binarized image features

Z. Mentouri[1,2], H. Doghmane[3], A. Moussaoui[4] and D. Boudjehem[2]

[1]*Research Centre in Industrial Technologies CRTI, Algeria*
[2]*Laboratory of Advanced Control-LABCAV, Université 8 Mai 1945, Algeria*
[3]*Laboratory of Electrical Engineering-LGEG, Université 8 Mai 1945, Algeria*
[4]*Laboratory of Inverse Problems-PI:MIS, Université 8 Mai 1945, Algeria*

In steel industry, the product surface control is essential for ensuring the required quality level, mostly, defined for an intended use of the product. Particularly in hot rolling process, the strip being shaped, may exhibit surface flaws, as scratches, crazing, holes and so on, of which the origin could be some internal discontinuities in the input product or the material transformation during the rolling process itself. Such defects are of a random occurrence and of different severity. Thus, the purpose of the product on-line quality control is the detection and identification of any surface defect that starts appearing, to allow a fast decision making. Such a product monitoring is assured by automatic systems meeting the requirements of speed, accuracy and robustness, and mainly based on a discriminant features extractor and on a reliable classifier.

Filtering operations are usually used for feature extraction. However, applying a filter to an image may result in some unintended effects. As using an increased size filter, to remove a noise, may result in more blurred edges. Whereas a small spatial support area of 3x3 pixels of size, for instance, enhances edges, but allows capturing the information of only small-scale structures.



General scheme of a multiresolution BSIF procedure

In this paper we explore pre-learnt image filters and work on a procedure, depicted in the figure above, to achieve an improved flaw recognition rate, and to realize the best trade-off between this recognition level and the computing time.

The proposed method is a multiresolution approach, based on Binarized Statistical Image Features. The applied filters stand as new revelators of the metallic surface structure of the two experimented dataset and provide a quite discriminant image description. This allows an efficient classification of the defective hot rolled products, compared to some previous works, as shown in the table below.

Method Num.	F. Descriptor	Parameters	Classifier	Labelled samples (/900)	Results (%)
01	Gabor_LDA$_{PCA}$	O=4, S=2	KNN	667	74.16±1.26
			SVM	674	74.90±1.28
		O=8, S=5	KNN	800	88.86±0.95
			SVM	791	87.89±0.99
02	LPQ_LDA$_{PCA}$	W.S=9x9	KNN	866	96.18±0.57
			SVM	861	95.71±053
03	Gabor_LPQ_LDA$_{PCA}$	D=4, S=2, W.S=9x9	KNN	892	99.12±0.29
			SVM	888	98.67±0.32
		D=8, S=5, W.S=9x9	KNN	891	98.98±0.25
			SVM	886	98.44±0.86
04	Gabor_LPQ_PCA	D=4, S=2, W.S=9x9	KNN	829	92.16±0.84
		D=8, S=5, W.S=9x9	KNN	829	92.15±0.94
05	BSIF_LDA$_{PCA}$	S7B12	KNN	893	99.18±0.30
			SVM	761	84.50±1.07
06	MRBSIF_LDA$_{PCA}$	S3,5B8+S13B11+S9,15B12	KNN	896	**99.60±0.20**
			SVM	893	99.03±0.41
07	MRBSIF_PCA		KNN	855	95.62±0.61

Table: Recognition rates of strip surface defects of the Northeastern University (NEU) Database

Biography

Z. Mentouri obtained his PhD in 2018 and his academic accreditation in 2020 from the University of May 8th, 1945, Guelma, Algeria. He started working as an engineer at the Applied Research Department of the National steel company in Algeria. He joined the Research Center in Industrial Technologies in 2005, where he worked as a research engineer and then as a senior researcher. His fields of interest are computer vision, image processing and artificial intelligence in industrial applications for the measurement and control of products. Another area of interest is the implementation of supervisory systems for measurement and accuracy of laboratory testing, with respect of international standards.

Selective oxidation of styrene to benzaldehyde over niobium modified phosphomolybdic acid catalyst

B. Viswanadham[1] and **Komandur V R Chary**[2]

[1]*GMR Institute of Technology, India*

[2]*Catalysis Division, Indian Institute of Chemical Technology, India*

Niobium substituted phosphomolybdic acid with various Nb/P mole ratio of catalysts were successfully synthesized by hydrothermal method. These materials were characterized by X-ray diffraction, FT-IR spectroscopy, Raman spectroscopy, temperature programmed desorption of ammonia and BET surface area measurements to be investigate the structural and acidity properties of catalyst. The activities of the materials were evaluated for the solvent free oxidation of styrene to benzaldehyde and the best catalytic activity was achieved for the catalyst with Nb/P mole ratio is 2.0. This catalytic system provides one of the most straight forward syntheses of carbonyl compound from styrene. The synthesized material can be recovered and reused for same reaction.

Biography

Dr Balaga Viswanadham (1985), working as Associate Professor at GMR Institute of Technology-Rajam Affiliated to JNTU-Kakinada, Andhra Pradesh, India. He also worked as Assistant Professor in Rajiv Gandhi University of Knowledge Technologies, Andhra Pradesh, India. He has completed his MSc from Andhra University, Vishakhapatnam, India. He has completed his PhD degree in Chemistry from CSIR-Indian Institute of Chemical Technology (JNTU), Hyderabad, India in 2015 under the guidance of Prof. Komandur V. R. Chary. He completed his Post-Doctoral study from University of KwaZulu-Natal, Durban, South Africa under the supervision of Prof. Holger B. Friedrich and Prof. Sooboo Singh for 3 years. His research mainly focuses on developing novel heterogeneous solid acid catalysts for biomass conversion and sustainable organic transformations, and also CO2 utilization study. He authored about 16 peer-reviewed journal articles with an h-index of 11 and more than 238 citations. He has been received several national and international awards/fellowships/Editorial Board Member, such as AES Post-Doctoral Fellowship-2015 (UKZN, Durban), CSIR-Junior Research Fellowship -2008 (CSIR-India), GATE -2008 (All India Rank-150 in Chemical Science conducted by IISC, Bangalore, India), APSET-2012 (Andhra Pradesh, India) and acting as Editorial Board Member and Reviewer in several professional societies. He also worked as Research Scientist at Jubilant Life Sciences Ltd, India.

Biodiversity and agricultural heritage: A path to sustainability

Liane Portuondo Farías[1] and **Dariellys Martínez Balmori**[2]

[1]*Institute of Technologies and Applied Sciences (InSTEC), Cuba*

[2]*University of Havana, Cuba*

Tobacco cultivation in the Viñales Valley is carried out most authentically and traditionally following an ancestral culture. The use of organic matter and crop residues by the peasants adds nutrients to the soil thus increasing biogeochemical cycles and soil conservation. To preserve this heritage, the country is enacting regulations for the appropriate use of the land to ensure the preservation of tobacco cultivation and biodiversity conservation, including the provision of food products with strict environmental protections. This makes it possible to guarantee the care and development of natural resources for future generations. The application of humic acids from the decomposition of soil organic matter applied in the leaves to different crops in the area showed that parameters such as leaf mass and specific root mass, the content of photosynthetic pigments and enzymatic systems were modified. The experimental evidence obtained confirms a specificity in the tolerance level of crops to different types of stress, and an attenuation of the anatomical-morphological and biochemical-physiological effects that come through agro-ecological practices. In this context, Viñales was declared a Cultural Landscape registered on the UNESCO World Heritage List, and the local and state governments linked to the Ministry of Agriculture are working jointly to eventually attain the status of Globally Important Agricultural Heritage System. The most relevant characteristic of Viñales is its high degree of endemism, which places the Cuban island as the main center of evolution and speciation in the Antilles. That is why the research aims to discuss the role of rural ecological knowledge and socio-political factors in the implementation of agro-policies in the Viñales Valley.

Biography

Graduated as Agricultural Engineer with a Masters in Agricultural Chemistry (Agrarian University of Havana), Agricultural Heritage (University of Firenze), and Protection against CBRNe events (advanced course at the University of Rome Tor Vergata). Doctoral studies completed in the area of Biological Sciences - Biophysics at the Federal University of Rio de Janeiro, Brazil. Currently working as a Full Professor in the Environmental Department at the Institute of Technologies and Applied Sciences (InSTEC), Cuba. Professional experience in the areas of Environmental Pollution, Phytoremediation, Oxidative Stress, and Agroecology.

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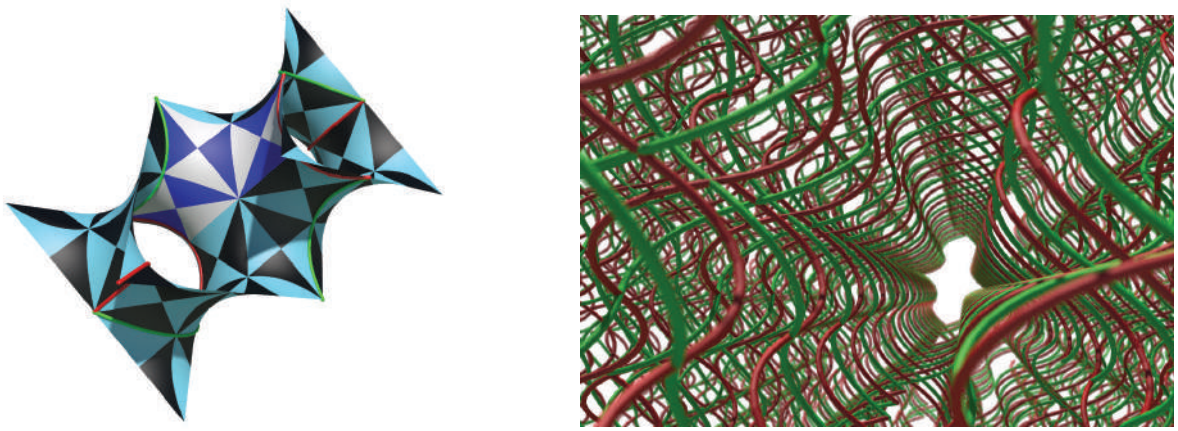
Hyperbolic tilings and crystallographic structures

Benedikt Kolbe[1] and **Myfanwy Evans**[2]

[1]*Hausdorff Center for Mathematics, Germany*

[2]*University of Potsdam, Germany*

Triply-periodic nets are one of the most important classes of structures in chemistry and materials science. Many triply periodic structures can be modeled as graphs embedded on prominent triply-periodic minimal surfaces, including the gyroid and diamond surface. We discuss some recent breakthroughs concerning an inherently interdisciplinary project between mathematicians, chemists, and computer scientists that attempts to produce different structures in three-dimensional Euclidean space from graph embeddings on triply-periodic minimal surfaces. The mapping class group of a surface is the group of homeomorphisms of the surface modulo isotopies of the surface. It has a long history in topology and represents an active area of research. We present in this talk a recent new application of MCGs relevant for crystallography, materials science, structure formation, and knot theory. We first explain the necessary set-up for the construction of candidates for new crystalline structures from graph embeddings on surfaces, where intrinsically hyperbolic triply-periodic minimal surfaces in three-dimensional Euclidean space are used as a scaffold for promising three-periodic structures. We then give an overview of new results on MCGs that facilitates an enumeration of isotopy classes of graph embeddings with a given group of symmetries. Lastly, we present a catalogue of three-dimensional structures that have resulted from this project and explain some of the difficulties involved as well as future directions.



A crystallopgraphic net shown on a part of the diamond triply-periodic minimal surface and in R3

Biography

Benedikt Kolbe completed his PhD in mathematics at the Technical University of Berlin under the supervision of John Sullivan and Myfanwy Evans in 2019. Before taking up his current position in Bonn, Germany, at the Hausdorff center for mathematics, he held a post at Inria in Nancy, France. The focus of his research has always been interdisciplinary, at the boundary between mathematics, computer science, and chemistry. His main interests lie in computational geometry, hyperbolic geometry, and the interplay of structure and function in chemical structures.

Biochemical reaction networks used in population dynamics and epidemiological modeling

S. Markov and **M. Borisov**

Institute of Mathematics and Informatics, Bulgarian Academy of Sciences, Bulgaria

The Susceptible-Exposed-Infectious (SEI) epidemiological model can be considered in the context of the Chemical Reaction Network Theory as a two-step exponential (radioactive) decay reaction chain (Bateman chain), such that the initial (first) reaction step: S is transformed into E, is catalyzed by species I. The reaction network thus defined is a generalization of the familiar logistic reaction network, wherein the first reaction step is self-catalyzed by I, leading thus to the logistic-type SI epidemiological model. More specifically, the logistic SI model is a special (limit) case of the SEI model, obtained when the rate of the first reaction step tends to infinity while the rate of the second reaction step is kept fixed. So, in the limit, the E-species disappears (meaning that there is no latent period), and the SEI model turns into the logistic SI model. Thus, we can speculate that in the biological life evolution, the SEI reaction network mechanism chronologically precedes the more involved biochemically self-catalytic logistic SI-type mechanism. This circumstance allows us to look at the SEI-mechanism as related to the logistic one and to denote the resulting growth function as ''pre-logistic'' function.

We study the time evolution of the masses/concentrations of the species involved assuming mass action kinetics, focusing on the growing pre-logistic function. We investigate the situation when one of the chain-links is much faster relative to the other one. We demonstrate that a pre-logistic reaction network can be ''approximated'' by a single-step reaction, which is either of logistic-type or of a first-order-type. We thus show that the time evolution graph of the growing species changes its shape between a sigmoidal logistic-type and a concave first-order-type, depending on the ratio of the two rate parameters. This fact motivates us to propose some instructions that may be useful for deciding on the choice of an appropriate class of growth functions when simulating a given measurement set resulting from biological (experimental) process.

Biography

Svetoslav Marinov Markov, DSci, PhD, Assoc. Member in dept. "Math Modelling and Numerical Analysis", Institute of Mathematics and Informatics, Bulgarian Academy of Sciences.

Academic qualifications:

- MS in Computational Mathematics, Sofia University, 1966;
- MA, Wolfson Colledge, University of Cambridge, UK, 1971;
- Ph. D. (mathematics), Sofia University, 1979;
- Professor, Center for Biology, Bulgarian Academy of Sciences (BAS), 1984;
- DSc. (math), Institute for Mathematics and Informatics, BAS, 2004.

Fields of interest:

Biomathematics, Mathematical Modeling in Biology, Reaction networks, Metabolic Processes, Enzyme Kinetics, Dynamical Models of Biological Processes, Validated Numerical Analysis, Convex and Interval Analysis, Error analysis, Interval and Computer Arithmetic, Interval algebra, Linear Algebra, Hausdorff Approximations.

Employment record:

- Faculty of Mathematics at Sofia University, Assistant professor, 1966-1974;
- Mathematical Institute of BAS, Researcher, 1974-1984;
- Research Group for Mathematical Modeling in Biology, Center for Biology, BAS, Professor and Head of the Research Group, 1984-1989;
- Professor, Head of Department "Mathematical Modeling in Biology'', Institute of Biophysics 1989-1995;
- Professor, Head of Department "Biomathematics", Institute for Mathematics and Informatics (IMI), BAS 1996-2010;
- Professor, Dept "Mathematical Modelling and Numerical Analysis (MMNA)", IMI- BAS, 2011;
- Assoc. Professor, Dept. "MMNA", Institute for IMI- BAS, 2011-present.

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N, S donor acetamide ligand: Silver (I) binding and test silver (I) extraction studies

A. Aderibigbe[1,2] and **A. Clark[2]**

[1]*School of Nursing, University of Connecticut, USA*

[2]*Department of Chemistry, University of Warwick, United Kingdom*

Ligands bearing soft donors including N- and S- have found applications in selective metal recovery due to the ability to preferentially bind soft acceptors like Ag+. Herein, N-(2-((4-vinylbenzyl)thio)ethyl)acetamide (L) bearing potential Ag+-selective N- and S-donors was prepared in a 76% yield under mild conditions. Reaction of L with silver perchlorate and silver nitrate gave complexes 1 and 2, as pastes, in yields of 98 and 77%, respectively. Physico-chemical and spectroscopic characterizations confirmed the chemical compositions of L, 1 and 2. ESI–MS data indicated that 1 and 2 each contain both the [AgL]+ and [AgL2]+ types complexes. Binding studies carried out by Job plot and 1H NMR titration using silver perchlorate indicated that L interacts with Ag+ to form the [AgL]+ type complex and that the N- and S-donors may be responsible for binding Ag+. Finally, L was observed to demonstrate excellent selectivity and moderate efficiency (36%) for Ag+ extraction from an aqueous solution also containing Cu2+ and Pb2+.

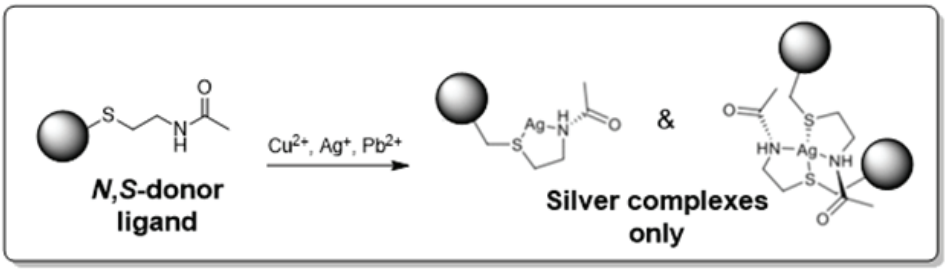

Figure 1. Acetamide ligand selectively binds to silver (I) to give both 1:1 and 1:2 complexes in solution

Biography

Dr. Abiodun Aderibigbe obtained his bachelor's in Industrial Chemistry from the Federal University of Technology Akure, Nigeria in 2011, his masters in Waste & Clean Technologies from the University of the West of Scotland, United Kingdom in 2014 and his PhD in Chemistry (supervised by Profs. Andrew Clark & Stefan Bon) from the University of Warwick, United Kingdom in 2020. As part of his PhD work investigating novel small molecules and materials for sustainable, selective, and efficient silver recovery from waste materials, and amongst other outstanding pioneering work, he designed, prepared, and tested an acetamide ligand which was observed to demonstrate excellent selectivity for silver binding from matrices also containing copper and lead. Currently he is a postdoctoral research associate at the University of Connecticut, USA. He lives in Willimantic, Connecticut with his wife and he enjoys watching football matches and football analyses.

Progressive Sperm Sorting Method using High-throughput Rheotaxis-based device

A. Ataei[1] and **W. Asghar**[2]

[1]*Department of Physics, Florida Atlantic University, USA*

[2]*Department of Computer and Electrical Engineering and Computer Science, USA*

Assisted reproductive technologies (ARTs) use different sperm sorting methods to select viable sperm from any given semen sample. The more commonly known ART techniques use centrifugation-based methods which damages the sperm morphology, induces DNA fragmentation and is time consuming. Microfluidic devices have been a novel substitute to conventional method to sort motile and morphological normal sperm for ARTs. However, they require more investigation in terms of DNA fragmentation, and effect of flow on the quality of sorted sperm. Rheotaxis, the ability of the sperm to reorient and align itself against the flow direction and swim upstream, has been suggested as a key long-range guidance mechanism. We have developed a microfluidic device inspired by the natural sperm selection that exploits the ability of sperm cells to swim against the flow (rheotaxis). We carried out an experiment for various flow rates to investigate the effect of rheotaxis on human sperm guidance and selection. The quality of the isolated cells was quantified by sperm motility, velocity parameters, morphology, and DNA integrity. Sperm selected with this microfluidic device have a higher motility (~100%) and normal morphology with lesser DNA fragmentation compared to commonly used centrifugation-based methods. Moreover, we have shown that the device is capable of washing out an infected semen sample by removing infected cells, but not cell-free viruses. Taken together, the constructed device responds to a request of selection of healthy sperm for ART procedures while suggesting the optimal flow rate for selection process that decreases the damage to the cells during sorting.

Biography

This is Afrouz Ataei PhD student in Physics in Florida Atlantic University. My current research centers on designing microfluidic devices to sort human sperm for assisted reproductive technology while studying the behavior of human sperm in a microfluidic channel. My interdisciplinary research project has been done under the supervision of my advisors from Physics and Engineering department. In addition to my PhD research project, I earned my degree in Professional Science master's in medical physics (PSMMP) along my PhD. I defended successfully in spring 2021. My research work addressed one of the greatest challenges facing modern medicine. I used my computational physics knowledge to design a novel algorithm that predict liver cancer risk from large database.

Combining machine learning and molecular modeling — CASTELO, a 4D submolecular motif identification method for drug discovery

Leili Zhang

IBM Thomas J. Watson Research Center, USA

Drug discovery is a multi-stage process that comprises two costly major steps: pre-clinical research and clinical trials. Among its stages, lead optimization easily consumes more than half of the pre-clinical budget. We propose a combined machine learning and molecular modeling approach that partially automates lead optimization workflow in silico, providing suggestions for modification hot spots. The initial data collection is achieved with physics-based molecular dynamics simulation. Contact matrices are calculated as the preliminary features extracted from the simulations. To take advantage of the temporal information from the simulations, we enhanced contact matrices data with temporal dynamism representation, which are then modeled with unsupervised convolutional variational autoencoder (CVAE). Finally, conventional and CVAE-based clustering methods are compared with metrics to rank the submolecular structures and propose potential candidates for lead optimization. With no need for extensive structure-activity data, our method provides new hints for drug modification hotspots which can be used to improve drug potency and reduce the lead optimization time. In addition to the small molecule hotspot identifications, we show that CASTELO can also be used for protein-protein interaction structures, such as antigen-MHC binding. In this use case, CASTELO predictions agree well with experimental binding results and free energy perturbation-predicted binding affinities. Our work supports the usage of structure-based deep learning techniques in antigen specific immunotherapy design.

