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**Virtual Event**

**4<sup>TH</sup> EDITION OF**  
**ADVANCED**  
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**WORLD**  
**CONGRESS**

**MARCH 28**  
**2023**

**ADV. CHEMISTRY 2023**

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# **YOUR FIRST CHOICE FOR RESEARCH INGENUITY**

**PROGRAM-AT-A-GLANCE**

**ADV. CHEMISTRY  
2023**

# Scientific Program

GMT-Greenwich Mean Time

07:45-08:00 Opening Ceremony

## Distinguished Speaker Talks

**Sessions:** Analytical Chemistry | Agricultural Chemistry | Biochemistry | Chemistry of Transition Elements | Chemical Engineering | Electrochemistry | Environmental Chemistry | Food Chemistry | Forensic Chemistry | Geochemistry | Green Chemistry | Industrial Chemistry | Inorganic Chemistry | Materials Science | Medicinal Chemistry | Metallurgy | Molecular biology | Natural Product | Neurochemistry | Organic Chemistry | Petrochemistry | Physical Chemistry | Polymer Chemistry

08:00-08:20 **Title: Ethics on the soil: She is a living substance**  
Katsuyuki Minami, *Kitasato University, Japan*

08:20-08:40 **Title: Magnesium production in China and the process optimization**  
Daxue Fu, *Northeastern University, China*

08:40-09:00 **Title: Novel therapeutic potential of the anti-cancer drug BIBR1532 in ischemic stroke**  
Chi Kwan Tsang, *The First Affiliated Hospital of Jinan University, China*

09:00-09:20 **Title: Recent advances of magnetic gold hybrids and nanocomposites, and their potential biological applications**  
Mirza Muhammad Faran Ashraf Baig, *The Hong Kong University of Science and Technology, China*

09:20-09:40 **Title: Free of cost energy conservation through behavioural training: An Indian perspective**  
Ali Shaikh Shamsar, *Energy Conservation Project Management, India*

09:40-10:00	<p><b>Title: Autoclave and pulsed low frequency ultrasound cavitation based thermal activation of persulfate for regeneration of hydrogen titanate nanotubes as recyclable dye adsorbent</b></p> <p><b>Satyajit Shukla</b>, <i>CSIR-National Institute for Interdisciplinary Science and Technology (NIIST), India</i></p>
10:00-10:20	<p><b>Title: Anticancer potency of N(4)-ring incorporated-5-methoxyisatin thiosemicarbazones</b></p> <p><b>Paras Nath Yadav</b>, <i>Tribhuvan University, Nepal</i></p>
10:20-10:40	<p><b>Title: Simulations of liquid chromatography using two-dimensional non-equilibrium lumped kinetic model with Bi-Langmuir Isotherm</b></p> <p><b>Sadia Perveen Ahsan</b>, <i>Air University, Pakistan</i></p>
10:40-11:00	<p><b>Title: Electrochemical sensing by novel copper oxide nanostructures</b></p> <p><b>Rupali Nagar</b>, <i>Symbiosis Institute of Technology, India</i></p>
11:00-11:20	<p><b>Title: Safety culture in Sri Lankan industrial chemical laboratories</b></p> <p><b>Udaya K Jayasundara</b>, <i>Institute of Chemistry Ceylon, Sri Lanka</i></p>
<b>Refreshment Break 11:20-11:30</b>	
11:30-11:50	<p><b>Title: Soft X-ray emission in plasma focus device</b></p> <p><b>Hadi Barati</b>, <i>Amirkabir University of Technology, Iran</i></p>
11:50-12:10	<p><b>Title: A new ant algorithmic approach for solving PFSP</b></p> <p><b>Shahriar Farahmand Rad</b>, <i>Payame Noor University, Iran</i></p>
12:10-12:30	<p><b>Title: Application of nanotechnology to monitor agricultural parameters that promote health and nutritional crop growth in order to provide sustainable economic growth in Aatma Nirbhar Bharat</b></p> <p><b>Sumanta Bhattacharya</b>, <i>Maulana Abul Kalam Azad University of Technology, India</i></p>