Biography

Dr. Leili Zhang is a research staff member at IBM Thomas J. Watson Research Center. His research interests include incorporating molecular modeling and machine learning to assist drug discovery, molecular modeling algorithm development, molecular structure analysis algorithm development and disease mechanisms. Recent highlights of his work include the development of CASTELO, a combined molecular dynamics and machine learning method that identifies weak spots in small-molecule drugs and biologic drugs for lead optimization; disease mechanism modeling of Huntington's disease; and drug mechanism modeling of small molecules and antibodies on SARS-CoV-2. He received his PhD from University of Wisconsin-Madison as a Hirschfelder fellowship recipient. He is a three-times A-level accomplishment award winner and two-times Outstanding Technical Achievement Award winner at IBM.

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Production water analysis by combining Electro Spray on Paper (EPS) and Laser-Induced Breakdown Spectroscopy (LIBS) techniques

C. Carreño, R. Cabanzo and **E. Mejia-Ospino**

Universidad Industrial de Santander, Colombia

Produced water in oil crude extraction contain high concentrations of salts and other compounds, so it is important to have a technique capable of analyzing liquid samples at high concentrations without any or minimal sample preparation. The electrostatic atomization on paper known as Electro Spray on paper (EPS) of brines and its application in the production of microdroplets and that are excited through the coupling of EPS with the technique Laser-Induced Plasma Spectroscopy (LIBS) and thus obtain the quantitative analysis of these solutions. The technique (EPS) allows to eliminate the difficulties associated with the interaction of the laser pulse with the liquid sample [1] and the LIBS technique provides unique advantages such as the ability to make quick measurements, in situ, to make a quantitative analysis of production waters at different concentrations [2]. By coupling these two techniques, LIBS- EPS, the quantitative analysis of production waters was carried out for the elements: Na, K, Mg and Ca. Quantitative analysis was performed by constructing calibration curves of solutions prepared from different salts.

Sample	*Theoretical Concentration (ppm)*	*Experimental Concentration (ppm)*	*%Error*
Production water	*6377*	*6408,05*	*0,49*
24-hour urine	*920-5060*	*4024,19*	-------
Blood serum	*3229,2*	*3158,45*	*2,19*
Solution prepared in the laboratory	*27480*	*28102,23*	*2,26*

Table 1. Determination of Na concentration of different samples

Unknown metabolites identification with high resolution GC-MS and IROA technology

Yunping Qiu and **Irwin Kurland**

Stable Isotope and Metabolomics Core Facility, Diabetes Center, Department of Medicine, Albert Einstein College of Medicine, USA

Determination and identification of real unknown metabolites is one of the major challenges for the metabolomics field. A typical untargeted GC-MS metabolomics run will generate thousands of mass features, only around 200 metabolites will be annotated. Here, we used a stable isotope-based technique to generate a recognizable mass pattern to discriminate real metabolites from background and artificial peaks and facilitate unknow metabolite identification (termed as Isotopic Ratio Outlier Analysis (IROA)), coupled with high-resolution GC-MS analysis.

With randomized 5% 13C and 95% 13C enriched substance as carbon sources, all metabolites generated from the cultured organism will produce mirror image isotopologue pairs in mass spectrometry based on the binominal distribution of 13C carbon. Each of the mirror pattern will represent one real metabolite, which can be easily differentiate biological signals from artifacts. The distance between Mn and M0 will be total carbon number of the metabolite, which largely reduce the metabolite candidates for the same molecular weight.

We applied this technique for the yeast metabolomics study. We used soft chemical ionization in the GC/MS analysis to produce molecular ions, which could be used for chemical formular generation (CFG) based on the accurate mass and the recognized carbon number. Fragmentations generated from electron impact (EI) reveals the carbon number for fragments of biological originated metabolites, easily discriminating against artifacts, and silylation adducts. The IROA EI spectra could be used to match fragmentations obtained from in silico fragmentation software such as Competitive Fragmentation Modeling for metabolites Identification (CFM-ID).

In summary, we developed a high-resolution GC-MS and IROA technology-based metabolites discrimination and identification workflow, which is of great potential in identifying novel metabolites of biological origin.

Biography

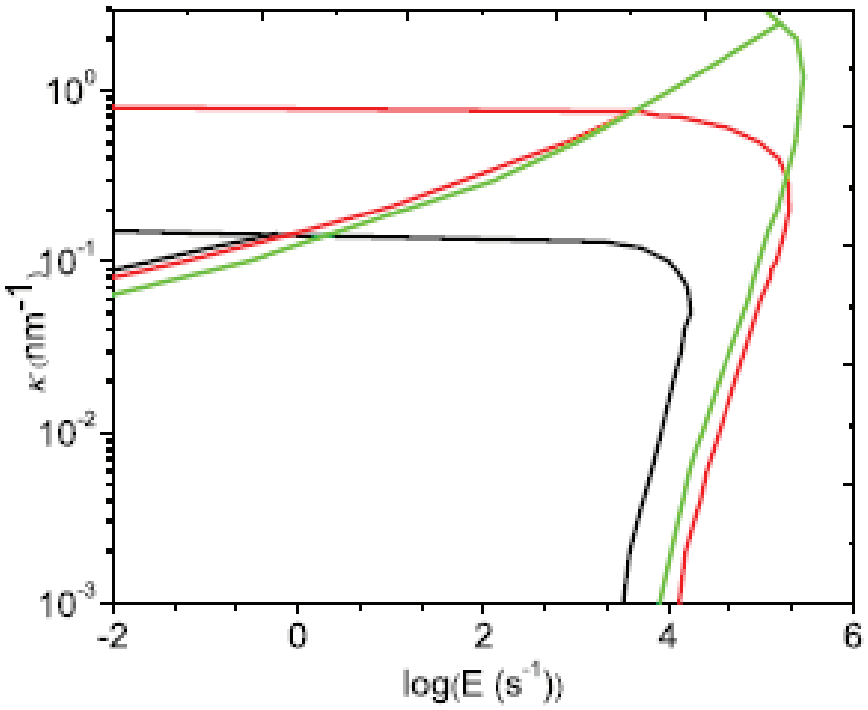
Dr. Qiu is a Research Associate Professor at Albert Einstein College of Medicine. He also serves as the operations manager for the stable isotope & metabolomics core of diabetes research center. He got his Ph.D. degree in Shanghai Jiaotong University, China, in 2008. He moved to the university of North Carolina at Greensboro in the year of 2009 and worked there for 5 years. He joined Albert Einstein College of medicine in 2014. His research focus is to use stable isotope labeling techniques to improve metabolomics research.

Stability characteristics of nanoparticles in a laminar linear shear flow in presence of DLVO- and non-DLVO forces

Vivekananda Bal

Massachusetts Institute of Technology, USA

Stability or coagulation of colloids is extremely important in the areas of milk processing, paint industry, food processing, protein stability, microemulsion etc. Previous works in the area of colloidal stability analysis are mostly based on experimental investigation. Fogler and Melik (J. Colloid Interface Sci. 1984, 101, 84-97), and Zeichner and Schowalter (AIChE J., 1977, 23, 243-254) are the only two theoretical analysis available in this area, and are applicable to only non-Brownian particles in rapidly flocculating system. With the emergence of the field of nanomaterials, analysis of the state of colloids is becoming increasingly relevant. We present a stability analysis of Brownian particles in a laminar linear shear flow. To achieve this, we developed a mathematical model based on Fokker-Plank equation including the effect of (i) Brownian motion, (ii) fluid convection, (iii) van der Waals force, and (iv) double-layer repulsion. Furthermore, this work, for the first time, studies the effects of solvation and steric repulsion on colloid's stability.



This work interestingly finds that stability of colloids initially increases with an increase in particle size followed by a decrease. In contrast to that, stability is observed to increase in an accelerating manner with an increase in surface potential. Similarly, it is found that stability shows a relatively stronger dependence on the solvation potential pre-exponential coefficient as compared to that found with the solvation potential decay length or surface potential. In the case of the coating thickness, though stability shows increasing behavior, the rate of increase is decelerating. The coating density is found to be the single most important parameter in controlling stability as observed by even higher self-accelerating rate of increase of stability as compared to that observed with particle size or the surface or solvation potential. Importantly, analysis reveals that stability to secondary minimum coagulation is not affected by either solvation or steric potential.

Biography

Vivekananda Bal received his B.Sc. in chemistry (honours) from the University of Calcutta in 2003 followed by B.Tech. in chemical engineering from the same university in 2006. He received his M.Tech. in chemical engineering from Indian Institute of Technology Kanpur. Then he moved to Indian Institute of Technology Bombay for pursuing PhD with prof. Rajdip Bandyopadhyaya. Thereafter, he went to the University of Illinois at Urbana-Champaign for postdoctoral research with Prof. Baron Peters. Presently, he is pursuing his second postdoctorate at Massachusetts Institute of Technology with prof. Richard Braatz. His research interests lie in the area of crystallization, colloids, coagulation, computational fluid dynamics, population balance modeling, data analytics and machine learning, and mathematical and statistical modeling. He is the author and co-author of 9 papers in international referred journals. He is also an active reviewer of peer-reviewed international journals.

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Validation of analytical model and identification of salt effect on wellbore temperature in underbalanced drilling

Olatunji Olayiwola[1], Vu Nguyen[1], Opeyemi Bello[2], Ebuka Osunwoke[1], Boyun Guo[1] and Catalin Teodoriu[2]

[1]University of Louisiana at Lafayette, USA

[2]Mewbourne School of Petroleum and Geological Engineering, University of Oklahoma, USA

Understanding the behavior of the borehole temperature recovery process, which has an impact on drilling operations, necessitates accurate fluid temperature estimation. The presence of salt in a saline formation alters the annular fluid's composition and has a substantial impact on fluid temperature distribution during drilling operations. As a result, it is critical to investigate the important parameter that provides an accurate estimation of fluid temperature while drilling a saline formation. This work presents a simplified user-friendly computational system that evaluates the drilling fluid systems performance evaluation and selection optimization using Python software and statistical quantitative approaches.

The fluid temperature distribution of China's X Field was investigated using the Shan mathematical model as a starting point. The model predicted the temperature distribution of the field with less than 10% error when compared to MWD data from the field. To account for changes in annular fluid composition while drilling a saline formation, an adjustment factor was added to the base model. Salt concentration has an effect on fluid temperature distribution during drilling, according to the data. With both high and low adjustment factors, the fluid temperature at the wellbore condition changes by at least 7%. The rheology of the fluid combination varies as the salt in the formation input dissolves in the drilling fluid towards the annulus.

Biography

Olayiwola Olatunji is a PhD candidate at the University of Louisiana Lafayette. He earned his bachelor's and master's degrees in petroleum engineering from THE University of Ibadan in Nigeria and the Technical University of Clausthal in Germany, respectively. He has several years of experience working as a Production and Process engineer in Oil and Gas service firms. His present study is centered on enhancing the utilization of Nano-silica gel for sealing micro-annuli and well cement fracture Sheath. He has published multiple journal publications and is an active member of the Society of Petroleum Engineers (SPE).

ACCEPTED ABSTRACTS

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March 21-22, 2022

ADV. CHEMISTRY 2022

Hollow–Shell–structured mesoporous silica-supported palladium catalyst for an efficient suzuki–miyaura cross-coupling reaction

F. Abdulelah Taher Ali Mohammed[1] and **S. Lijian Wang**[2]

[1]*Key Laboratory of Resource Chemistry of Ministry of Education, Shanghai Key Laboratory of Rare Earth Functional Materials, Shanghai Normal University, China*

[2]*Hadhramout University,Yemen*

The construction of high stability heterogeneous catalyst for privileged common catalysts is a benefit for the reuse and separation catalyst from reactants. Herein, a palladium diphenylphosphine-base Hollow-shell-structured mesoporous catalyst (HS@PdPPh2@MSN) is prepared by the immobilization of bis[(diphenylphosphino)ethyltriethoxysilane] palladium acetate onto the inner wall of mesoporous organicsilicane Hollow-shell whose surface be protected by -Si(Me)3 group. In detail Hollow-shell-structured (PPh2)2Pd(OAc)2-functionalized mesoporous silica nanoparticles, abbreviated as HS@PdPPh2@MSN , were synthesized through a simple post-grafting-complexation three-step procedure, as shown in Scheme 1. The first step was the co-condensation of tetraethoxysilane (TEOS) and 1,2-bis(triethoxysilyl)ethane, followed by the modification of hexamethyldisilazane (HMDS) leading to silylated core-shell-structured nanoparticles Me@SiO2@NPs. The second step was the post grafting of diphenyl(2-(triethoxysilyl)ethyl)phosphane within the inner surface of the silylated Me@HS@MSN (1), which was obtained by an etching process in toluene for 12 h under refluxing condition. The third step was the direct complexation of the immobilized diphenyl(2-(triethoxysilyl)ethyl)phosphane with Pd(OAc)2 in the cavity of the hollow-shell-structured mesoporous silica and producing of the coarse catalyst 3, which was subjected to a Soxhlet extraction to remove the unreactive materials providing its pure form as a gray powder. Structural analyses and characterizations of the heterogeneous catalyst reveal its well-defined single-site active species within its silicate network. Electron microscopies confirm its Hollow-shell-structured mesoporous material. As presented in this study, the newly constructed heterogeneous catalyst enables an efficient Suzuki-Miyaura cross-coupling reaction for a range of substrates with up to 95% yield in mild conditions. Meanwhile, the HS@PdPPh2@MSN possessed excellent stability and recyclability, which could be reused at least five times without significant loss of activity. Furthermore, the HS@PdPPh2@MSN is easily synthesized and cost-effective, which makes it a candidate for applications in fine chemical engineering.

Scheme 1. *Preparation of the heterogeneous catalysts 3*

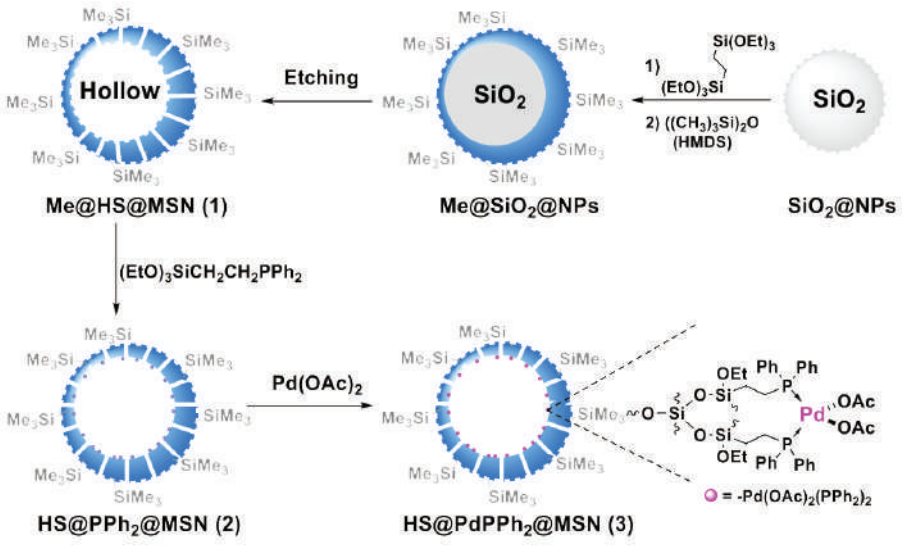
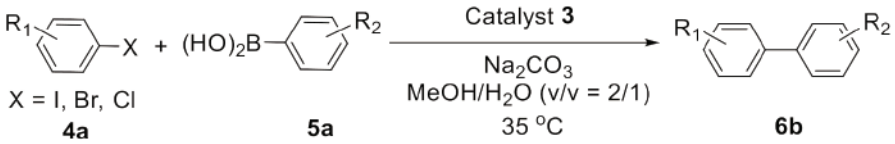


Table 1 . *The scope of the 3-catalyzed Suzuki–Miyaura cross-coupling reaction.a*



Entry	X	R_1	R_2	Time (h)	Yield (%)[b]
1	I	4-COMe	H	1	95
2	I	4-Cl	H	1	90
3	I	4-Me	H	1	90
4	Br	4-NO_2	H	1	85
5	Br	4-Cl	H	1	95
6	Br	4-OMe	H	1	90
7	Br	2-Me	H	1	90
8	Br	4-CN	H	1	92
9	Br	4-CH_3	H	1	92
10	Br	4-Cl	4-CF_3	1	95
11	Br	4-CN	4-CF_3	4	85
12	Br	4-Me	4-CF_3	1	93
13	Br	4-OMe	4-OMe	1.5	90
14	Br	4-CN	4-OMe	1	95
15	Br	4-Me	4-OMe	1.5	94
16	Br	4-Cl	4-OMe	1	92
17	Br	4-OH	H	1	95
18	Br	H	4-OMe	1	95
19	Br	H	4-CF_3	1	95
20	Br	COMe	H	1	95
21	Br	COMe	4-OMe	1	95

a Reaction conditions: *catalyst 3 (100.0 mg, 5.0 μmol of Pd based on the ICP analysis), aryl boronic acid (0.75 mmol), aryl halide (0.5 mmol), K_2CO_3 (1.0 mmol), in 3.0 mL of the co-solvent MeOH/H2O (v/v = 2/1), at 35°C, 1-3 h. b Isolated Yield*

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The effect of early application of a combined therapy of bone marrow mesenchymal stem cells and platelet-rich plasma on blood and bone parameters in ovariectomized rats

Arwa A. Hassan[1], Gehane M. Hamed[1], Noha A. Nassef[1], Rania S. A. E. Mansour[1], Mona K. E. Shawky[1] and **Asmaa A. Abo Zeid[2]**

[1]Department of Medical Physiology, Faculty of Medicine, Ain Shams University, Egypt

[2]Department of Histology and Cell Biology, Faculty of Medicine, Ain Shams University, Egypt

Background and Objectives: Osteoporosis is a common bone disorder with marked morbidity and mortality that occurs frequently in women after menopause. Inadequacy of current treatments and their side effects has driven the search for improved approaches. This study attempted to evaluate the early use of either bone marrow-derived mesenchymal stem cells (BM-MSCs), or platelet-rich plasma (PRP), or both combined to slow down bone loss, and improve bone formation in rats following ovariectomy.

Materials: In our study, female rats were divided into five groups: sham-operated (SHO) control, ovariectomized (OVX) untreated group, OVX-MSCs treated group, OVX-PRP treated group, and OVX-MSCs/PRP treated group. Body mass index (BMI) had been measured in all groups; furthermore, serum calcium (Ca^{2+}), phosphorus (P), alkaline phosphatase (ALP), collagen type 1 cross-linked C-telopeptide (CTx-1), malondialdehyde (MDA), and tumor necrosis factor alpha (TNF-α) were assessed. Additionally, specimens of tibia were analysed by light microscopy, morphometry and immunohistochemical staining for osteopontin (OPN).

Results: The results showed a significant increase of the final BMI in all groups. The OVX untreated group showed an insignificant change in the serum Ca^{2+} level, while the serum P level, together with ALP, CTX 1, MDA and TNF- α, showed a significant elevation. Administration of either BM-MSCs, or PRP, or their combination, significantly reduced serum levels of Ca^{2+}, ALP, CTX-1, MDA, and TNF-α, however, the combination therapy showed most significant results, including the final BMI. Histological examination also confirmed rapid bone formation in the combined therapy group with in vivo osteogenesis demonstrated via positive immunohistochemical staining of OPN.

Conclusion: The present study demonstrates that early administration of a combination therapy can have a therapeutic benefit over every monotherapy for the treatment of osteoporosis.

High-throughput 16S rRNA gene sequencing of the microbial community associated with palm oil mill effluents of two oil processing systems

Benedicte Ella Zranseu Aka and **Theodore N'dede Djeni**

Laboratoire de Biotechnologie et Microbiologie des Aliments, University Nangui Abrogoua, Cote d'Ivoire

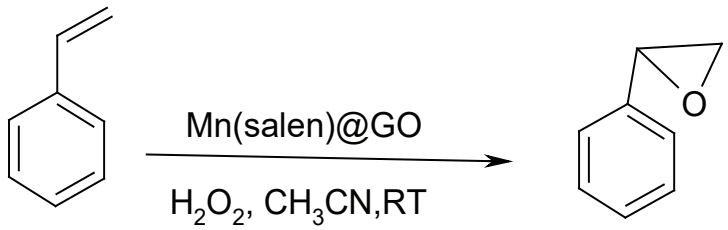
Palm Oil Mill Efuents (POME) are complex fermentative substrates which habour diverse native microbial contaminants. However, knowledge on the microbiota community shift caused by the anthropogenic efects of POME in the environment is up to date still to be extensively documented. In this study, the bacterial and archaeal communities of POME from two palm oil processing systems (artisanal and industrial) were investigated by Illumina MiSeq Platform. Despite the common characteristics of these wastewaters, we found that their microbial communities were signifcantly different with regard to their diversity and relative abundance of their different Amplicon Sequence Variants (ASV). Indeed, POME from industrial plants harboured as dominant phyla Firmicutes (46.24%), Bacteroidetes (34.19%), Proteobacteria (15.11%), with the particular presence of Spirochaetes, verrucomicrobia and Synergistetes, while those from artisanal production were colonized by Firmicutes (92.06%), Proteobacteria (4.21%) and Actinobacteria (2.09%). Furthermore, 43 ASVs of archaea were detected only in POME from industrial plants and assigned to Crenarchaeota, Diapherotrites, Euryarchaeota and Nanoarchaeaeota phyla, populated mainly by many methaneforming archaea. Defnitively, the microbial community composition of POME from both type of processing was markedly different, showing that the history of these ecosystems and various processing conditions have a great impact on each microbial community structure and diversity. By improving knowledge about this microbiome, the results also provide insight into the potential microbial contaminants of soils and rivers receiving these wastewaters.

Mn (salen) complexs on graphene n oxide as highly efficient catalyst for Epoxidation of Styrene

Ali Zarnegaryan

Department of Chemistry, Yasouj University, Iran

Graphene oxide and its derivative have attracted extensive interests in many fields, including catalytic chemistry, organic synthesis, and electrochemistry, recently. Transition metal complexes are one of the most useful and powerful catalysts for industrial processes. However, the practical applications of homogeneous metal complexes are hampered by their high costs with problems of separating from the reaction mixtures. Therefore, designing heterogenized metal complex catalysts is of great interest for economic and environmental reasons in recent years [1-5]. Catalytic epoxidation [6] of styrene is an important practical reaction for producing styrene oxide which is an important industrial organic intermediate and is used in the synthesis of fine chemicals and pharmaceuticals [7].A Mn (salen) complex has been homogeneously immobilized on a modified graphene oxide (GrO) support via covalent bonding. The loading of Mn (salen) complex on GrO nanosheets was monitored by FTIR, TG-DTA, and elemental analyses. The catalytic properties of Mn (salen) - Graphene oxide compound in the oxidation of styrene with H2O2 as oxidant were investigated and compared with the properties of their homogeneous analogues. It was found that both heterogeneous Mn (salen) catalysts were more active than their homogeneous analogues and that the product selectivity varied in cases of different oxidants. The supported Mn (salen) complex showed high yield of styrene oxide (86.0%) and good recoverability when using air as oxidant.



Scheme 1. *Epoxidation of Styrene*

Evaluation of different Sudan dyes in Egyptian food samples utilizing liquid chromatography/ tandem mass spectrometry

S. Mohamed[1,2], A. Salim[3], Y. Issa[1], M. Atwa[4] and **R. Nassar[4]**

[1]Chemistry Department, College of Science, Jouf University, Saudi Arabia

[2]Chemistry Department, Cairo University, Egypt

[3]Basic science Department, Faculty of engineering and applied science, Nile University, Egypt

[4]Regional Center for Food and Feed, Agriculture Research Center, Egypt

A sensitive and a precise method was developed for the quantification of different Sudan dyes in some Egyptian food samples. They were analyzed utilizing two fragment ion transition under multiple reactions monitoring (MRM) mode. Separation was carried out on Kinetex 2.6u C18 100 A (75 mm ×4.6 mm) phenomenex using isocratic elution with 10:90% water and acetonitrile containing 2.0 mmol/L ammonium formate and 0.2% formic acid. The validation parameters were obtained and verified. The linearity was 0.2-10.0 ng/mL with r2> 0.9975. LOD and LOQ were 0.06 and 0.19 ng/mL, respectively for Sudan (I, II) whereas they were 0.07 and 0.23 ng/mL, respectively for Sudan (III and IV), and Sudan Orange G. Recoveries are ranged from 78.79 to 110.49%. The method has been successfully applied for the quantification of these dyes in 60 food samples such as spices, chili powder, turmeric, paprika, and curry. The results show that about 55% of the randomly selected food samples were adulterated with the banned dyes.

Bio-based polymer membranes for a possible Recovery of bioactive material

S. Ananda Kumar and **P.Tamilazhagan**

Department of Chemistry, Anna University, India

Bio-based membranes are widely used in many separation processes such as Gas separation (GS), Nano-filtration (NF), Ultra-filtration (UF), etc. In this work, PLA and its blends has been used for a bio-based polymeric membranes synthesis that can be applied for fractionation of bioactive materials. PLA manufacturers around the world have been working seriously to develop solutions to some chronic limitations especially brittle behavior. The limitations also include their susceptibility to degradation and loss of inherent properties during processing and reprocessing. In addition, bio-based polymers and blends have less flexibility in polymer design as that of copolymers. In many applications, biopolymers require additives that do not inhibit their ability to compost. Very limited research had been cited on toughening properties of bio-based membranes suited for bioactive recovery. Hence, we attempted to formulate and synthesize PLA membrane with its appropriate blend to increase it toughness. From the study conducted, it was observed that the blend composition of PLA with PCL (Polycarprolactone), CNSL (Cashewnutshell liquid), PEG (Polyethyleneglycol) are the appropriate blends for toughness improvement and reproduceable hydrophilic nature.

Development of Ni+TiB_2 metal matrix composite coating on AA6061 aluminium alloy substrate by gas tungsten arc cladding process

Anil Kumar Das and **Omkar Verma**

Department of Mechanical Engineering, National Institute of Technology Patna, India

In the present research work Ni+TiB_2 metal matrix composite coating was deposited on AA6061 aluminium alloy substrate using nickel and titanium diboride as precursor by gas tungsten arc cladding process. The TIG torch was used as heat source to melt the preplaced powder mixture. The mixture of TiB_2 and Ni powders were taken as 10 wt. % and 90 wt. % respectively. The three level of currents were used as variable parameters to melt the pre-placed powder layer viz. 120Amp, 140Amp and 150Amp. The microstructure of coated layer was investigated by field emission scanning electron microscope (FESEM) and the chemical composition of the coated layer was detected by energy dispersive spectroscopy (EDS). From the microstructural study it was found that the coating exhibits good metallurgical bond between coated layer and substrate. For analyzing the micro-hardness of coated layer Vickers micro hardness testing was performed along the cross-section of the coated samples. The maximum microhardness value of coated layer was 1233 HV, for sample cladded at current of 150 Amp. It was observed that increase in micro hardness value of coated sample was about 11 times higher than that of the aluminium alloy substrate (110HV). It was found that with increase in applied current, amount of microhardness of coated sample increased.

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Synthesis and properties of R-phenoxy-substituted phthalocyanines with gadolinium and neodymium

A. N. Bychkova, T.V. Tikhomirova, A.A. Botnar, N. P. Domareva and **A.S. Vashurin**

Ivanovo State University of Chemistry and Technology, Russian Federation

Phthalocyanines (Pc), which contain peripheral and non-peripheral substituents and include rare-earth elements, are important objects of research and practical applications in various fields of science and technology. The most relevant are double-decker complexes of phthalocyanines with lanthanides, which suggest a variety of uses due to their distinctive optical and electrical properties. Sandwich-type complexes are used as organic semiconductors, catalysts, photodetectors and electrochemical sensors. The architectural flexibility of these compounds can be used to adjust molecular properties such as aggregation, solubility and optical absorption.

The aim of this study is to search for selective approaches to the synthesis of tetra- and octaphenoxy-substituted metal complexes of phthalocyanine with gadolinium and neodymium. Introduction of steric substituents into peripheral and non-peripheral positions of the phthalocyanine macrocycle will improve their solubility and reduce the ability to aggregate in solutions. The presence of axial ligands and the high coordination capacity of lanthanides will also contribute to improving the solubility of the target complexes.

Synthesis of metal complexes was carried out by template condensation of the corresponding phthalonitriles with gadolinium and neodymium salts in a molar ratio of 3:1 in the presence of DBU. Product separation was carried out on a chromatographic column on silica gel. The obtained compounds were infected using modern physicochemical methods.

The work includes study of the introduction of peripheral and non-peripheral substituents effect and the nature of the salt on the yield of target products. Spectral characteristics in organic solvents (chloroform, THF, DMF) of the obtained complexes were studied.

It was determined that the preferred product of the syntheses is a sandwich-type complex. It was also found that when used in the synthesis of double-deck complexes of gadolinium and neodymium by template condensation by fusion in the presence of DBU leads to the formation of a sandwich molecule, which, due to the presence of a base, is in a mixture of neutral-radical and reduced forms.

This work was supported by the Russian Science Foundation (grant № 17-73-20017).

Sequence variants in biopharmaceuticals

Anushikha Thakur

Former Employee, RnD, Biocon Biologics, India

Among various other product impurities sequence modification in protein bio-therapeutics can be categorized as undesired product variant. These sequence variants (SV) may possess altered physicochemical and or biological properties compared to wild-type product, which can affect the overall efficacy, stability or safety of the biomolecule drug. Early detection of specific sequence modifications is therefore desirable in product manufacturing. Because of their low abundance, and finite resolving power of conventional analytical techniques, they are often overlooked in early drug development. However, once the mutation is identified: genetic or misincorporation, the clone is rejected and the cell line is changed or further optimized in upstream media supplements, respectively. Depending on the stage of the development, this approach may incur a moderate to significant delay in reaching the drug to patients. In case, the sequence variant is in a functionally inactive region of the protein the impact can be nullified theoretically and the development can move forward with a risk possibility of failing in immunogenicity during the clinical trial. The present topic discusses a case study where trace amount of a sequence variant is identified in a monoclonal antibody (mAb) based therapeutic protein by LC–MS/MS. The sequence variant was enriched during downstream processing of the antibody for further extensive characterisation using biophysical techniques and biological assays to exploit its physicochemical properties for downstream purification of desired drug product. Using a very sensitive selected reaction monitoring (SRM) technique, this SV was quantitated in in-process samples which revealed both prominent and inconspicuous nature of the variant in process chromatography assisting in devising control strategy for sequence variant in the final product. This way as low as <0.05% upper limit could be achieved for sequence variant in the drug product utilizing SRM based mass spectrometry method during the purification steps.

Effect of silver nanoparticle treatment on the expression of key genes involved in flavonoids biosynthetic pathway in *Viola tricolor* L. Plant

A. Hassanvand[1], S. Saadatmand[1], Hossein Lari Yazdi[2] and **Alireza Iranbakhsh[1]**

[1]*Department of Biology, Science and Research Branch, Islamic Azad University, Iran*

[2]*Department of Biology, Boroujerd Branch, Islamic Azad University, Iran*

Heartsease (*Viola tricolor* L) of the Violaceae family is used for biological and pharmacological usages due to its antioxidant substances. Nanotechnology plays an important role in increasing agricultural productivity using biological nanoparticles Silver nanoparticles (AgNPs) are new metallic compounds with numerous physiological and biological properties, which are widely used in medical industries and so on. In the present study, plant-mediated nanosilver was produced from aqueous extract of Pansy flower as a good covering and stabilizing agent using the green synthesis method. Silver nanoparticles (AgNPs) are new metallic compounds with numerous physiological and biological properties, the presence of synthesized Ag-NPs was first confirmed with Dynamic light scattering, transmission electron microscopy, and zeta potential analyses. In this study, the effect of different concentrations of bio nanosilver 0, 10, 50, and 100 mg/L on phytochemical and physiological properties, and the expression of some key genes involved in flavonoids biosynthesis including phenylalanine ammonia-lyase (pal), chalcone synthase (chs), flavonoid '3', '5-hydroxylase (f3'5'h), and flavonoid 3'-hydroxylase (f3'h) were determined in V.tricolor plant.The results showed nanosilver treatments cause the accumulation of manganese, zinc, and silver elements and increasing the content of phenolic, flavonoid, anthocyanin and antioxidant activity . Using AgNPs also cause the increase of activity of antioxidant enzymes such as superoxide dismutase, ascorbate peroxidase, phenylalanine ammonia-lyase, and peroxidase. Besides, treatment with a concentration of 10 mg/L of silver nanoparticles significantly causes an increase in flavonoids compounds such as rutin, apigenin, and quercetin. In general, we found that silver nanoparticles could increase of secondary metabolites content in the V.tricolor plant. Nanoparticles can exert the inhibitory effect of DDPH free radicals in a dose-dependent manner. According to the results, AgNPs stimulated the antioxidant activity and increased secondary metabolites (flavonoid content).

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New capsaicinoids: Biological activity and theoretical calculation

Arif Khan, Fatima Naaz and **Syed Shafi**

Department of Chemistry, SCLS, India

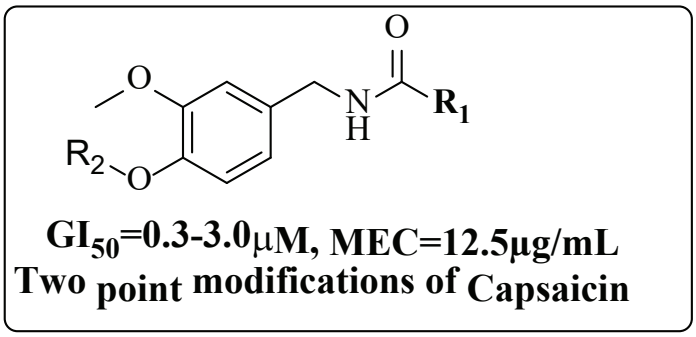
Backbround: Natural product is organic substance produced by living organism found in the nature. It can be in form of primary and secondary metabolites. These have pharmacological activity which is beneficial various kinds of diseases. Natural products have been an important source for drug development over the years as more than 70% of the currently available drugs are either directly from natural sources or semi-synthetic analogues of natural products or molecules developed inspired by natural products.

Aims/Objectives: Keeping in view of the importance of natural product scaffolds in cancer and bacterial drug discovery, we aimed at the development of some new secondary leads based on capsaicin and their computational calculation.

Methodology: A library of new capsaicinoids has been synthesized through a two point modification around 4-hydroxy-3-methoxy-benzyleamine moiety by varying the nature and the length of lipophilic side chain and by bringing modifications at phenolic group. All the synthesized compounds were screened for their anti-proliferative activity against NCI panel of 60 human cancer cell lines, and bacterial NorA efflux pump inhibitors. All synthesized compounds were screened DFT and QSAR calculation.

Results: New capsaicinoids resulted from the two point modification of capsaicin have demonstrated promising anti-proliferative activities with GI50s 0.3-30 μM against NCI panel of 60 human cancer cell lines. Among the cancer cell lines tested Colon cancer cell lines were found to be more susceptible to this class of compounds. The inhibitor displayed a minimum effective concentration of 12.5 μg/mL against SA1199B which was better than its parent conjugates capsaicin (MEC 50μg/mL) and standard drug reserpine (MEC 25μg/mL). In computational study, some compounds revels good co-relation with colon cancer cell line (HCT-15, HT29 and KM12).

Conclusion: In conclusion a promising lead molecule has been generated through two point modifications of capsaicin.



Application of nano bubbles in wastewater treatment: Challenges, applications and futuristic developments

Arijit Dutta Gupta[1,2] and **Harinder Singh**[2]

[1]*UPL University of Sustainable Technology, India*

[2]*Motilal Nehru National Institute of Technology Allahabad, India*

In the last decade, researches on bulk micro and nano bubbles have been attracting the attention of scientists and environmentalists in the field of wastewater treatment. Many patented and open-sourced literatures reports on the techniques on the bulk generation of nanobubbles and its underlying research and applications. However, the major drawback in these studies are the bubble concentration and their size distribution. Moreover, there are challenges related to scale-up applications (particularly on pilot and industrial scale) which limits their applications for handling wastewaters with high flow rates. Nano bubbles (1 – 100 nm diameter) present excellent and interesting characteristics such as high surface to volume ratio, high longevity and stability, good surface charge density and tendency to form aggregates of hydrophobic particles. These results demonstrate the futuristic technological advancements not only with nano bubbles but also in combination with macro (diameter = 100 µm – 2 mm) or micro bubbles (1 – 100 µm diameter). Nevertheless, most of the research has been devoted to the generation of nano bubbles by hydrodynamic cavitation or depressurization of air (saturated with water) in various flow constrictors (orifice, needle valves, venturi). In the field of metallurgy, nanobubbles serve the purpose of accelerating the recovery rate and flow kinetics of both ultrafine and fine particles at lower amounts of collector and frother. In wastewater treatment, nano bubbles significantly enhance the removal of different pollutants (organic/inorganic precipitates, ions, colloidal solids, emulsified oils, residues) via floatation accompanied with bigger bubbles (micro or macro). Future researches on nano bubbles should focus on more promising bubble generation techniques with high rate of mass transfer, studies on economic analysis through experiments on pilot scale handling real wastewater with continuous injection of bubbles.

Melvin Calvin, Nobel in Chemistry

A. Nonomura

Northern Arizona University, USA

Melvin Calvin won the 1961 Nobel Prize in chemistry for the discovery of the canonical photosynthetic carbon reduction cycle in collaboration with Andrew A. Benson and James A. Bassham and a personal glimpse provides insight into this American force in physical chemistry and inspiration for the future of innovations in chemistry. He was born in St. Paul, Minnesota, USA, on April 8, 1911, and lived until 1997. His father was from Lithuania and his mother was from Russia. Calvin investigated artificial photosynthesis, the physical chemistry of color in porphyrins, the origin of life, cancer, the biochemistry of learning, moon rocks, and avenues to grow gasoline, as well as its related optimization of photosynthesis. The Calvin lab sought to modulate glycoregulation in the field, and yet this significant advancement has been achieved only today. Based on the discovery of the plant lectin cycle, BRANDT GlucoPro® plant growth regulator puts control of crop photosynthesis in the hands of farmers.

Synthesis and physic-chemical properties of metal complexes with bulky phthalocyanine ligands

A. Vashurin

Ivanovo State University of Chemistry and Technology, Russian Federation

Complexes of d- and f-metals with phthalocyanine ligands are promising compounds for creating materials with controlled photophysical and photochemical properties, as well as catalytic and sensory activity [1-2]. The presence of promising physicochemical properties of metal phthalocyanines is primarily due to the specifics of the coordination center of the macromolecule and its functional environment. The nature of the substituents in the peripheral and non-peripheral positions of the phthalocyanine macrocycle, on the one hand, determines their solubility in various media, and on the other hand, the possibility of the formation of oligomeric and polymeric molecular systems that retain the specified physicochemical properties due to ionic, coordination and covalent interactions.

In addition, the nature of substituents in the macrocyclic backbone can determine the possibility of obtaining various materials with the participation of metal phthalocyanines. We have previously shown that immobilization of macrocycles on inorganic carriers, for example, silica, is promising in this case. It should be noted that in this case, not only the set of functional groups in the composition of the substituent, but also their spatial arrangement has a significant effect on the physicochemical properties of the materials obtained.

The report presents the synthesis of a wide range of promising complexes of d- and f-metals with phthalocyanine ligands containing functional groups in peripheral and non-peripheral positions (cyano-, sulfo-, nitrocyclohexyl fragments, etc.), separated from the macrocyclic backbone by spacer phenoxyl chains of various length. An analysis is given of the relationship between the nature of the spacer fragment of macrocycles and their aggregation, spectral, luminescent properties, as well as the processes of molecular complexation in liquid-phase systems.

Interdisciplinary approaches to environmental assessments: Cases in architecture

A. OZTURK

Cyprus International University, Turkey

The architectural design and construction processes bring a building into existence. In this existence the "body" of the building is the hardware; and the "soul" of the building consists of the environmental characteristics of that body. Most of the environmental assessment tools deal with the evaluation of the hardware such as outer shell, building materials, constructional details, building services, etc., and physical phenomenon of the indoor environment such as IAQ, thermal quality, lighting, etc. However the conceptual meaning of the environment includes relations and dependencies as well as the physical conditions and surroundings. Physical surroundings and conditions are based on real, objective facts such as climate, energy, water, etc. which can be measured by devices; whereas relations and dependencies are based on more abstract, subjective facts such as socio-cultural characteristics, norms, beliefs etc. which cannot be measured by any device. While the science and technology deal with the physical aspects social science examines the relations. Those of conceptual approaches come and knot in many cases, and necessitate the interdisciplinary approaches.

In this presentation two cases will be demonstrated as samples of interdisciplinary work. First is consideration of IAQ and the architectural design process within the building system; and the second is placing social criteria within the green building assessment tools. Since the speaker is an architect and the congress is on advanced chemistry, the aim of this sampling is to share the idea of realizing something related to one's professional area in another professional's field; and realizing something related to the another professional's area in one's professional field. Those of metaphorical approaches bring the uniqueness and richness in knowledge.

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Study of β-Cyclodextrin nanoparticle on essential oil content and expression of key genes in biosynthesis of bioactive compounds and biochemical parameters of medicinal plant *(Ocimum basillicum L.)*

A. Loni[1], S. Saadatmand[2], H. Lari Yazdi[3] and **A. Iranbakhsh[2]**

[1]*Department of Biology, Payame Noor University, Iran*

[2]*Department of Biology, Science and Research Branch, Islamic Azad University, Tehran, Iran*

[3]*Department of Biology, Islamic Azad University, Iran*

Bioelicitors are one of the management methods to induce the improvement of quantitative and qualitative performance of medicinal plants. The use of beta-cyclodextrin nanoparticles is described as a new protection strategy of the plant and induces a plant defense response. In this study, β-cyclodextrin nanoparticles (β-CDNPS) were synthesized. The nanoparticle profile was determined by UV-VIS spectrum, transmission electron microscopy (TEM) and dynamic light scattering (DLS). Then different concentrations of β-CDNPs including 0, 10, 50, 100 mg / l were used for foliar spray of basil (Ocimum basilicum c.v. Keshkeni luvelou). The amount of chlorophyll pigments and basil essential oil was significantly different (P≤ 5%) compared to the control. The maximum amount of chlorophyll b was observed in 100ppm treatment. Membrane stability index was assessed by measuring the electrolyte leakage of leaves and roots. A significant reduction (P≤5%) of ion leakage and malondialdehyde of roots and leaves was observed in the treatment of 50mg/l β-Cyclodextrin nanoparticle which indicates an increase in enzyme activity. Soluble sugars and proline of basil leave and root in 50ppm treatment had a significant increase (P≤%5) compared to the control, so that insoluble sugars in leave and root showed the opposite trend. In the presence of β-CDNPS, phenylpropanoids and terpenoids concentration, in the basil showed a significant difference (P≤5%) compared to the control group. Induction of β-Cyclodextrin nanoparticle in the biosynthesis pathway of secondary metabolites results in plant productivity. According to molecular analysis, eugenol O-methyltransferas(EOMT) and chavicol O-methyltransferas(CVOMT) genes expression in methyl eugenol and methyl chavicol biosynthesis pathways were significantly improved when treated with 50 ppm concentration compared to the control. Therefore, foliar spray at the right concentration can act as an inducer while stimulating, preserving the active ingredients in basil and increase the content of essential oil for food and drug consumption.