12:30-12:50	<p><b>Title: Absorption spectra of dissolved oxygen molecules in aerated solvents. A review of laser activation experiments</b>  <b>Alexander Krasnovsky Jr.</b>, <i>Federal Center of Biotechnology Russian Academy of Science, Russian Federation</i></p>
12:50-13:10	<p><b>Title: Locus of chemical reactions domains in the freely falling drop impact flow</b>  <b>Yuli D. Chashechkin</b>, <i>Ishlinsky Institute for Problems in Mechanics RAS, Russia</i></p>
<p><b>Lunch Break 13:10-13:40</b></p>	
13:40-14:00	<p><b>Title: The relationship between the efficiency of energy conversion, fertility and the presence of branched ears as indicators for the determination of the optimal dosage for disease resistance mutation breeding when gamma irradiation is applied to kernels of <i>Triticum aestivum</i> L.</b>  <b>Eben von Well</b>, <i>ARC-Small Grain Institute, South Africa</i></p>
14:00-14:20	<p><b>Title: Spectroscopic features of NH-tautomers of the free base corroles</b>  <b>Yousef H. Ajeeb</b>, <i>Modern University for Business and Science, Lebanon</i></p>
14:20-14:40	<p><b>Title: High-temperature hydrogen attack on 2.25Cr-1Mo Steel: The roles of residual carbon, initial microstructure and carbide stability</b>  <b>Mohammed Alshahrani</b>, <i>Saudi Aramco Research and Development Centre, Saudi Arabia</i></p>
14:40-15:00	<p><b>Title: Economic performance of certified cocoa-based agro-forestry systems in Cameroon</b>  <b>Ngoucheme Rene</b>, <i>Institute of Agricultural Research for Development (IRAD), Cameroon</i></p>
15:00-15:20	<p><b>Title: Carbon and nutrient cycling in tree plantations vs. natural forests: Implication for an efficient cocoa agroforestry system in West Africa</b>  <b>Michel K. Yao</b>, <i>Université Nangui Abrogoua, Côte d'Ivoire</i></p>
15:20-15:40	<p><b>Title: Phosphogypsum as secondary resource in the circular economy</b>  <b>Katarzyna Kiegiel</b>, <i>Institute of Nuclear Chemistry and Technology, Poland</i></p>

15:40-16:00

**Title: Tunable polycationic organohalloysite electrocatalyst**

**Francis Merlin Melatagua Tchieno**, *Leibniz Institute for Solid State and Materials Research (IFW Dresden), Germany*

**Refreshment Break 16:00-16:10**

16:10-16:30

**Title: Optimization of essential oils yield extracted from *Curcuma longa* residue through solid state fermentation**

**Sylvie Nguikwie Kwanga**, *University of Douala, Cameroon*

16:30-16:50

**Title: Improved surface morphology and corrosion resistance performance of 2205 duplex stainless steel by low temperature gas nitriding**

**Nsikan Etim Dan**, *Federal University of Technology Owerri, Nigeria*

16:50-17:10

**Title: Healthy humans can be a source of antibodies countering COVID-19**

**Antonietta M. (Mietta) Lillo**, *Los Alamos National Laboratory, USA*

17:10-17:30

**Title: Peukert generalized equations with due consideration of internal resistance of automotive-grade lithium-ion batteries for their capacity evaluation**

**Nataliya Nikolaevna Yazvinskaya**, *Don State Technical University, Russia*

17:30-17:50

**Title: Quantum-classical mechanics: Principles, applications and prospects**

**Vladimir V. Egorov**, *FSRC Crystallography and Photonics, Russia*

17:50-18:00

**Title: Quantification of kinetic rate constants of oxygen reduction reaction pathways over Pt-free electrocatalysts and its application in Tafel slope evaluation**

**Yun Wu**, *Guangdong University of Petrochemical Technology, China*

18:00-18:10

**Title: Mercury prediction in groundwater of Naameh Landfill (Lebanon) using an Artificial Neural Network (ANN) model**

**Farah Kanj**, *Lebanese University, Lebanon*

**Panel Discussions**

**Closing Remarks**





*SCIENTIFIC  
ABSTRACTS*

**DAY 2**

VIRTUAL EVENT

**4<sup>th</sup> Edition of**

Advanced  
Chemistry  
World  
Congress

March 28, 2023

ADV. CHEMISTRY 2023



## Ethics on the soil: She is a living substance

**Katsuyuki Minami**

*Kitasato University, Japan*

The time has come to promote a new paradigm for promoting the concept that soil is alive and an object of ethics. A long time has passed since an abnormality occurred in the soil where living things have born and grown from old times to now, and into the future.