Production of energy sources and reduction of environmental hazardous solid wastes

Bijoy Kumar Mondal

Department of Chemistry, Uttara High School & College, Bangladesh

Post consume waste plastics (WP) and coal fly ash (FA) have been regarded as great environmental hazard because suitable disposal pathways has yet not been established for them. The amount of waste plastic is increasing because of the rapid growth of polymer consumption, short service life and non-degradable properties. On the other hand, FA, a coal combustion residue of thermal power plants has been regarded as a problematic solid waste all over the world. In this study, FA samples were modified with NaOH and H2SO4. The mineralogical and microstructural characterization were carried out by means of X-ray diffraction (XRD), fourier transform infrared spectroscopy (FTIR), scanning

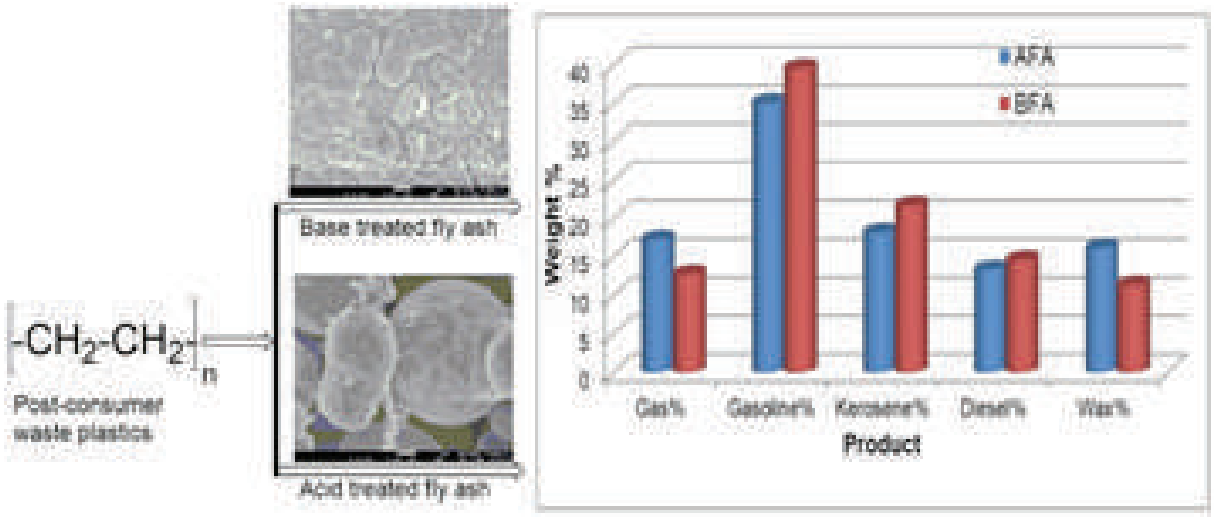

Figure 1: Effects of alkali and acid treated fly ash catalysts on post-consumer waste plastic pyrolysis

electron microscopy with energy dispersive X-ray spectroscopy (SEM/EDS) and Braunauer-Emmett-Teller's multilayer adsorption theory (BET). Waste low-density polyethylene (LDPE) and high-density polyethylene (HDPE) were degraded using a semi-batch reactor along with modified fly ash catalysts. The liquid products were analyzed using FTIR, nuclear magnetic resonance (1H, 13C, and DEPT-135 NMR), and gas chromatography–mass spectrometry (GC–MS). Experimental data showed that cenospheres were dominated with quartz and mullite glasses with both amorphous and crystalline phases. The acid treatment increased Si/Al ratios by removing impurities and dealuminations, whereas alkali treatment significantly increased total pore volume. Both of the waste plastics were degraded at 400–450°C., and the highest yield of liquid fuel product (about 87.24 wt%) was achieved for base treated FA at a polymer and catalyst ratio of 25 w/w. The NMR results accompanied by GC–MS data ensure that obtained fuels contain both aliphatic (saturated and unsaturated) and aromatic hydrocarbons, and FA is an efficient catalyst to pyrolize waste plastics into light weight liquid (gasoline and kerosene) hydrocarbons. This plastic-to-fuel technology should be commercialized owing to be profitable and eco-friendly.

Discovery of novel cyclic salt bridge in thermophilic bacterial protease and study of its sequence and structure

Debanjan Mitra and **Pradeep K. Das Mohapatra**

Department of Microbiology, Raiganj University, India

The plausible explanation behind the stability of thermophilic protein is still yet to be defined more clearly. Here an insilico study has been undertaken by investigating sequence, structure of protease from thermophilic (tPro) bacteria and mesophilic (mPro) bacteria. Results showed that charged and uncharged polar residues have higher abundance in tPro. Total 6 conserve regions have been found in tPro sequences which are 100% conserved. In extreme environment, the tPro is stabilized by high number of isolated and network salt bridges. A novel cyclic salt bridge (R415-D502:R415-E419:K416-E419: K416-D502:R480-D502) is also found in a structure of tPro. High number of metal ion

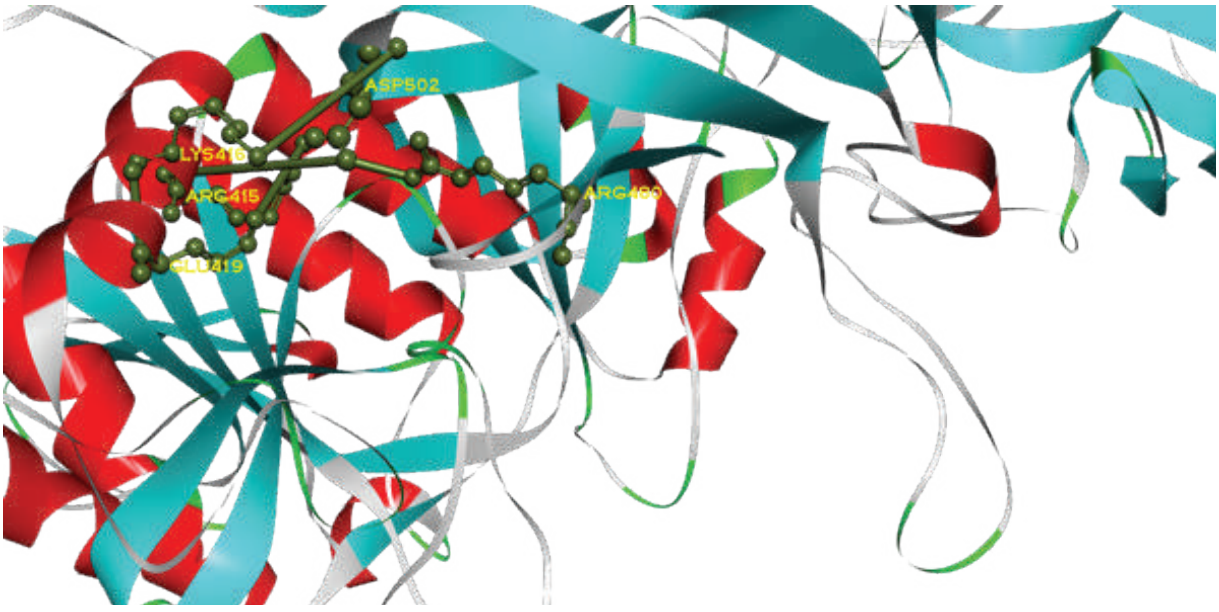

Figure- *A novel cyclic salt bridge found in Fervidobacterium pennivorans (1R6V)*

binding site also helps in protein stabilization of thermophilic protease. Aromatic-aromatic interactions also play a crucial role in tPro stabilization. Formation of long network aromatic-aromatic interactions also first time reported here. the high value of solvation free energy indicates that tPro are more stable than mPro. Presence of high number tyrosine phosphorylation site specially helps in tPro stabilization. This is a remarkable outcome of this study which also helps in protein engineering. This thermophilic protease can widely use in industrial application. Cause it can stable at very high temperature. It does not easily breakdown. Due to high stability, it can tolerate very extreme condition.

Dissolution studies of MOX nuclear fuel during the PUREX process

N. Desigan, S. Ganesh, K. A. Venkatesan and **K. Ananthasivan**

Indira Gandhi Centre for Atomic Research, India

The fundamental information required for designing a continuous FBR MOX spent fuel dissolution system is the fuel pellet's intrinsic kinetics of dissolution under typical PUREX process conditions. Hence the dissolution behaviour of a typical FBR MOX fuel pellet in nitric acid was investigated. Influence of parameters, such as plutonium content of the MOX pellet, initial concentration of nitric acid, intensity of mixing and the temperature of the reaction mixture, on the dissolution behavior of typical FBR MOX pellets in nitric

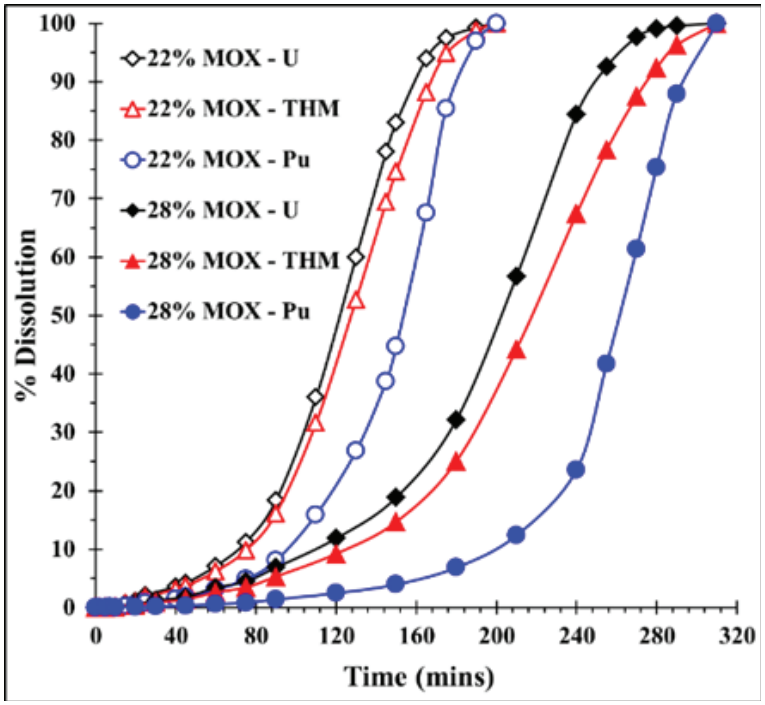

Figure 1: *Influence of Pu content on the kinetics of dissolution of MOX pellets in 8 M nitric acid at 348 K*

acid was examined. The results clearly bring out the differential rapid dissolution behavior of UO_2 over PuO_2 from the same MOX pellet under all the conditions of investigation. This differential dissolution was found to be inversely proportional to all the above evaluated influencing parameters except for the Pu content of the pellets in which case it was directly related. These results had paved way for better understanding of the dissolution mechanism of a typical FBR Pu rich MOX fuel under the conventional PUREX process conditions.

Table 1: *Consolidated table of results of MOX fuel dissolution experiments*

No.	Parameter studied	Its influence on the MOX fuel dissolution
1	Pu content of MOX pellets	Directly related to the differential rapid dissolution of UO_2 over PuO_2 from the same MOX pellet
2	Initial concentration of nitric acid	Inversely related to the rate of dissolution and the differential rapid dissolution behaviour
3	Rate of stirring of the reaction mixture	Inversely related to the overall dissolution rate of MOX pellets and the differential dissolution behaviour up to 600 RPM but has no effect on further increasing its intensity
4	Temperature of the reaction mixture	Directly related to the rate of dissolution and inversely to the differential dissolution behaviour

Synthesis and study of spectroscopic-luminescent properties of magnesium aryloxy substituted phthalocyaninates as promising fluorescent biomarkers

D. Erzunov, S. Tonkova, I. Sarvin, A. Alekseeva, A. Belikova and **A. Vashurin**

Ivanovo State University of Chemistry and Technology, Russian Federation

The variety of applications of materials based on macroheterocyclic molecules is due to the wide possibilities of adjusting the structure of the resulting compound for a specific task by choosing a specific class of compounds, introducing suitable peripheral and non-peripheral substituents, and varying the central metal atom. Phthalocyanine complexes have established themselves as one of the most promising types of macroheterocycles due to the presence of an extended conjugated aromatic circuit, as well as intense light absorption in the area of the "therapeutic window". In turn, the introduction of a luminescent active metal atom into the coordination center of a molecule opens up opportunities for the use of complexes in the medical field as elements of diagnostics and PDT of tumor diseases.

This work describes the synthesis and study of the spectral-luminescent properties of aryloxy-substituted phthalocyaninates with magnesium. The complexes were obtained by template fusion of substituted phthalodinitriles with magnesium (II) acetate in the absence of a solvent at 190 °C for 10 min. Purification was carried out using a column (silica gel M60, gradient elution with a mixture of ethanol (0 to 15 vol.%) in chloroform) and gel permeation chromatography (gel Bio-Beads S-X1, elution with a mixture of 2.5% ethanol in chloroform). The structure of the obtained complexes was confirmed using NMR, IR and electronic absorption spectroscopy, mass spectrometric analysis. Absorption maxima and molar light absorption coefficients of compounds in various organic media are determined, Stokes shifts, quantum yields and fluorescence lifetimes are calculated.

The use of enhanced hydrophobicity of nanofibrillated cellulose derived from oil palm empty fruit bunches as nano-reinforcing agent for poly (lactic acid) nanocomposite films

DY. Hastati[1], E. Hambali[2,3], K. Syamsu[2], E. Warsiki[2,3] and **NE. Suyatma[4]**

[1]College of Vocational Studies, Bogor Agricultural University (IPB University), Indonesia

[2]Department of Agro-Industrial Engineering, Bogor Agricultural University (IPB University), Indonesia

[3]Surfactant and Bioenergy Research Center (SBRC), Bogor Agricultural University (IPB University), Indonesia

[4]Department of Food Science and Technology, Bogor Agricultural University (IPB University), Indonesia

Nanofibrillated cellulose derived from oil palm empty fruit bunches (NFC-OPEFBs) has a high potential for nano-reinforcement in polymer composites. However, the hydrophilic surface of NFC-OPEFBs limits their usage as nanofiller for the hydrophobic polymers. To overcome the limitation, the enhancement hydrophobicity of NFC-OPEFBs was performed using a sustainable cationic surfactant, i.e., cetyltrimethylammonium chloride derived from palmityl alcohol through surface modification method. In this study, a modified NFC-OPEFBs was reviewed in terms of their effects on mechanical, water vapor permeability, and thermal properties of polylactic acid (PLA) nanocomposite films. The PLA nanocomposite films were prepared with the addition of unmodified NFC-OPEFB (unmodNFC) 0.5 wt%, with the addition of various amounts of modified NFC-OPEFB (modNFC) from 0.5 to 3.0 wt% into PLA matrix by the solvent casting method and neat PLA film as the control. The ultimate tensile strength of PLA films was increased by using 3.0 wt% of the modNFC 87.8 %, while it was decreased by using 0.5 wt% the unmodNFC. This result proved that the hydrophobicity of NFC could improve interfacial adhesion between PLA and NFCs. The water vapor permeability of PLA film was decreased by 36.0 % and 33.3 % with the addition of 2.0 wt% and 3.0 wt% modNFC, respectively. Moreover, the PLA+modNFC films exhibited overall higher crystallinity and higher glass transition temperature than those of neat PLA film. The transparency of PLA nanocomposite films with the incorporation of modNFC was clearer than that of unmodNFC at the same loading level observed with the visual transparency test using background images. This research revealed that the enhanced hydrophobicity of NFC might be used as nanofillers for other hydrophobic matrices such as polypropylene, polyethylene, and other hydrophobic polymers.

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Artificial neural network and multi-criteria decision-making models for flood simulation in GIS: Mazandaran Province, Iran

E. Shahiri Tabarestani[1] and **H. Afzalimehr**[2]

[1]*School of Civil Engineering, Iran University of Science and Technology, Iran*

[2]*Natural Disasters Prevention Research Center, School of Civil Engineering, Iran University of Science and Technology, Iran*

Flood is one of the most destructive natural disasters globally and is a concern due to its high vulnerability. In this study for identification of flood susceptible areas, artificial neural network (ANN) and Multi-Attributive Border Approximation Area Comparison (MABAC) combined with Weights of Evidence (WoE) and Analytical Hierarchy Process (AHP) Models were used in Mazandaran province, Iran. MABAC method was used for the first time to evaluate the flood-prone areas in this study, and Attempts have been made for evaluate the performance of this new method by comparing with ANN model. The output of the neural network was discharge values in hydrometric stations. Using Geographic Information System (GIS) with eight effective factors including rainfall, distance from rivers, slope, soil, geology, elevation, drainage density, and land use, a flood model developed. Three precision parameters containingR^2, RMSE and MAE were applied to show the performance of the ANN model which yielded the values of 0.89, 0.0024 m^3/s, and 0.0018 m^3/s, respectively for testing data. The verification results indicated satisfactory agreement between the predicted and the real hydrological records. Also, based on flood inventory map and using the area under receiver operating curve, predictive power of the MABAC-WoE-AHP model was evaluated. The AUC value for prediction rate of this model was 86.1% which indicates the very good accuracy in predicting flood-prone areas. The results of ANN and MABAC-WOE-AHP methods indicated that respectively 48.83% and 46.93% of Mazandaran Province was located in high and very high risk of flooding area. Comparison of flood susceptibility maps for ANN and MABAC-WoE-AHP models showed the good agreement between two models that clarifies the efficiency of the new proposed method for future preventive measures.

Combating nuclear terrorism: Characterization of an orphan Ra-Be neutron source

E. Elish

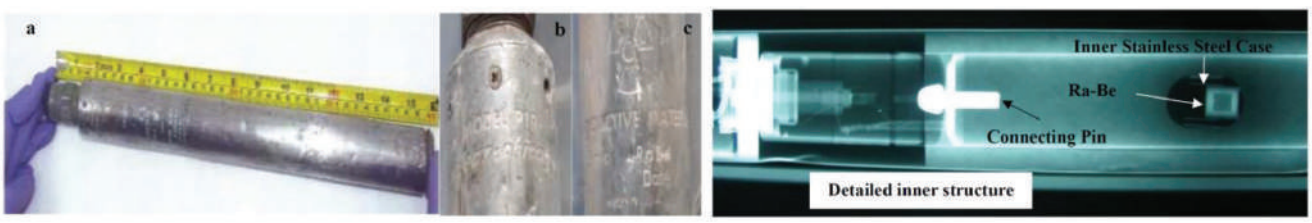
Nuclear Research Center Negev, Israel

Radio-active sources are wildly used in the oil industry, building cites, hospitals, agriculture and more, for various applications. Being so widespread, they have a high potential to be easily diverted from their legal use, to serve as "dirty bombs" – Radioactive Dispersive Device. Nuclear forensics aims at the development of scientific capacity needed to prevent such terror acts, and attribution capabilities in the occurrence of such an event.

An orphan radium-beryllium (Ra-Be) neutron source (Nuclear Chicago Corporation) detected inside a scrap metal shipping container, was seized and subjected to nuclear forensic analysis. Physical and chemical characterization methods were used before and after source dismantling. Non-Destructive Testing (NDT) proved to be most useful for initial analysis of the source. Dissolution of the Ra-Be capsule was followed with elemental analysis by Inductively Coupled Plasma (ICP) Atomic Emission Spectroscopy (AES) and Mass Spectrometry (MS). Model age determination by ICP-MS (81.6 y ± 4.08) was found to be sensitive to insufficient accuracy in measuring daughters present in the parent solution.

Within this presentation, the term nuclear forensic will be discussed in view of the global threat of nuclear terror, following by a detail description of the Ra-Be neutron source characterization.

The Ra-Be outer case (a), and magnification of text shown on the case (b): "Model P19 Nuclear Chicago" and (c): "Radioactive Material RaBe", are presented in the figure below, aside the neutron radiography of the source.



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Co substrate facilitated charge transfer for bioelectricity evolution in a toxic blue green alga fed microbial fuel cell technology

Fabrice Ndayisenga[1], Zhisheng Yu[1], Telesphore Kabera[2], Bobo Wang[1], Hongxia Liang[1], Irfan Ali Phulpoto[1], Telesphore Habiyakare[1,2], Yvan Kalisa Ndayambaje[2] and **Xinyu Yan[1]**

[1]College of Resources and Environment, University of Chinese Academy of Sciences, China

[2]College of Science and Technology, University of Rwanda, Rwanda

This study has investigated the key contribution of sodium acetate as co-substrate on the performances of microbial fuel cells (MFC) during the conversion of a toxic blue-green algae (BGA) biomass into bioelectricity. Microcystis aeruginosa biomass was employed as a target substrate and sodium acetate (AC) as a co-substrate. Compared with MFC treated with BGA alone (MFC-BGA), the MFCs treated with BGA together with acetate (MFC-BGA-AC) significantly magnified the voltage output by 261.3%. Moreover, the addition of co-substrate extended the electric batch cycle by 253.1% and 7.9% compared with MFC-BGA-AC and its corresponding MFC treated only with AC (MFC-AC), respectively. The co-substrate strategy also enhanced the maximum power density by a factor of 3.53 MFC-BGA and 1.2 MFC-AC. It has also displayed the smallest charge transfer resistance of 12.01 Ω which was approximately 45.8% lower than that of MFC-BGA and even slightly lower than the control. Based on the transmission electron microscope results, the cell morphology was also less affected in MFC-BGA-AC. Thus, our new study revealed that the co-substrate could empower the bio-electrochemical active bacteria for toxin survival and make a crucial contribution in alleviating the internal resistance within the operating reactors, which consequently promote the transfer of the generated charges to the bio-anode for power production evolution. The current investigation will conspicuously help in paving ways toward sustainable clean energy production and durable wastes control in the aquatic environment. However, more studies exploring the feasibility of using non-commercial renewable wastes such as wastewater to replace commercial acetate as co-substrate are still needed to make this MFC technology more economic and sustainable.

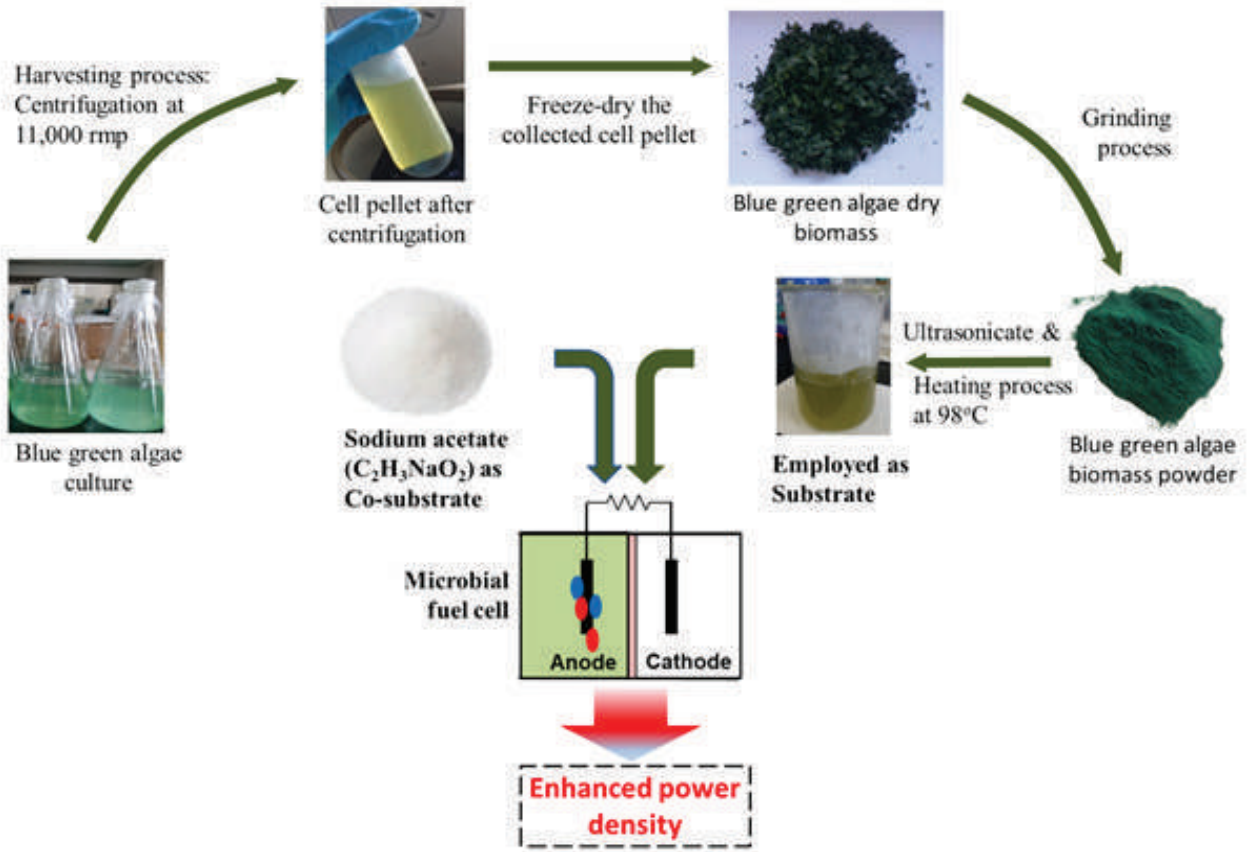


Figure 1: *General diagram summarizing the conversion process of the blue-green algal biomass into bioelectricity via MFC assisted with co-substrate.*

Mechanism of few-layer graphene growth from coal via a catalytic process

Faridul Islam[1] and **Jianglong Yu**[2]

[1]*Chemical Engineering, School of Engineering, The University of Newcastle, Australia*

[2]*Monash Research Institute of Science and Technology (Suzhou Industrial Park), Southeast University—Monash University Joint Graduate School, China*

Graphene has recently attracted a significant attention with wide applications owing to its unique thermal, electronic, composite, and mechanical properties. Few-layer graphene was synthesized via a microwave-assisted catalytic graphitization. The microwave irradiation temperature and time played a key factor to synthesize the few-layer graphene. The highest degree of graphitization value and a well-developed pore structure was fabricated at 1300 °C using a 10% iron catalyst for 20 min. The produced FLG has been examined by Raman spectroscopy, X-ray diffraction, Transmission electron microscopy, and Atomic force microscopy. A high-resolution transmission electron microscopy analysis confirmed that the fabricated few-layer graphene consisting of 3–6 layers. In addition, the 2D band at 2700 cm−1 in the Raman spectrum indicated the presence of graphene layers. The Raman mapping also represented the catalyst loaded sample was homogeneously distributed and displayed a few-layer graphene sheet. The highest I2D/IG value indicated a few-layer graphene sheet at 10% iron loaded sample. Moreover, the few-layer graphene growth process was induced when iron oxide was reduced to metallic iron. The graphene nucleation and growth occurred via the dissolution-precipitation mechanism of bituminous coal and catalyst droplets. Finally, this technique assists in developing a cost-effective and environmentally friendly few-layer graphene fabrication process using a coal-based carbonaceous material.

Wnt5A and TGFβ1 converges through YAP1 activity and integrin alpha v up-regulation promoting epithelial to mesenchymal transition in ovarian cancer cells and mesothelial cell activation

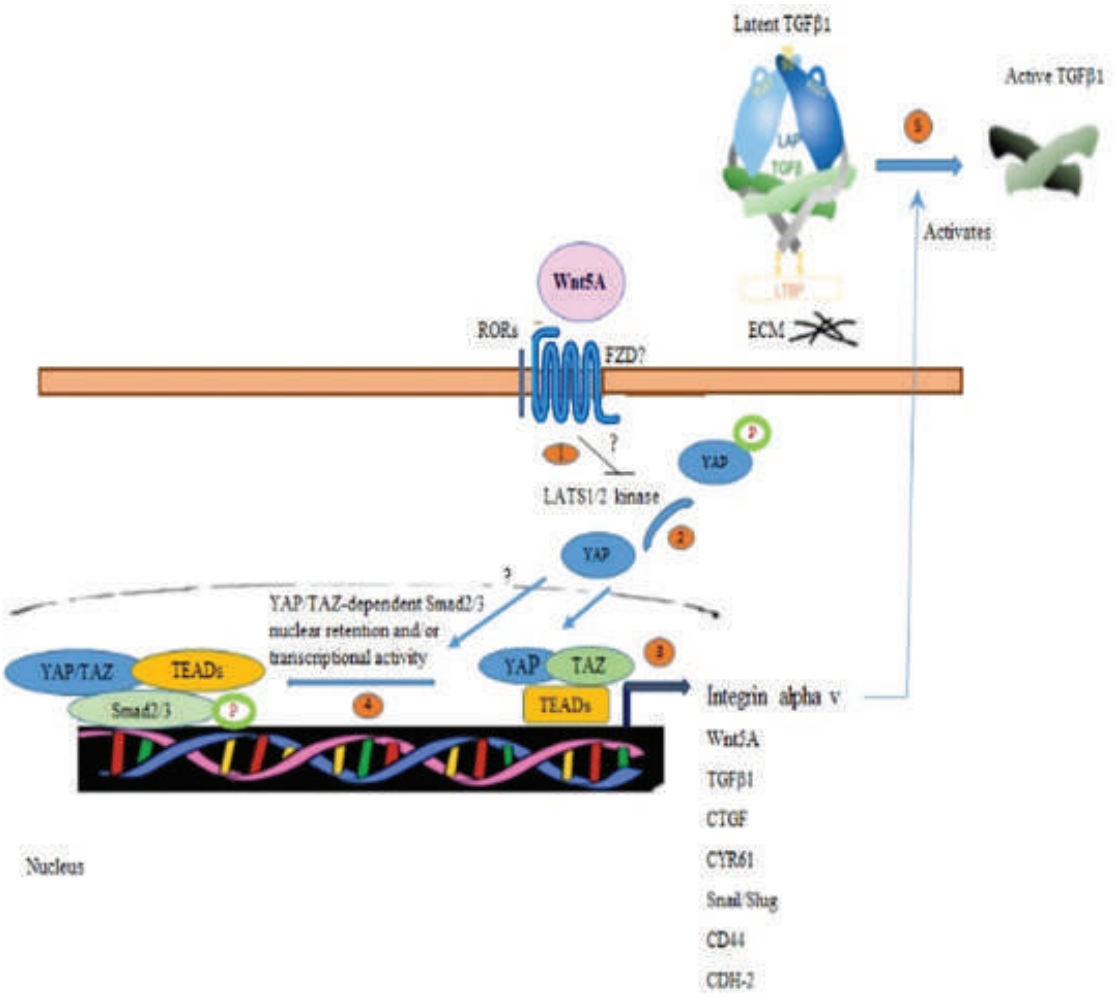
Zeinab Dehghani-Ghobadi[1], Shahrzad Sheikh-Hassani[2], Ehsan Arefian[3] and Ghamartaj Hossein[1]

[1]Department of Animal Biology, Developmental Biology Laboratory, School of Biology, College of Science, University of Tehran, Iran

[2]Department of Gynecology Oncology Valiasr, Imam Khomeini Hospital, Tehran University of Medical Science, Iran

[3]Department of Microbiology, School of Biology, College of Science, University of Tehran, Iran

Here we investigate whether Wnt5A is associated with TGF-□1/Smad2/3 and Hippo-YAP1/TAZ-TEAD pathways implicated in epithelial to mesenchymal transition (EMT) in the epithelial ovarian cancer. We used 2D and 3D cultures of human epithelial ovarian cancer cell lines SKOV-3, OVCAR-3, CAOV-4, and different subtypes of human serous ovarian cancer compared to normal ovaries specimens. Wnt5A showed a positive correlation with TAZ and TGF□1 in high- and low-grade serous ovarian cancer specimens compared to borderline serous and normal ovaries. Silencing Wnt5A by siRNAs significantly decreased Smad2/3 activation and YAP1 expression and reduced nuclear shuttling in ovarian cancer (OvCa) cells. Furthermore, Wnt5A showed to be required for TGF□1-induced cell migration and invasion. In addition, inhibition of YAP1 transcriptional activity by Verteporfin (VP) altered OvCa cell migration and invasion through suppression of Wnt5A expression and inhibition of Smad2/3 activation, which was reverted in the presence of exogenous Wnt5A. We found that the activation of TGF□1 and YAP1 nuclear shuttling was promoted by Wnt5A-induced integrin alpha v. Lastly, Wnt5A was implicated in the activation of human omentum-derived mesothelial cells subsequent invasion of ovarian cancer cells. Together, we propose that Wnt5A could be a critical mediator of EMT-associated pathways.


Latent TGFβ1
Active TGFβ1
Activates
Wnt5A
RORs
FZD?
ECM
YAP
LATS1/2 kinase
YAP/TAZ-dependent Smad2/3 nuclear retention and/or transcriptional activity
YAP/TAZ
TEADs
Smad2/3
YAP
TAZ
TEADs
Integrin alpha v
Wnt5A
TGFβ1
CTGF
CYR61
Snail Slug
CD44
CDH-2
Nucleus

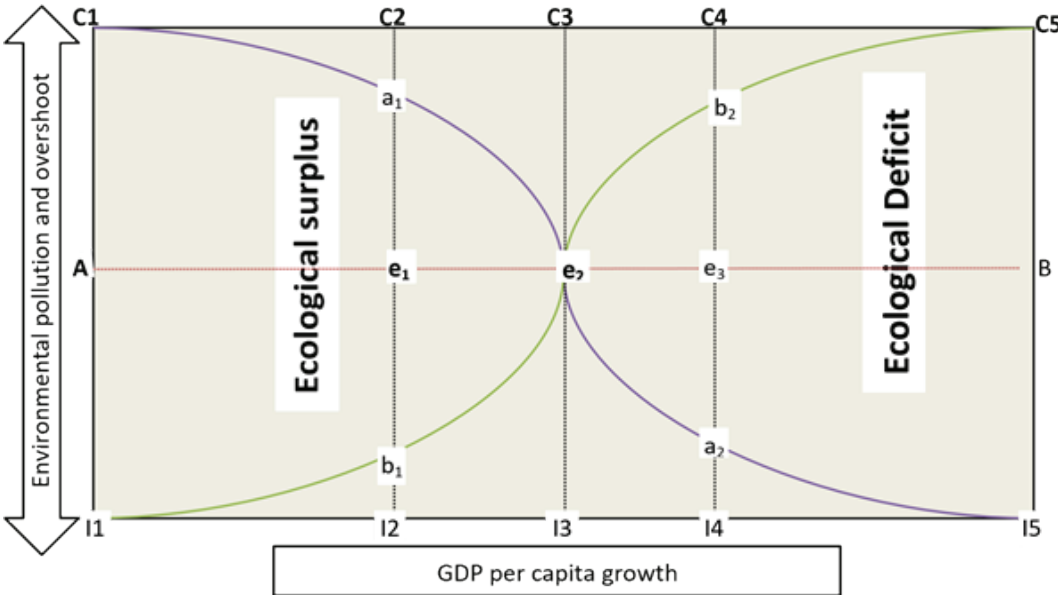
Primal-dual approach to environmental Kuznets curve hypothesis: A demand and supply side analyses of environmental degradation

Gildas Dohba Dinga[1], Dobdinga Cletus Fonchamnyo[2] and **Elvis Dze Achuo[3]**

[1,2]The University of Bamenda, Cameroon

[3]The University of Dschang, Cameroon

The unavoidable negative effects of global warming have been a key if not the most important issue occupying policy makers in the world at large today. The much talked about green economy nowadays seeks to achieve sustainable economic growth and development without compromising environmental quality. The relationship between environmental degradation and economic growth is largely explained by



Baseline primal dual relationship

Table 2. *Sign analyses of the demand side and supply side approach of EKC.*

Case 1.	α1	$\alpha_2>0$	$\beta_1<0$	$B_2<0$			No dual U/∩ -shaped EKC
Case 2.	$\alpha_1>0$	$\alpha_2<0$	$\beta_1<0$	$B_2>0$			Dual U/∩ -shaped EKC
Case 3.	$\alpha_1>0$	$\alpha_2<0$	$\alpha_3>0$	$\beta_1<0$	β2>0	$\beta_3<0$	Dual N-shaped EKC
Case 4.	$\alpha_1>0$	$\alpha_2>0$	$\alpha_3<0$	$\beta_1<0$	β2<0	$\beta_3>0$	No N-shaped EKC but U-shaped
Case 5.	$\alpha_1>0$	$\alpha_2<0$	$\alpha_2<0$	$\beta_1<0$	β2>0	$\beta_3>0$	No N-shaped EKC but U-shaped

the environmental Kuznets Curve (EKC) hypothesis. By employing the basic postulation of the baseline EKC framework, this study proposes and tests the existence of a dualistic approach of the EKC hypothesis. Geometry is used to illustrate the proposed dualistic model. Meanwhile, the novel dynamic common correlation effect econometric technique is employed to test the existence of the dualistic EKC within a panel of 109 countries from 1995 to 2016. The outcome from the estimated models shows that, in the global sample, the existence of the dualistic U-shape and N-shape EKC hypothesis is validated. When the sample is split into sub samples based on income levels, the U-shape EKC hypothesis is validated for lower income and high income economies meanwhile, the N-shape dualistic EKC is mostly associated with high income economies.

Thermostability, elasticity, and tenacity of rna RNA as rubbery anionic polymer in third milestone drug development------ Cancer targeting with undetectable toxicity

Peixuan Guo

The Ohio State University Wexner Medical Center, Arthur G. James Comprehensive Cancer Center and Richard J. Solove Institute, USA

RNA nanotechnology resembles LEGO accretion or architecture construction with RNA as the major composition material including the scaffolding and functional groups. The ideal building material should have the following properties: 1) versatility and controllability in shape and stoichiometry; 2) spontaneous self-assembly when mixed together; and 3) thermodynamic, chemic, and enzymatic stability with a long shelf-life. RNA building blocks exhibits all of the above properties. In addition, RNA nanoparticles hold many unique and favorable properties that further enhance their applicability. RNA is a polynucleic acid making it a polymer. RNA is negatively charged, which prevents nonspecific binding to negatively charged cell membranes. RNA can be designed and manipulated with a level of simplicity of DNA while displaying versatile structure and enzymatic function attributed to proteins. RNA folds into a large variety of single stranded loops or bulges suitable for inter molecular or domain interactions. These loops or bulges can serve as mounting dovetails alleviating the need for external linking dowels in the nanoparticle construction. RNA nanoparticles display rubber- and amoeba-like properties, leading to compelling vessel extravasation to enhance tumor targeting and fast renal excretion to reduce toxicities. RNA nanoarchitectures are stretchable and shrinkable through multiple repeats like rubber, leading to an unusually high tumor targeting efficiency since their rubber- or amoeba-like deformation property enables them to squeeze through leaky vasculature enhancing the EPR effect. RNA nanoparticles remain non-toxic since they can be rapidly cleared from the body via renal excretion into urine with little accumulation in organs and tissues. It was predicted in 2004 that RNA will be the third milestone in pharmaceutical drug development. The recent approval of several RNA drugs and the COVID mRNA vaccine by FDA suggests that this milestone is coming to realization.

Multifunctional textile auxiliary: Part 1: Preparation and application on polyester and acrylic fabrics

H. El-Sayed, M. Abou Taleb, A. Hussein and **A. F. El-Fiky**

Proteinic and Man-made Fibres Department, Textile Industries Research Division, National Research Centre, Egypt

Huge amounts of textile wastes and by-products are discharged into the surroundings causing environmental problems and loss of possible profits. Wool wax is produced as a by-product from scouring of raw wool fleece and many small and medium enterprises don't utilize them properly. Herein, we propose a novel approach for adopting green technologies for synthesis of new softener based on fatty acids derived from wool wax. The extracted fatty acids were condensed with a dihydroxy amino aliphatic short chain organic compound. The formed condensate was applied to acrylic fabric to enhance its performance attributes; Viz. imparting soft hand and reducing electrostatic charge. FTIR, GC-MS, ^{13}C NMR, were adopted to assign the mechanism of reaction between fatty acid and the bifunctional compound. The alteration in the structure of the treated fabric was assigned using XRD, FTIR, SEM analyses. The comfort characteristics as well as mechanical properties of the treated fabrics were also investigated.

Preliminary results indicate that the prepared condensate is a suitable candidate for improvement of comfort characteristics of acrylic fabrics without any adverse effect on its inherent properties.

Machine learning investigation of the micromechanics of granular materials

J. Wang

City University of Hong Kong, Hong Kong

There is a dearth of machine-learning investigations of the micro-mechanics of granular soils. The micro-mechanics deals with the mechanics of granular materials at the micro-scale (often particle scale) or meso-scale and is contrasted with the macro-mechanics which focuses on the macro-scale behavior measured at the laboratory sample scale or field scale. In this talk, a poineering investigation of the micromechanics in quasi-statically sheared granular materials using machine learning methods is conducted. An artificial neural network (ANN) based on discrete element method (DEM) simulation data is developed and applied to predict the anisotropy of contact force chains (CFC) in an assembly of spherical grains undergoing a biaxial test. An excellent model performance manifested in a close match between the rose diagrams of CFC from the ANN predictions and DEM simulations is obtained. In addition, some preliminary results of the prediction of the constitutive response of granular materials using the machine learning method are also presented.

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Effects of the addition of laser in the synthesis process of PZT nanopowders-microstructure and optical properties

K.H. Omran[1,2], M.S. Abd El-sadek[1], M.Mostafa[2], O.M. Hemeda[3] and **R. Ubic[4]**

[1]Nanomaterials Lab., Physics Department, South Valley University, Egypt

[2]Laser Tech. & Environment Lab., Physics Department, South Valley University, Egypt

[3]Physics Department, Tanta University, Egypt

[4]Micron School of Materials Science & Engineering, Boise State University, USA

Lead zirconate titanate, PbZr.52Ti.48O3, nano-powder has been synthesized via simple procedures based on the Pechini-type reaction route method. Laser radiation was applied during the preparation process. The influence of the laser radiation on the obtained nanopowders was studied. The thermal behavior of the dried gel was investigated via thermal gravimetric analysis (TGA) and differential scanning calorimetry (DSC). The obtained powders were characterized via XRD, UV–VIS–NIR, FT-IR, SEM and TEM techniques. The obtained X-ray powder diffraction patterns were analyzed by MATCH software to identify the existing phases, then a profile fit was carried out using the FullProf software package. The Goldschmidt tolerance factors and modified tolerance factors were estimated for the prepared nanopowders while the fractional of the observed individual phases were evaluated via the Rietveld method. The XRD measurements and TEM images confirmed the formation of nanoparticles. Williamson–Hall (W–H) and size strain plot (SSP) methods were used to evaluate the crystallite size and the lattice microstrain of the calcined nanopowders. The optical band-gap energy was determined using diffused reflectance measurements and the transformed Kubelka-Munk function. The band-gap energy values of the synthesized nanopowders were found to be slightly changed when laser radiation was applied.

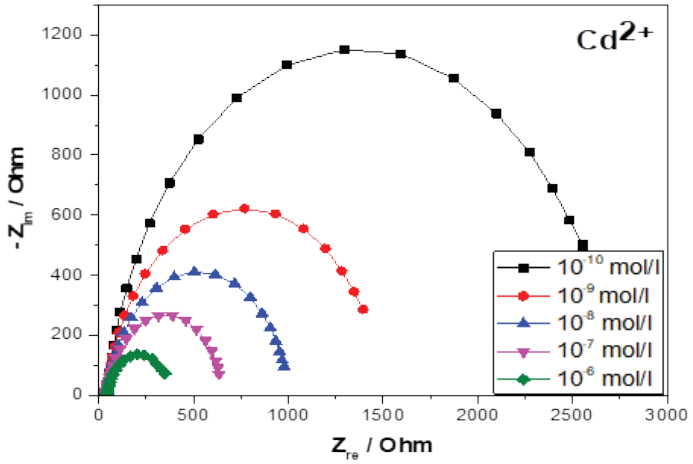
New selective modified glassy carbon electrode based on 6-furfurylaminopurine ligand for cadmium detection in real samples

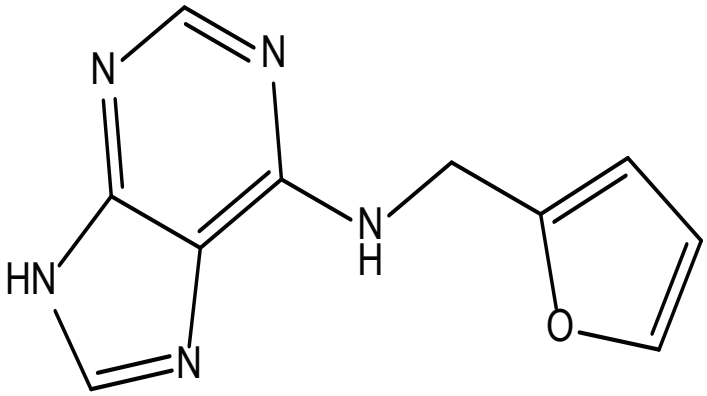
S Kouchar[1], M Benounis[1] and **N Jaffrezic-Renault[2]**

[1]Laboratory of Sensors, Instrumentations and Process (LCIP) Institute of Science and Technology, University of Khenchela, Algeria

[2]Institute of Analytical Sciences of the Claude Bernard University Lyon 1, France

This work presents a simple, inexpensive, and highly sensitive electrochemical sensor based on new polymeric membrane incorporating kinetin (6-furfurylaminopurine) as a specific sensitive molecule deposited on the surface of a glassy carbon electrode for the detection of cadmium in water. The electrochemical characterization was examined using electrochemical impedance spectroscopy and cyclic voltammetry. Additive effect and selectivity for cadmium over many common cations, such as copper, lead, and zinc, at pH 4.5 are studied. We showed that the cadmium selectivity is better for membrane based on potassium tetrakis(4-chlorophenyl)borate (KTpClPB) with a significant decrease of the Rct and an increase in constant phase element CPE, the sensor exhibits a LOD of $3{,}96\times10^{-10}$ M with a linear response towards cadmium ions over a wide concentration range of 10^{-6} to 10^{-9} M. vFinally, the proposed sensor was applied to the determination of cadmium in water and can be proposed to use successfully in real water samples.

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Impact of graphene-based nanomaterials (GBNMs) on the structural and functional conformations of hepcidin peptide

Krishna P. Singh[1,2], Lokesh Baweja[4], Olaf Wolkenhauer[1,5], Qamar Rahman[3] and **Shailendra K. Gupta[1,2]**

[1]*Department of Systems Biology & Bioinformatics, University of Rostock, Germany*

[2]*CSIR-Indian Institute of Toxicology Research, India*

[3]*Amity Institute of Biotechnology, Amity University, India*

[4]*Indian Institute of Technology Gandhinagar, India*

[5]*Stellenbosch Institute for Advanced Study (STIAS), Wallenberg Research Centre at Stellenbosch University, South Africa*

Graphene-based nanomaterials (GBNMs) are widely used in various industrial and biomedical applications. GBNMs of different compositions, sizes and shapes are being introduced without thorough toxicity evaluation due to the unavailability of regulatory guidelines. Computational toxicity prediction methods are used by regulatory bodies to quickly assess health hazards caused by newer materials. Due to the increasing demand of GBNMs in various sizes and functional groups in industrial and consumer-based applications, rapid and reliable computational toxicity assessment methods are urgently needed. In the present work, we investigate the impact of graphene and graphene oxide nanomaterials on the structural conformations of small hepcidin peptide and compare the materials for their structural and conformational changes. Our molecular dynamics simulation studies revealed conformational changes in hepcidin due to its interaction with GBMNs, which results in a loss of its functional properties. Our results indicate that hepcidin peptide undergo severe structural deformations when superimposed on the graphene sheet in comparison to graphene oxide sheet. These observations suggest that graphene is more toxic than a graphene oxide nanosheet of similar area. Overall, this study indicates that computational methods based on structural deformation, using molecular dynamics (MD) simulations, can be used for the early evaluation of toxicity potential of novel nanomaterials

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4-(2/4-cyclohexylphenoxy) phthalonitrile and phthalocyanine metal complexes based on it

K. Kazaryan, T. Tikhomirova, A. Botnar and **A. Vashurin**

Ivanovo State University of Chemistry and Technology, Russian Federation

Complexes of phthalocyanines with metals are known as the compounds with promising properties such as high chemical and thermal stability, as well as unique optical and electrical ones. The nature of the central metal ion and substituents are a tool for fine-tuning the physicochemical characteristics of compounds. The disadvantages of phthalocyanines associated with low solubility and a tendency to aggregation can be overcome by chemical modification of the macrocycle periphery by introducing functional- substituents.

In this regard, this work is devoted to the synthesis and study of properties of 4-(2/4-cyclohexylphenoxy)phthalonitrile as well as phthalocyanine based on it and its complexes with s, d and f- metals.

One of the simple and effective methods for obtaining phthalocyanines is a nitrile one. Initially, 2-cyclohexylphenoxy– and 4-cyclohexylphenoxy phthalonitriles were obtained, which afterward being used for the synthesis of corresponding phthalocyanines and their metal complexes. Complexes with s- and d- metals synthesis were carried out by template fusion of substituted nitriles with appropriate metal salts at 180-190 oC. The preparation of metal complexes with f- elements was carried out by boiling phthalonitriles with metal acetates in boiling iso-amyl alcohol in the presence of DBU.

All synthesized compounds were isolated and purified using column chromatography.

The identity of all the compounds obtained characterized by 1H NMR, IR spectroscopy and elemental analysis.

Due to the good solubility of the synthesized compounds in organic solvents, their spectral and luminescent properties were studied. The effect of the nature of the metal and solvent on the position of the main band and the behaviour of the spectral curves is shown.

This work was carried out with the financial support of the Russian Science Foundation (Grant No. 17-73-20017) using the resources of the Center for Collective Usage of the ISUCT.

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Experimental study of CdI_2 revaporization behavior in reactor cooling system condition after a nuclear severe accident

E. Le Fessant[1], A. C. Gregoire[1], L. Martinet[1], L. Cantrel[1], J. F. Paul[2] and **A. S. Mamede[2]**

[1]*Institut de Radioprotection et de Sûreté Nucléaire, Prais*

[2]*Unité de Chimie Catalytique et du Solide, Université de Lille, Paris*

During a severe accident occurring in a nuclear power plant, many Fission Products (FP) are released from the degraded fuel and transported in the Reactor Coolant System (RCS). This was the case for the Fukushima Daiichi (FD) accident with important FP releases. One of the main FP found around the FD power plant after the accident was iodine. If early phase releases were well predicted by SA simulation codes, delayed releases were not correctly predicted1,2,3. Such discrepancies are attributed to the deposits revaporization composed of metallic iodide (CsI, CdI_2, AgI…) inside the RCS which were not yet modeled in the SA simulation tools. Cadmium iodide revaporization behavior was investigated experimentally, mixed with CsI4 and by DFT calculation5 highlighting possible revaporization as cadmium oxide and molecular iodine (I2).

However, up to this day, no specific analytical study on revaporization of cadmium iodide in isotherms conditions and depending on oxygen concentration has been performed.

This study is scheduled within the OECD/NEA/ESTER project. The present work aims at determining the CdI_2 revaporization mechanism and quantifying revaporized species in isotherm conditions (temperature between 200 and 400°C) and oxygen partial pressure (between 1.10^{-4} and 4.10^{-2} atm). Thanks to a new experimental setup coupled with ICP-MS, Tof-SIMS and XPS analyses, Cd and I speciation are determined and quantified. On the one hand, with a steam/air atmosphere (oxygen partial pressure at 4.10^{-2} atm) significant I revaporization is observed even with isotherms at 400°C resulting in the transport of both gaseous and aerosols I species. On the other hand, when oxygen partial pressure increases, I gaseous species revaporization increases with different iodine species.

New technological and instrumental solutions for thermal reactors' SNF reprocessing

V. Volk[1], L. Podrezova[1], V. Rubisov[1], V. Alekseenko[2] and **A. Dyachenko[2]**

[1]SK «A.A. Bochvar High-Technology Scientific Research Institute for Inorganic Materials (VNIINM), Russia

[2]FSUE «Mining and Chemical Combine», Russia

Currently, the Russian Federation is completing the construction of a Pilot Demonstration Center (PDC) for the innovation-based spent nuclear fuel (SNF) of VVER-1000 treatment. Minimization of the generated liquid radioactive waste volume is one of the most important PDC tasks. To implement this approach VNIINM has developed a scheme for SNF processing using new technological and instrumental solutions (Figure 1).

According to the technological scheme,

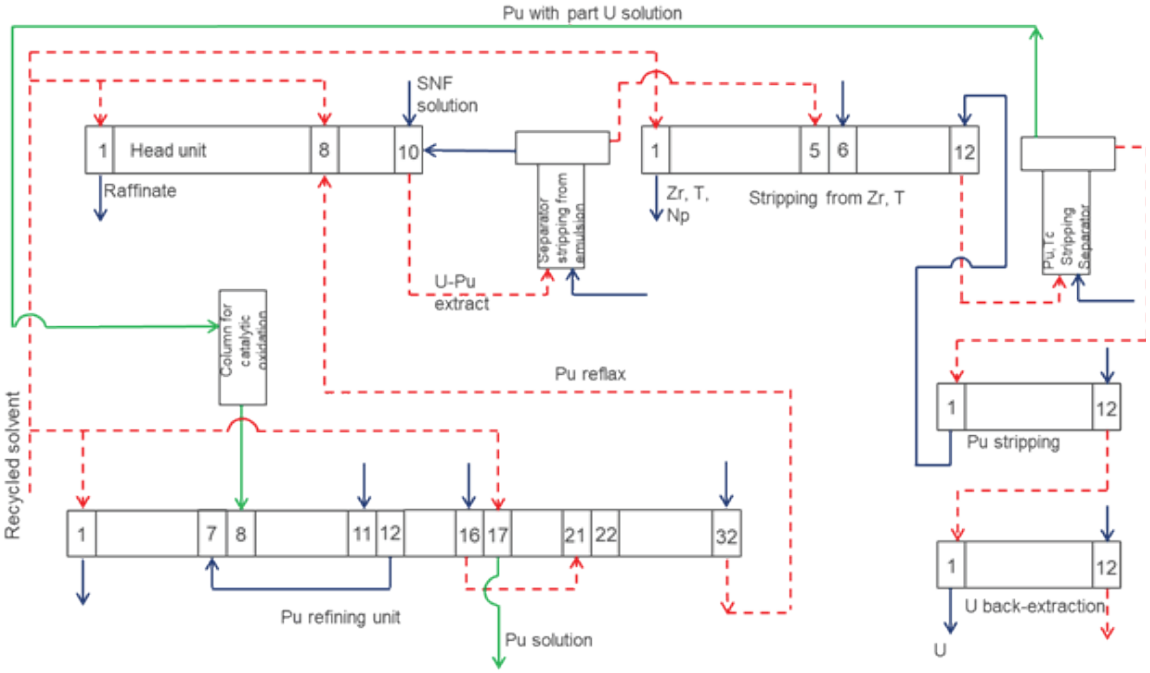


Figure 1 - Scheme of VVER-1000 SNF reprocessing, proposed by VNIINM

uranium, plutonium, and relevant elements are extracted from the nitric acid solution. Then the extract is scrubbed, plutonium is back-extracted with a part of uranium, and then the uranium extract is stripped from the remains of plutonium, neptunium, and technetium. Plutonium (III) in the solution of back-extraction is oxidized to plutonium (IV) and is extracted again together with U. The extract of the second stage is then scrubbed and plutonium is back-extracted. The first back-extraction of plutonium with a part of uranium is carried out in a mass-transfer separator by an aqueous stream containing Pu (IV) and Tc (VII) reducing agents at a high organic phase/aqueous solution ratio (up to 30). Additional purification of the uranium extract is carried out by a weakly acidic solution of the complexone. The spent complexone solution is directed to the U-Pu extract scrubbing stage. Then the plutonium-technetium solution goes through a catalytic oxidation column with a carbon catalyst. The oxidized Pu-Tc solution is directed to the refining unit.

A complex test of the VNIINM scheme of the VVER-1000 SNF reprocessing was successfully carried out in a PDC hot cells using a simulator of plutonium solution as well as the solution of spent nuclear fuel of the thermal reactor.

The main technological indicators of the scheme and high efficiency of the mass-transfer separators usage have been confirmed. The feasibility of the two-stream input of the circulating solvent to the head extraction unit and the process of a two-stage U and Pu separation with a concentrated plutonium solutions obtaining at the first stage has been confirmed, as well as the process of additional U-extract purification from plutonium residues at the second stage with the spent scrubbing solution utilization inside the extraction cycle.

The efficiency of the catalytic oxidation of Pu (III) → Pu (IV) process without the introduction of additional oxidizing reagents has been also confirmed. The efficiency of the refining plutonium sub-cycle unit with the return of excess uranium to the technological scheme with a return organic flow is shown.

Excellent color rendering index single system white light emitting carbon dots for next generation lighting devices

Manasa Perikala and **Asha Bhardwaj**

Department of Instrumentation and Applied Physics, IISc Bangalore, India

Recently, quantum dots (QDs) are fnding enormous application in white light emitting diodes (WLEDs) and WLEDs with high color rendition are in high demand. QD-WLEDs use diferent color (Red, Blue, Green) emitting QDs to obtain white light. Use of diferent color emitting QDs afect purity of white light due to self-absorption losses and QD degradation, in the long run afecting color rendering index (CRI) of WLEDs. Herein, we report low cost, environment friendly, open air atmosphere synthesis of single system white light emitting carbon dots (CDs) with broad emission bandwidth ranging 116 –143 nm and quantum yields (QY) ~ 5 – 13 % in colloidal state by modifying CD surface. Furthermore, carbon dot polymer phosphor (CD-PDMS phosphor) is fabricated which emits white light under UV illumination with a record emission bandwidth of ~ 154 nm and QY~ 16 % in solid state. Moreover, CD-PDMS phosphor exhibit excellent color rendering index (CRI)~ 96, the highest reported so far with CIE co-ordinates (0.31, 0.33) that are quite akin to pure white light. Such high performances are achieved due to high quality of CDs and CD-PDMS polymer phosphors by precise control in passivation/functionalization of nanoparticle surface. This work will set platform for the application of CD-phosphor based WLEDs in lighting systems.

"Using LIBS to answer the query, "Grandma, what is my rock made of?""

Marilyn D. Duerst[1] and **Richard W. Duerst**[2]

[1]*Retired, Dept of Chemistry, University of Wisconsin-River Falls, USA*

[2]*Retired*

The development of a hand-held device utilizing laser-induced breakdown spectroscopy (LIBS) has revolutionized the elemental analysis of solid samples, since it can be used in-the-field for geological and mineralogical exploration. The increasing need for lithium, precious metals, and rare earth elements for the manufacture of electronic gadgetry has spurred this endeavor.

Our full LIBS spectra from 190-950 nm of over 75 elements were obtained and used to confirm the presence of those elements in a large number of mineralogical samples, the metals present in antique and souvenir spoons from all over the world, in jewelry, coins and other alloyed objects.

Detection of non-metals in samples has been challenging, since the intensity of their emission lines are often at least two orders of magnitude smaller than the intensity of metal emission lines. We determined the relative intensity ratios of halogen/alkali metal in 20 alkali halide samples in order to develop a method to aid in confirming the presence of Cl, F, Br and I in mineralogical samples. How to confirm the presence of sulfur in solid samples will be illustrated.

LIBS (in particular the hand-held device), is a valuable addition to our arsenal of analytical techniques for elemental analysis of myriad solid samples

Fabrication of a sensitive biosensing system for Cu^{2+} ion detection by gold-Decorated Graphene Oxide Functionalized with Gly-Gly-His

M. Azizi

Institute of Biochemistry and Biophysics, University of Tehran, Iran

Incorporation of nanomaterials and nanostructures into sensors causes remarkable advances in device operation due to sensitivity, selectivity, multiplexed detection capability, and portability. In this study, a nanographene sensor coated with gold nanoparticles and tripeptide Gly–Gly–His was designed for Cu^{2+} ion detection at low concentrations. Graphene oxide synthesized by the modified Hummer's method and analyzed by UV–Vis spectrometry, x-ray diffraction (XRD), and transmission electron microscopy (TEM). The optimum conditions based on the maximum gold loading were evaluated 71 min for incubation time and 1 for HAuCl4/HEPES concentration ratio. Gold-coating on graphene oxide was approved by TEM, UV–vis spectrometry, XRD, and FTIR. The EDC/Sulfo-NHS method was used to stabilize Gly-Gly-His to graphene oxide-gold, which has a high affinity toward Cu. The performance mechanism of this nanosystem was based on the localized surface plasmon resonance (LSPR) property of gold nanoparticles. The sensor was extremely selective and sensitive to Cu^{2+} with the detection limit of 8.83 nM without cross-binding to other metal ions. The response time was evaluated about 9 min. The GO-Au-GGH biosensor was also very stable and easily reused, which further confirms it as an efficient and sensitive Cu^{2+} ion detection device.

Isolation, characterization and identification of pesticide degrading bacteria from contaminated soil for bioremediation

Akshita Mehta, Kamal Kumar Bhardwaj, Mayorin Shaiza and **Reena Gupta**

Department of Biotechnology, Himachal Pradesh University, India

In this study, malathion and chlorpyrifos degrading bacteria were isolated from agricultural soil samples taken from the Himachal region in India. A total of 52 organisms were isolated which were further screened for their efciency for chlorpyrifos and malathion degradation. Screening was done by checking the growth on Nutrient Agar, Mineral Salt Medium and MacConkey agar plates containing chlorpyrifos and malathion; 37 isolates showed growth in these. Biomass assay and minimum inhibitory concentration (MIC) determination were carried out for the selection of most efficient bacterial isolates. Out of the seven isolates which showed good biomass assay and MIC, only three isolates (PDM-2, PDM-15 and PDM-20) were selected for further studies. These were characterized by various biochemical tests, Gram staining, indole test, methyl red test, Voges-Proskauer test, citrate utilization test and carbohydrate fermentation test. Out of three isolates, PDM-15 showed good resistance against the antibiotics such as erythromycin, chloramphenicol, ampicillin and penicillin and identifed as Kocuria assamensis. Degradation of 71.3% of chlorpyrifos and 85% of malathion was observed by the gas chromatography.

Nowadays, the problem of pesticides pollution is increasing and it causes the environmental hazard. Microorganisms are essential for bioremediation of environmental pollutants because they play a considerable role in the degradation of insecticides. The strain with good degradation capability, i.e. Kocuria assamensis was isolated from agricultural soil of diferent regions of Himachal Pradesh. It has shown that this strain was able to grow in the presence of chlorpyrifos and malathion and it utilized these pesticides as carbon source. Results obtained in this study have shown that the isolate PDM-15 was found to be Gram-positive coccus and was identifed as Kocuria assamensis which was capable of degrading pesticides and tolerating antibiotics as well as metal ions.

Level of organochlorine pesticides in the barents sea sediments

M.A. Novikov

Polar Branch of VNIRO (PINRO named after N.M. Knipovich), Russia

GIS-technology facilitated the study of organochlorine pesticides' (hexachlorobenzene, hexachlorocyclohexane and DDT) distribution in the Barents Sea bottom sediments. The study aims at reviewing the pesticides' distribution in the sediments and the ways they are transported in the Barents Sea. The results from the analysis of samples of the sediments' upper layer at 696 stations were processed. The sampling was conducted in 2003-2019 during research cruises of PINRO named after N.M. Knipovich. The pesticides were identified by using the chromatography/ mass spectrometry instrument and applying the capillary gas chromatography method. Mapping was done in the ArcGIS application environment. There were additionally six sites identified: the Spitsbergen ¬¬– a shelf area south of Spitsbergen, the Bear Island Trough region including the Hopen Trench, The Northeast area, the Southeastern area (the Pechora Sea), the Eastern (Central) Basin and the Kola Bay region. There was separate statistical data processing conducted for each site. The pesticides contents in the sediments were compared between the sites and the Barents Sea in general. During the study, there were maps made of the distribution of the pesticides in the Barents Sea sediments. The sediments of the Eastern Basin and the Bear Island Trough sites were identified as the most contaminated by the organochlorine pesticides in the Barents Sea, with the average total content of 5.86 and 4.36 ng/g of dry weight respectively. The sediments of the Barents Sea southeastern part were found to be the least contaminated, with the average content of 1.53 ng/g of dry weight. Long-distance trans-border transfer, contaminants coming from the Arctic due to melting pack ice and glaciers on the Spitsbergen archipelago, the Franz Josef Land archipelago and Novaya Zemlya (long-term accumulated contamination) are likely the main sources of the sediments contamination by pesticides in the northern part of the Barents Sea.

Computed distribution of quaternary complexes of Cu (II), Zn (II) Co (II) and Ni (II) with Citrulline and tryptophan as primary ligand and thymine as secondary ligand

Monika Singh[1], Surabhi Sinha[2] and **Vijay Krishna[3]**

[1]Department of Chemistry, CMP Degree College, A Constituent College of University of Allahabad, India

[2]Department of Chemistry, United College of Engineering and Sciences, India

[3]Department of Chemistry, University of Allahabad, India

Investigation in solution exhibits the interest of chemist in thermodynamic aspects, which include knowledge of the stability constant of complexes with ligands of biochemical interest. It has been relevant for the experimental modeling of both reactions of metal ions with biomolecules and non-covalent interactions occurring in biological system. Stability constant data have been utilized to compute the equilibrium constant of ternary and quaternary complexes of citrulline/tryptophan and thymine with Cu(II), Zn(II) Co(II) and Ni(II) using SCOGS computer program at 37 ± 1°C and in ionic strength I = 0.1 M $NaNO_3$. The metal–ligand formation constant of MA, MB, MAB and M1M2AB type of complexes follows Irving William order. The distribution curves of various complex species occurring at the different physiological pH have been discussed, and solution structures with an explanation of plausible equilibria have been proposed.

Adsorbent coated adsorption cycle performance investigation

Muhammad Wakil Shahzad[1], Kim Choon Ng[2], Nida Imtiaz[1], Muhammad Ahmad Jamil[1] and **Ben Bin Xu[1]**

[1]*Mechanical & Construction Engineering Department, Northumbria University, UK*

[2]*Water Desalination and Reuse Centre, King Abdullah University of Science and Technology, Saudi Arabia*

The adsorption cycles are employed in cooling as well as in desalination industries due to its many advantages including waste heat utilization, solar thermal energy application and low maintenance cost. The major bottleneck in conventional adsorption cycles commercialization is its large footprint due to poor heat transfer in adsorbent packed bed heat exchangers. The recent development in coating technologies enabled powder adsorbent to be coated on heat exchanger to improve heat transfer and reduce the footprint of adsorption cycle. We designed an adsorption cycle based on adsorbent coated heat exchanger to investigate the two major parameters such as, the best binder suitable with most commonly silica-gel adsorbent and reliability of adsorbent and binder for commercial applications. The initial experimental investigation showed that silica-gel and hydroxyethyl cellulose (HEC 3% by weight) binder improved the overall heat transfer coefficient to 100-120W/m2-K as compared to 30-40W/m2-K in conventional packed bed AD cycle. In terms of pore surface area, the HEC only block 5-10% of total adsorbent area that showed insignificant impact on performance. We also developed detailed mathematical model to simulate adsorbent coated bed AD cycle performance and to compare with experimental results. Both have good agreement in terms of heat transfer coefficient values. It can be concluded that, the proposed coated bed AD cycle can produce double the amount of desalinated water or cooling effect with same amount of waste heat available.

Transformer oil Depolarization Ratio Index (DRI) for incipient fault analysis

Nor Asiah Muhamad

Universiti Teknologi Brunei, Brunei Darussalam

Preventive tests and diagnosis of in-service power transformers require system outage and need experts' knowledge and experiences in interpreting measurement results. Techniques such as insulating oil analysis may cause significant variance to measurement results due to different practices in oil sampling, storage, handling and transportation of insulating oil. The principal objective of this thesis is to develop a cost effective, fast, and reliable measurement technique for incipient fault analysis of in-service power transformers. An extended application of Polarization and Depolarization Current (PDC) measurement for characterization of different fault conditions of in-service power transformer was investigated in this research. The unique characteristic pattern of each condition was determined by a unique numerical dimensionless quantity known as the Depolarization Ratio Index (DRI) to express the changes of depolarization current shape. In addition, a graphical representation of DRI was also used as a technique to identify the incipient fault. Changes in the molecular properties of the insulating oil material due to different fault conditions were found to influence the initial time response. Sensitivity analysis using Artificial Neural Network (ANN) indicated that depolarization current provided better accuracy in identifying and classifying different transformer conditions as compared to the polarization current. A range of DRI between 5/100 and 10/100 was found to have a correlation of at least 90% with the incipient fault in power transformer. A DRI of 5/100 was observed to have a higher accuracy when detecting units with normal, overheating, and arcing conditions, compared to that for partial discharge condition. Both DRI and its graphical representation were validated using fresh field data and were more than 90% accurate. Both were able to identify and correctly classify the transformer condition as normal, overheating, or arcing. This demonstrated that the PDC measurement technique can be used to determine incipient faults in a power transformer.

Features of sorption of hexavalent chromium ions with magnetite

O.D. Linnikov

Institute of Solid State Chemistry, Ural Branch of the Russian Academy of Sciences, Russia

The report is devoted to the features of sorption properties of magnetite with respect to hexavalent chromium ions and the possibility of its use as a sorbent for removing these toxic ions from contaminated aqueous solutions. It has been shown that during the sorption of chromium(VI) ions by magnetite, two processes occur simultaneously: ordinary adsorption and chemisorption (redox reaction between hexavalent chromium ions and magnetite). The latter is accompanied by the oxidation of iron(II) in magnetite to iron(III) and the reduction of chromium(VI) ions to chromium(III) with the formation in the surface layer of magnetite (or on its surface) maghemite and a number of other compounds, including mixed chromium compounds(III) with iron. It is shown that the kinetics of the redox process between chromium(VI) and magnetite is described by the first-order reaction equation with respect to the concentration of chromium(VI) ions in solution. The parameters of the equation are found. As a result of chemisorption, unlike conventional sorbents, irreversible binding of chromium(VI) to magnetite occurs, which excludes the re-entry of its ions into the environment. In this case, the sorption capacity of magnetite, as it is saturated with chromium, irreversibly decreases. In addition, the sorption capacity of magnetite with respect to chromium(VI) ions also decreases with increasing pH of the solution being purified, and at pH>11 it is practically zero.

Device design optimization of highly efficient perovskite solar cell

Piyush K. Patel

Renewable Energy Laboratory, Department of Physics, Maulana Azad National Institute of Technology Bhopal, India

In order to provide experimental guidance, a theoretical study was performed on transparent conduction oxide (FTO)/TiO_2/ interface defect layer 1/$CH_3NH_3SnI_3$/interface defect layer 2/Cu_2O/ back contact solar cell. The simulation was performed under the illumination of 1000 W/m2, at 300 K and an air mass of AM 1.5G. The diffusion lengths of electron and hole were set to 260 nm and 560 nm in absorber layer, respectively. The set value is very near to recently observed experimental values. The device performance is severely influenced by the thickness of absorber layer, acceptor density, defect density and work function of various back contact electrode materials. Oxidation of Sn^{2+} into Sn^{4+} was considered and it is found that the reduction of acceptor concentration of absorber layer significantly improves the device performance. Further, optimizing the defect density (1014 cm^{-3}) of the perovskite absorber layer, encouraging results of the Jsc of 40.14 mA/cm2, Voc of 0.93 V, FF of 75.78% and PCE of 28.39% were achieved. This theoretical simulation provides an appropriate direction for devolving photovoltaic technology.

Comparison of interproximal reduction techniques and proximal strips: An atomic force microscopic and confocal microscopic study

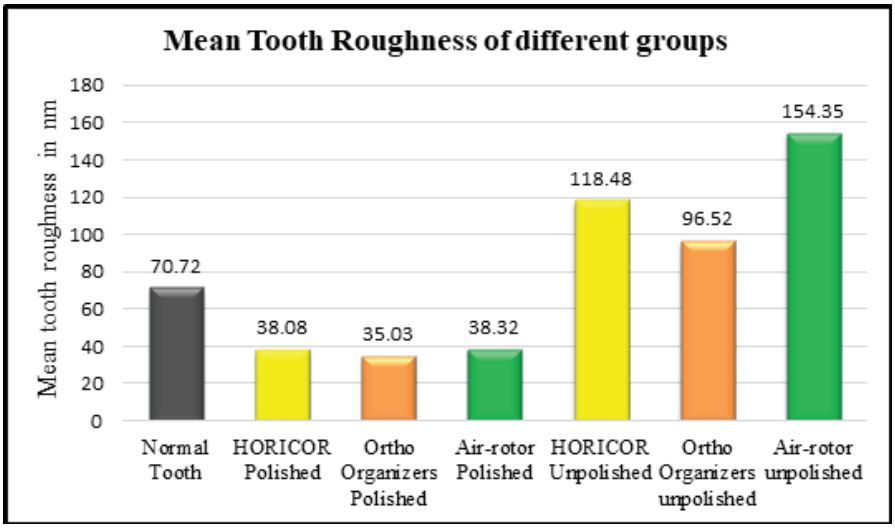
Pooja Harish[1] and **Karunakara B C**[2]

[1]*Yenepoya Dental College, Yenepoya (Deemed to be University), India*

[2]*KLE Society's Institute of Dental Sciences, Indi*

Introduction: An in vitro study was conducted to evaluate the surface roughness produced by two different methods: hand-held mechanical and air-rotor stripping and also by HORICOR and Ortho Organizer strips, before and after polishing with 3M Sof-Lex™ Finishing Strips under Atomic Force Microscope.

Methodology: Study included 44 proximal surfaces of extracted premolars divided into control group and three experimental groups with 12 surfaces in each. Hand held mechanical stripping was done by forty passages of 6cm long abrasive strips and Air-rotor stripping using high-speed air-rotor turbine hand piece. Polishing was done using 3M Sof-Lex™ finishing strips. Reduced teeth samples were viewed under AFM and the proximal strips under Confocal microscope for surface roughness.



Mean tooth roughness of different groups under atomic force microscope

Results: Air-rotor stripping produced more surface roughness compared to mechanical reduction technique (P = 0.009). There was no significant difference between the roughness produced by two different proximal strips. Tooth surface after IPR with polishing had less roughness compared to unpolished surface. There was no mean difference between the wear of proximal strips (Fig 1).

Conclusion: The mechanical reduction technique of interproximal surface produces less surface roughness compared to air-rotor stripping. Polishing with 3M Sof-Lex strips after reduction irrespective of the technique and material used gives smoother surface than even normal enamel.

Polyoxometalates: Innovative environmental technologies

Rami Al-Oweini

Kamal A. Shair Central Research Science Laboratory, Faculty of Arts and Sciences, American University of Beirut, Lebanon

The oxygen-evolving complex of photosystem II (PSII) in green-plants, where wateroxidation takes place, is the fundamental element of photosynthesis, where sunlight is transformed into renewable chemical energy. Prior studies led to the discovery of highly effective, molecular, homogenous catalytic systems of noble metals such as Ru or Ir. Nevertheless, their high cost, toxicity, and low abundance are unfavorable for using them as bulk water oxidation catalysts (WOCs).1,2 Hence, switching focus to environmentally benign, thermally stable, oxidatively robust, and redox-active Mn-substituted polyoxometalates (POMs) are of special interest, also due to the nature of the active center of PSII. Along these guidelines being inspired by nature with the principal aim to design new and efficient oxidation systems employing natural O2 as primary oxidant, a novel Mn-substituted POM was tested as artificial photosynthetic WOC [MnIII3MnIVO3(CH3COO)3(A-α-SiW9O34)]6- (Mn4POM), using the RuII(bpy)32+ (P) / Na2S2O8 sacrificial cycle,1,2 and was found to be active with higher turnover number and frequency than amorphous Mn-based oxides

Thermal analysis of the physicochemical properties of organic waste to application in the compost process

G. Aparicio and **N. Carmona**

Universidad Autónoma de Occidente, Colombia

The thermal and physicochemical characteristics of the husk of rice, pineapple, banana, potato, papaya, and lettuce were studiedto evaluate their effectiveness in a composting process as a harvesting alternative. Thermogravimetry (TGA) was used to assessthe thermal stability of the shells, mass spectrometry (MS) to identify volatile compounds, differential scanning calorimetry(DSC) to find the possible phase transitions caused by the increase of temperature, and elemental analysis to determine the C/Nratio. In the composting process, four mixtures were made through the quantitative balance of nitrogen, carbon, and humidity,and the process was controlled and monitored until the compost was obtained. The results in the TGA showed three characteristicstages present in organic materials that absorb heat: the dehydration of the samples in a temperature range between 25and 230 °C,the decomposition in a range of temperatures that occurred between 240 and 370 °C, and degradation in a temperature rangebetween 380 and 600 °C. DSC showed the endothermic processes were associated with melting followed by the evaporation ofthe aqueous content, and decomposition and a degradation of the samples associated with volatile contents. The exothermicprocesses were associated with the oxidation of the elements released during evaporation of the aqueous content, and theenthalpies of the processes varied between 5.90 and 91.60 J/g. Mass spectrometry identified that the volatile compounds releasedwere H2O, CO2,CO,CH4, and N. In the composting, the effective mixture was a 20% concentration of each of the biowastes thatdemonstrated better conditions for decomposition, where alkaline pH and acid indicated the decomposition of fatty acids,nitrogen, and carbon. Finally, it was concluded that the thermal stability of the shells is associated with the presence of lignin,cellulose, and hemicellulose. In addition, the compost obtained is a fertilizer applicable to soils and plants

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Teaching humanitarian engineering through environmental chemistry

R. Hanson[1] and **C. Hanson**[2]

[1]*University of Education, Ghana*

[2]*Kwame Nkrumah University of Science and Technology, Ghana*

The purpose of this paper is to describe a possible best practice to teaching environmental chemistry from a humanitarian engineering perspective using microchemistry equipment. The interest in teaching chemistry by focusing on humanitarian engineering arises from the economic and environmental concerns that the country of this study faces, some of which are poverty, climatic changes, food crisis, inadequate health care, water crisis and pollution. As an educator, there is an interest in educating future generations to be able to cope with environmental changes that face their countries and the world at large. This exposition of a possible new approach, with appropriate pedagogies that is presented here may be an answer that under-developed, developing and emergent economies may adopt to close the gap between themselves and other industrialised nations. A case of a study where a topic in an environmental study course is presented. The theoretical framework2 which supported the study in which 19 students were involved was constructivism1. Findings indicated that teaching humanitarianism and humanitarian engineering through chemistry education in an integrated manner through student-centred approaches3 had massive potential.

Prenatal diagnosis for a novel missense mutation in X-linked intellectual disability

Sangeeta Khatter, Ritika Bajaj, Nidhi Sharma, Sheetal Jindal and **Umesh Jindal**

Jindal IVF Sant Memorial Nursing Home, India

Intellectual disability (ID) is still unexplained in 60% of cases and prenatal diagnosis is very challenging for this condition. A second gravida presented to us at 6weeks of gestation for counselling. Her previous child had been diagnosed with intellectual disability and autism. A detailed family history showed that her brother also had intellectual disability. Screening investigations were normal for affected child. Exome sequencing report revealed variation of unknown significance (VOUS) on SIN3A gene and *UPF3B* gene. The variation in X linked *UPF3B* gene was reclassified as novel pathogenic variation after segregation studies with parents and affected maternal uncle for both the genes variations. An amniocentesis was done at 18 weeks gestation for the novel mutation in UPF3B gene and fetus was found unaffected. Patient delivered a healthy male child who is doing well at two years of age. To conclude, we should not disregard VOUS on exome sequencing. Identification of VOUS requires careful genotype phenotype correlation and segregation studies to counsel parents regarding risk of having another affected child

Pyran derivatives for the prevention of mild steel in acid medium: Experimental and computational studies

J. Saranya and K. Lavanya

Gokaraju Rangaraju Institute of Engineering and Technology, India

Natural products contain pyran moiety have interesting biological and pharmacological activities. The structural importance of the pyran class of organic molecules and the effectiveness of this kind of molecules as corrosion inhibitors have prompted their recognition by the chemistry network as privileged structures. This present article aimed to synthesize pyran derivatives namely ethyl 2-amino-4-(4-hydroxyphenyl)-6-(p-tolyl)-4H-pyran-3-carboxylate (HP), ethyl 2-amino-4-(4-methoxyphenyl)-6-(p-tolyl)-4H-pyran-3-carboxylate (MP) and ethyl 2-amino-4-(4-hydroxy-3,5-dimethoxyphenyl)-6-(p-tolyl)-4H-pyran-3-carboxylate (HDMP) and characterized by FTIR, NMR and Mass spectroscopy. Weight loss and electrochemical measurements were done to study the corrosion mitigation of mild steel (MS) in 1M sulphuric acid solution

Name of the Inhibitor	Maximum inhibition efficiency (%) (2 mM) at 303 K		
	Weight loss method	Polarization method	Impedance method
HP	91.6	88.1	89.7
MP	92.5	89.0	90.4
HDMP	95.0	92.2	93.8

Table: *Maximum inhibition efficiencies obtained at the optimum concentration (2 mM) in 1M H2SO4 at 303 K*

and their adsorption followed Langmuir isotherm. Polarization measurements showed the inhibitors act as mixed-type. Surface of the metal with and without inhibitors in acid medium was studied by SEM-EDS, XRD and AFM methods. Quantum chemical studies have been performed for the non-protonated and protonated forms of the inhibitors. The obtained results by MD simulations have revealed that the studied molecules bind onto iron area spontaneously with binding energies of 438.465 kJ/mol, 434.934 kJ/mol, and 456.854 kJ/mol for HP, MP and HDMP respectively.

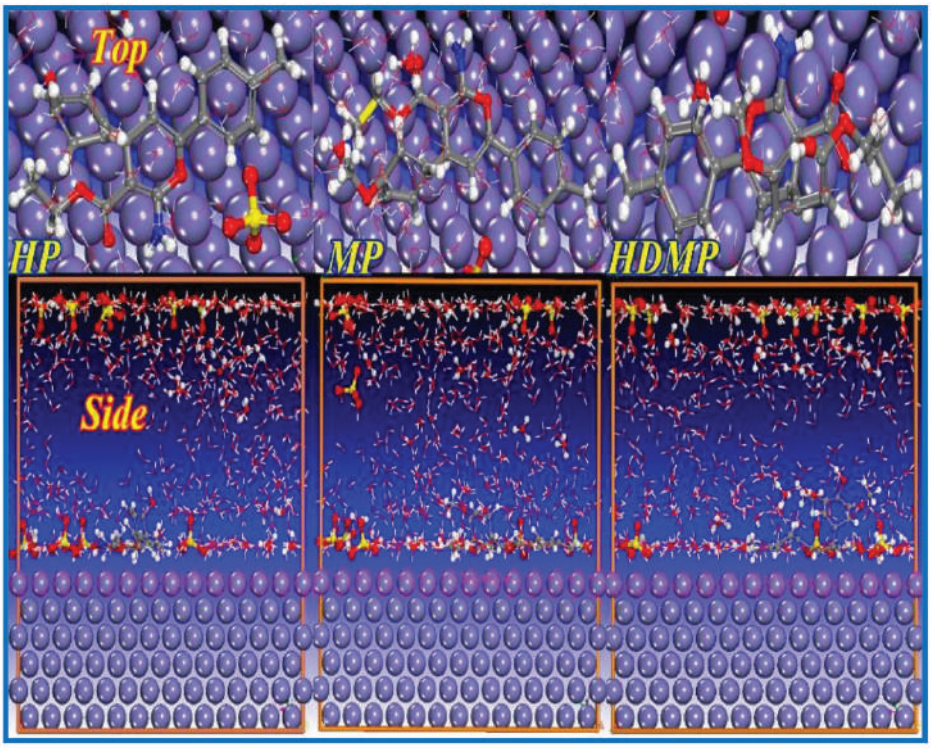

Figure: *Simulated stable adsorption configurations (side and top view) of HP, MP and HDMP molecules on the Fe (110) surface by MD simulations*

Sewage sludge amendment affects spinach yield, heavy metals bioaccumulation and soil pollution indexes

Satish Kumar Singh, Abhik Patra and **Adyasha Swain**

Department of Soil Science and Agricultural Chemistry, Institute of Agricultural Sciences, Banaras Hindu University, India

Use of sewage sludge (SS) in crop production is a feasible strategy for its disposal however, its application may pose an adverse impact on soil and human health. Therefore, identification of permissible level of SS is essential to prevent soil contamination. This research not only evaluated the impact of SS application on spinach (Spinacia oleracea L.) biomass yield but also tracked the accumulation of heavy metals in soil and plants. A pot experiment was conducted on Inceptisol with different levels of SS (0, 5, 10, 15, 20, 25, 30, 35, and 40 t ha-1) with recommended dose of fertilizers (RDF). Applications of SS at 20 t ha-1 resulted, the highest biomass yield however, the concentration of zinc (Zn) and cadmium (Cd) has exceeded the safe limit in leaves. Heavy metals accumulation in the plant was the highest in SS at 40 t ha-1. Spinach grown at 20 t ha-1 and higher dose of SS exceeded the safe limit of Zn and Cd concentration in leaves and translocation factor (TF) of lead (Pb) and Cd was found to be > 1. Hazard quotient (HQ) of Pb > 1 at higher doses of SS indicate health hazard if spinach is used for consumption. Assessment of health risk showed that, there was a possibility of Pb hazard at a high dose of SS (HI > 1). Evaluation of various soil pollution indexes revealed that the addition of SS enhanced the buildup of Cd and chromium (Cr) in soil. This study advocated the use of SS at 10 t ha-1 to sustain soil quality with no risk of food chain contamination.

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Development of green tire tread, by reducing carbon black with eco-friendly filler

Sohail Muhammad[1], Hamna Siddiqui[1], Usama Athar[1], Arsal Sohail[1], Asad Raza[1], Moiz Sarwar[2] and **Mudassir farooque[1]**

[1]Department of Materials Engineering, NED Unviersit of Engineering and Technology, Pakistan

[2]GTR Pakistan, Pakistan

Carbon black is traditionally used in tires as filler, but it possess a major challenge of CO2 emission during manufacturing stage. In the past few decades, the focus has been shifting on silica fillers to develop low rolling resistance tires resulting in low CO2 emissions contributing thus establishment of healthy eco system. In the present study Silica is used as a filler to reduce the amount of Carbon. Materials that can impact the wet traction, rolling resistance and dry traction of a silica filled compounds are studied by varying six different factors i.e SSBR Rubber, Silica, Carbon Black, Zinc Oxide, CBS and DPG in recipe. Use of eco-friendly filler, silica in compound reduced the carbon foot print of vehicle. One can observe here that Green tyres have RR very lower than conventional one, with low rolling resistance vehicle requires less force to move forward and hence less fuel will be consumed thus decreasing carbon dioxide emissions and ultimately its carbon footprint will also be decreased. The main hurdle for tire designers in green tyre manufacturing is to tradeoff between the dry traction and rolling resistance values, while here we can observe through our research that various compounds have DT values comparable with that of conventional tyres. Green tires have improved wet grip compared to conventional tires. Thus it will prevent the skidding of vehicle on wet surface hence increasing its safety

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Enhancing the crystallization phenomena and strength of porcelain stoneware: The role of CaO

T. Tchakouteu Mbakop[1,2,4], Juvenal G. Nemaleu Deutou[2,4], Likiby Boubakar[2], Ndigui Billong[2], U. Chinje Melo[1], Elie Kamseu[2,3] and **Vincenzo M. Sglavo[4]**

[1]Laboratory of Applied Inorganic Chemistry, Faculty of Science, University of Yaounde I, Cameroon

[2]Local Materials Promotion Authorithy, Cameroon

[3]Department of Engineering "Enzo Ferrari", Università di Modena e Reggio Emilia, Italy

[4]Department of Industrial Engineering, University of Trento, Italy

Limestone was used to modify the fluxing action of two potash feldspars (a pure potash feldspar and a sodo-potash feldspar) labelled P and C respectively in the formulation of porcelain stoneware based on Cameroonian raw materials. The effect of limestone addition (0 to 10 wt. %) was investigated in the range of sintering temperature between 1125 and 1300°C. Characterization of sintered samples including thermal behavior (DTA, TG and dilatometry test), phase evolution, densification parameters, flexural strength, morphology as well as pores structure were investigated in details. The maximum flexural strength (138 MPa) was obtained at 1175°C with P series (7 wt% addition of limestone) and at 1200°C (122 MPa) for C series. The maximum density (≈ 3.1g/cm3) and lower water absorption (≈ 0%) were obtained at 1200°C. Mullite and anorthite were identified as main crystalline phases. Starting from 1175°C and mostly at 1200°C, the two series compositions (with 7wt% addition) presented a self-glazing phenomenon which gave them significant brightness and high aesthetic quality; these properties were accomplished only at 1300°C for reference samples with no lime addition (P0 and C0). A proper addition of limestone (3 to 7wt. %) with potash feldspar, significantly reduced the sintering temperature (~150°C) and permits the production of high strength (122 – 138 MPa), low energy and sustainable porcelain stoneware.

A novel detection system for fragmented cytokeratin 18 using new antibodies

Minori Yamada[1], Koji Okuno[2], Koji Sakaguchi[1] and **Tetsuji Yamaguchi[3]**

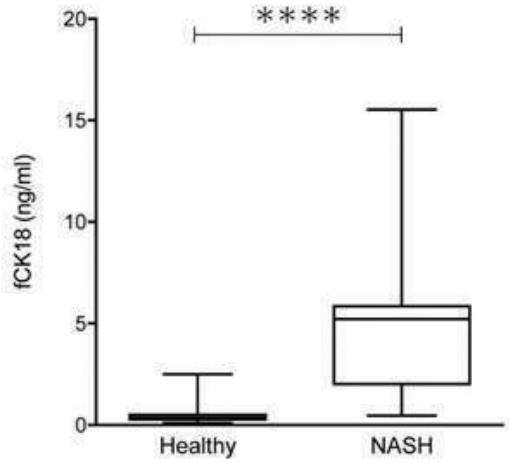
[1]Bio-Reagent Material Development, Bio-Diagnostic Reagent Technology Center, Sysmex Corporation, Japan

[2]Scientific Affairs, Sysmex Corporation, Japan

[3]Manufacturing Technology Development 2, Sysmex Corporation, Japan

Background: Fragmented cytokeratin 18 (fCK18) released from epithelial cells undergoing apoptosis is widely studied in various diseases. However, fCK18 measurement is not utilized in clinical practice due to imprecise disease-state cutoff values. Therefore, we generated new monoclonal antibodies (mAbs) and developed a highly sensitive chemiluminescent enzyme immunoassay (CLEIA).

Methods: Capture (K18-624) and detection (K18-328) mAbs were generated from mice immunized by either a synthetic peptide or a commercial recombinant protein. The mAb characterization was performed using immunoblotting, immunoprecipitation and reactivity with synthesized peptides. A recombinant fCK18 (rfCK18) produced in Escherichia coli was purified by affinity column chromatography. Analysis of performance and measurement of human fCK18 were evaluated



using K18-624 and K18-328 in a highly sensitive CLEIA.

Results: K18-624 had a high binding ability compared to the current commercial antibody. K18-328 recognized 323S-340G of CK18. A rfCK18 was expressed in the soluble fraction of E. coli when the N-terminal region (260 amino acid residues) of CK18 was truncated. Based on the fCK18 CLEIA performance, the coefficients of variation (CV) for within-run and between-day repeatability were below 10% and the recoveries were in the range of 15%. The detection sensitivity was 0.056 ng/mL. Serum fCK18 levels were significantly increased in NASH patients when compared to healthy individuals.

Conclusions: Our new fCK18 mAbs showed high affinity and sensitivity. CLEIA using our new antibodies will be useful in measuring fCK18 in human blood thereby generating accurate clinical diagnoses of human liver diseases.

Novel selectivity algorithm for metaloxide chemical sensor on volatile and hazardous gases in the air

V.Chistyakov[1], A.Sokolov[2] and **S. Soloviev[1]**

[1]Ioffe Institute, Russia

[2]OSTEK Enterprise Ltd, Russia

New algorithm is presented for selective identification such gases and vapors in the air as hydrogen, methane, propane, ethanol, acetone etc by use of ZnO and SnO2 based sensors doped with PdO and La2O3. The conductivity responses Δσ(μS) vs z=1000/T (K-1) from temperature modulation process are interpolated by following parameterized l discriminating functions

$$F_1(z)=\frac{A_1}{z^4+b_1z^3+c_1z^2},F_2(z)=zF_1(z),F_3(z)=\frac{A_3}{z^4+b_3z^3+c_3z^2+d_3z},F_4(z)=\frac{A_4}{z^4+b_4z^3+c_4z^2+d_4z+h_4},$$

$$F_5(z)=\frac{A_5}{b_5z^4+c_5z^3+d_5z^2+h_5z+1},F_6(z)=\frac{A_6}{b_6z^4+c_6z^3+d_6z+1}\ (1)\ -\ (6),$$

which parameters are estimated via nonlinear regression method. The dependences of the principal ones Ai(CY) on analyte Y concentration CY compose multivariate calibration portrait fitting to which an unknown analyte X is identified as the Y (e.g. ethanol in dry air— Fig). And the common abscissa of all intersection points of the level lines AiX and calibration curves Ai(CY) defines the analyte concentration in the units used (mg/m3, Fig). In case the abscissas are different or some of them are missing the analyte X is not Y. The method allows selective detection of broad list of analytes in synthesized dry and real wet air and even distinguishes the substances of the same homological group: methane/ propane/ hexane and ethanol/methanol/isopropyl alcohol. Actually, the method is breakthrough in solving the very important problem among 3S-problems:selectivity, stability, sensitivity.

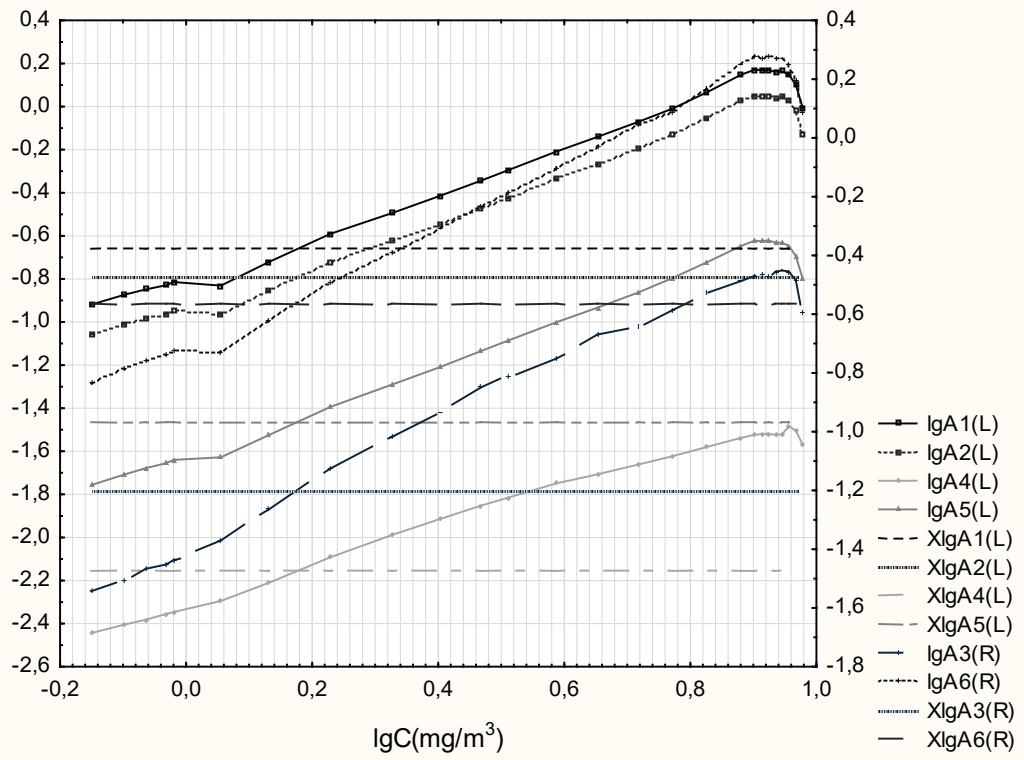


Figure. *1.5 mg/m3 absolutized ethanol is identified as ethanol due to Multivariate Gauge C2H5OH on SnO2. All abscissas of intersection points are visually equal.*

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On the charge instability and the metastable equilibrium state of a conducting droplet during liquid electrospraying

Yu. V. Samukhina[1], D. D. Matyushin[1], P. A. Polyakov[2] and **A. K. Buryak[1]**

[1]Frumkin Institute of Physical Chemistry and Electrochemistry, Russian Academy of Sciences, Russia

[2]Moscow State University, Russia

It is known that highly charged droplets formed in the course of electrospraying disintegrate into a number of smaller droplets. The criteria for the instability and disintegration of conducting liquid droplets in the course of electrospraying have been considered in this study. The development of charge instability may lead to the formation of droplets with a complex nontrivial shape. Some forms of the perturbation of a spherical liquid droplet have been shown for the case when the Rayleigh stability criterion is exceeded. The energy of droplets having complex shapes has been studied. The calculations were performed within the Wolfram Mathematica package using the numerical integration and iteration methods. The study of the development of the charge instability has given a new result: it has been shown that a quasi-stable state may exist during the disintegration of a liquid droplet at Rayleigh parameter values exceeding the critical one. A new nonspherical droplet shape has been found, for which the disintegration process is very slow, and the magnitude of the change in the energy is almost equal to zero.

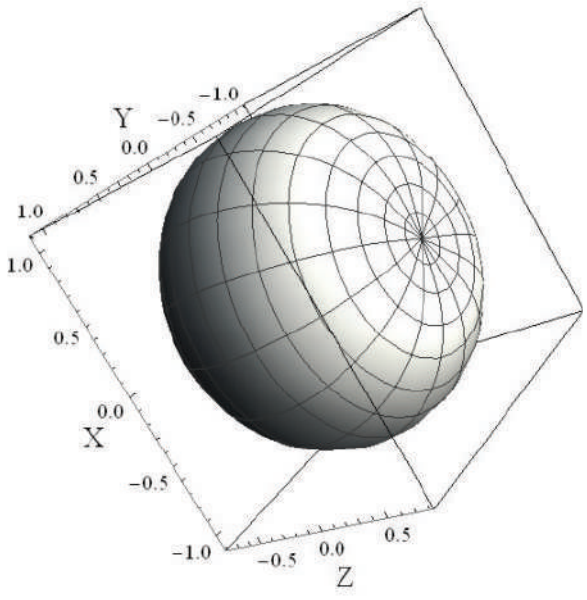

Fig. 1. *The shape of a perturbed spherical droplet occurring in a quasi-stable state*

Nanofluids, thermophysical properties and heat transfer

Zafar Said

Dept. of Sustainable and Renewable Energy Engineering, University of Sharjah, UAE

Research studies about nanofluids are on the rise owing to the mounting interest and demand for nanofluids as heat transfer fluids in a wide variety of applications in recent years. The stability of nanofluids is one key challenge hindering the widespread practical application of nanofluids. Studies showed that stability depend on pH, sonication time, different types of shapes, and sizes of nanoparticles with different base fluids, nanofluid preparation methods, volume fractions, and surfactants as well as functionalizing.

The incorporation of nanoparticles in the base fluid leads to change in the thermophysical properties such as thermal conductivity, viscosity, and specific heat that affect the convective heat transfer. Several factors affecting the thermophysical properties; including types of nanoparticles, solid volume fraction, different base fluid, stability, temperature, particle size, shape, pH, sonication, and surfactants. There are many contradictory results found in the literature on the influence of effective parameters on thermophysical properties. It has been observed that the thermophysical properties are affected by the mentioned parameters.

The recent development in this field indicates that the application of nanofluid in this thermal system showed promising performance. Proper characterization of nanofluids (with hybrid nanofluids as well recently) results in more efficient heat transfer fluids compared to single nanoparticle-based nanofluid. However, more intense research is needed towards the selection of proper hybrid nanoparticles, their preparation, characterization, and long-term stability to exploit their full potential. Finally, various application areas of nanofluids, such as transportation, electronic cooling, energy storage, mechanical applications, solar energy etc. are discussed.

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Novel approaches to circumvent devastating effects of pest on sugarcane

Zahida Qamar[1], Idrees Ahmad Nasir[1], Mounir G Abouhaidar[2], Kathleen L Hefferon[3], Abdul Qayyum Rao[1], Ayesha Latif[1], Qurban Ali[5], Saima Anwar[4], Bushra Rashid[1] and **Ahmad Ali Shahid[1]**

[1]Centre of Excellence in Molecular Biology, University of the Punjab Lahore, Pakistan

[2]Department of Cell and Systems Biology, University of Toronto, Canada

[3]Department of Microbiology, Cornell University Ithaca, USA

[4]Pakistan Biomedical Engineering Centre University of Engineering and Technology, Pakistan

[5]Institute of Molecular Biology and Biotechnology, The University of Lahore, Pakistan

Sugarcane (Saccharum officinarum L.) is a cash crop grown commercially for its higher amounts of sucrose, stored within the mature internodes of the stem. Quality and yield of sugarcane production is always threatened by the damages of cane borers and weeds. In current study two problems were better addressed through the genetic modification of sugarcane for provision of resistance against insects and weedicide via the expression of two modified cane borer resistant CEMB-Cry1Ac (1.8kb), CEMB-Cry2A (1.9kb) and one glyphosate tolerant CEMB-GTGene (1.4kb) genes, driven by maize Ubiquitin Promoter and nos terminator. Insect Bio-toxicity assays were carried out for the assessment of Cry proteins through mortality percent of shoot borer Chilo infuscatellus at 2nd instar larvae stage. During V0, V1 and V2 generations young leaves from the transgenic sugarcane plants were collected at plant age of 20, 40, 60, 80 days and fed to the Chilo infuscatellus larvae. Up to 100% mortality of Chilo infuscatellus from 80 days old transgenic plants of V2 generation indicated that these transgenic plants were highly resistant against shoot borer and the gene expression level is sufficient to provide complete resistance against target pests. Glyphosate spray assay was carried out for complete removal of weeds. In V1-generation, 70-76% transgenic sugarcane plants were found tolerant against glyphosate spray (3000mL/ha) under field conditions. While in V2-generation, the replicates of five selected lines 4L/2, 5L/5, 6L/5, L8/4, and L9/6 were found 100% tolerant against 3000mL/ha glyphosate spray. It is evident from current study that CEMB-GTGene, CEMB-Cry1Ac and CEMB-Cry2A genes expression in sugarcane variety CPF-246 showed an efficient resistance against cane borers (Chilo infuscatellus) and was also highly tolerant against glyphosate spray. The selected transgenic sugarcane lines showed sustainable resistance against cane borer and glyphosate spray can be further exploited at farmer's field level after fulfilling the biosafety requirements to boost the sugarcane production in the country.

A functional dromedary UF-yogurt co-fermentation with carob powder or autochthonous strains

JRAD Zeineb[1], OUSSAEIF Olfa[1] and **EL-HATMI Halima[2]**

[1]*Arid Land Institute, University of Gabes, Tunisia*

[2]*Higher Institute of Applied Biology, University of Gabes, Tunisia*

Co-fermentation process is a potential tool to improve benefits of fruit and lactic acid bacteria to human health, beyond their technological functions. This study was conducted to compare the properties of dromedary bio-yogurt obtained by co-fermentation process with plant (carob powder) or autochthonous bacteria (Enterococcus faecium and Streptococcus macedonicus). For this reason, the total solids required for yogurt preparation were obtained by ultrafiltration (UF). Carob powder or autochthonous bacteria were incorporated at the level of 2% in UF milk. Then mixtures were fermented using conventional microorganisms for yogurt and obtained products named respectively CFC (yogurt with carob) and CFS CFS (yogurt with autochthonous strains). During the storage period, CFC and CFS maintained Streptococcus at appropriate levels (> 8 log CFU/g). Moreover, CFC showed the lowest syneresis, highest textural properties and oleic acid (C18:1n9; 26.315%). However, CFS yogurt resulted in higher aroma compounds formation than CFC and control (without co-fermentation). The principal component analysis (PCA) applied to the aroma compounds allowed the CFC to be differentiated to CFS and control on the one hand, and the CFC correlated with 4 volatile compounds where isobornyl propionate was the major, on the other hand. Although both control and CFS exhibited DPPH• inhibition, because of protein proteolysis during fermentation, significant increased radical scavenging activity was found in CFC samples. Meanwhile, the yogurt co-fermentation with carob powder displayed enhanced both the antioxidant and textural properties, which indicated that it has the potential value to be utilized as a novel functional food

Synthesis, characterization, and cytotoxic evaluation of new Triazole derivatives of Osthol

Zubaid-ul Khazir Rather and **Javid Ah. Banday**

National Institute of Technology, India

Osthol [7-methoxy-8-(3-methylbut-2-en-1-yl) chromen-2-one] isolated from Prangos pabularia was used as a starting material for the synthesis of its various derivatives via modifications of the lactone ring. The resulting compounds were fully characterized by spectral techniques and evaluated for their anticancer activity against Hep-G2 (human hepatoma), HeLa (cervical carcinoma), U-87 (brain cancer) and MCF-7 (breast cancer) cell lines using MTT assay. All synthesized derivatives exhibited higher activity than that of osthol. Among this series, 4-bromophenyl, 3-hydroxyphenyl, and p-tolyl derivatives showed excellent cytotoxic activity against U-87 and MCF-7 cancer cell lines with IC50 values of 6–7.3 μM.

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A survey on diagnosing neurodegenerative diseases

K.P.Sanal Kumar[1] and **S.Anu H Nair**[2]

[1]*PG Department of Computer Science, R.V Government Arts College, India*

[2]*Department of CSE, Annamalai University, India*

Neurodegenerative disorders are termed as diversified group of disorders which comes under characterization of progressive degeneration in functioning of nervous system. Alzheimer and Parkinson's disease comes under neurodegenerative disorder. Recent studies have identified that it is caused due to the mechanisms of cellular and molecular functions based on the aggregation of protein. The disease is basically diagnosed pathologically. Autopsy has become essential for diagnosing the disorder. Advanced research on this particular field has led to perspective that pathological changes can be made in the brain without an autopsy. The changes are reflected through molecular brain imaging techniques. The study focuses on various functional and cognitive assessment that has been followed until recent times in the field of medical image processing. Recent methodologies in diagnosing through molecular image techniques without an autopsy is a successive progress in the field of medical research. The challenges in functional and cognitive assessment perspective of the disorder is also focused. The complications include difficulties in memory. This survey provides an insight for future research direction in medical image processing.

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Membrane interactions of Ocellatins. Where do antimicrobial gaps stem from?

José Muñoz-López[1,2], Jade C. L. Oliveira[1], Daniel A. G. R. Michel[3], Carolina S. Ferreira[3], Francisco Gomes Neto[4], Evgeniy S. Salnikov[2], Rodrigo M. Verly[3], Burkhard Bechinger[2,5] and **Jarbas M. Resende[1]**

[1]Departamento de Química, Instituto de Ciências Exatas, Universidade Federal de Minas Gerais, Brazil

[2]Université de Strasbourg / CNRS, Institut de Chimie, France

[3]Departamento de Química, Universidade Federal dos Vales do Jequitinhonha e Mucuri, Brazil

[4]Laboratório de Toxinologia, Instituto Oswaldo Cruz, Fundação Oswaldo Cruz, Brazil.

[5]Institut Universitaire de France, France

The antimicrobial peptides Ocellatin-LB1, -LB2 and -F1, isolated from frogs, are identical from residue 1 to 22, which correspond to the -LB1 sequence, whereas -LB2 carries an extra N and -F1 additional NKL residues at their C-termini. Despite the similar sequences, previous investigations showed different spectra of activities and biophysical investigations indicated a direct correlation between both membrane-disruptive properties and activities, i.e., ocellatin-F1 > ocellatin-LB1 > ocellatin-LB2. This study presents experimental evidence as well as results from theoretical studies that contribute to a deeper understanding on how these peptides exert their antimicrobial activities and how small differences in the amino acid composition and their secondary structure can be correlated to these activity gaps. Solid-state NMR experiments allied to the simulation of anisotropic NMR parameters allowed the determination of the membrane topologies of these ocellatins. Interestingly, the extra Asn residue at the Ocellatin-LB2 C-terminus results in increased topological flexibility, which is mainly related to wobbling of the helix main axis as noticed by molecular dynamics simulations. Binding kinetics and thermodynamics of the interactions have also been assessed by Surface Plasmon Resonance and Isothermal Titration Calorimetry. Therefore, these investigations allowed to understand in atomic detail the relationships between peptide structure and membrane topology, which are in tune within the series -F1>> -LB1 ≥ -LB2, as well as how peptide dynamics can affect membrane topology, insertion, and binding.

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