This soil change is largely due to the activities of the anthroposphere since the Industrial Revolution. The population pressure of 8 billion has been a great influence on not only the pedosphere but also geosphere, biosphere, hydrosphere, troposphere, and stratosphere, especially the collapse of soil, global warming, and biodiversity.

Soil is also closely connected to not only agricultural production but also the culture and civilization of an ethnic group living in each place, including their religion, thoughts, and others. Today, it is very important for people to protect the soil, their agriculture, and the environment because the collapse of soil leads to the collapse

of human culture, civilization, and livelihood.

In order to feed the increasing population, agriculture has been forced to overcome the limit of environmental capacity of the soil. Only the input of material and energy influenced the crop production. Soil has come to be treated as a mere medium for production. As a result, environmental problems such as soil erosion, salinization, desertification, and soil pollution have occurred. In addition, environmental changes in the pedosphere have had a great impact on the other spheres.

However, soil is a living substance. If we do not have soil ethics, just as we have for humans, there is no future for humanity. In order to restore soil ethics, it is necessary to recognize that soil is alive like organisms. For that purpose, I will try to utilize Living Systems Theory (LST) as proof to demonstrate that the soil is alive. Then we will have ethics on our soil.

### Biography

Education and Employment 1971: Ph.D. (Agriculture); Tohoku University, Sendai, Japan, 1971: The Ministry of Agriculture, Forestry and Fisheries, Japan, Nat. Inst. of Agri. Sci., 1977-78: Visiting Prof., Iowa State University, 2000: DG., Nat. Inst. for Agro-Environmental Sciences, 2005: Prof. Kitasato University, 2006: Vice President, Kitasato University, 2012: Emeritus Prof. Kirasato University, Principal, Agri. Collage of Inst. for Agri. Health, and the Environ., 2020: Retirement

Awards and Honors 1990: Award of Japanese Society of Soil Science and Plant Nutrition, 1991: Director Award of Agency of the Environment, Japan, 1995: Special Award of Nikkei Global Environment Award, Japan, 1996: Japan Prize of Agricultural Science and Award of Yomiuri Agricultural Science, 1998: The First Yuan T. Lee Award, International Union of Air Pollution Prevention and Environmental Protection Associations (IUAPPA) , 2008: Appreciation letter from IPCC for 2007 Nobel Peace Prize, 2015: Award of Nippon Agricultural Research Institute, 2019: The Order of the Sacred Treasure, Gold Rays with Neck Ribbon, Japan





## Magnesium production in China and the process optimization

**D.X. Fu and N.X. Feng**

*Northeastern University, China*


In this work, current situation of Mg production in China is reviewed firstly. Then, our works on improvement of Mg production are introduced. Pidgeon process as one of the silicothermic processes is the main method for Mg production. China has produced over 80% of the global production since 2010. The process requires high energy input and discharges a large amount of CO<sub>2</sub> gases, despite significant process development that reduced the energy consumption and CO<sub>2</sub> emission, such as automatic control and regenerative combustion. Three problems encountered in the process: low heat transfer efficiency, slow chemical reaction rate, and semi-continuous production. For low heat transfer efficiency, the authors studied the effects of some factors, such as pellet size,

charge type, reduction temperature on temperature distribution and reduction ratio distribution in the bed by numerical methods. The results show that the pellet with 22.3mm diameter obtain the maximum reduction ratio; the reduction temperature should be increased as much as possible in the production process. The closer to the central area of the bed, the lower the temperature is, and the lower the reduction ratio is. The method by making an empty central region can effectively shorten the reduction cycle and improve the utilization ratio of raw materials. The optimal size of the empty central region is less than 27mm diameter based on Mg yield per unit volume and unit time by taking operation time and reduction time into consideration.

### Biography

Dr.Fu (1986-), Ph.D, associate professor. He mainly focuses on the silicothermic and aluminothermic processes. He has studied the process since his doctoral study. During his doctoral study, Dr. Fu took part in the projects "Key industrial project of Liaoning Province: study on advanced magnesium production technology". After taking the job (2013-present), Dr. Fu is in charge of the project supported by National Natural Science Foundation of China: "study on CaSi<sub>2</sub> formation in calcinations process of pre-prepared pellet and strengthened reduction mechanism of magnesia". He also took part in a key project of Natural Science Foundation of China: "Basic research on magnesium production by continuous thermal reduction in relative vacuum".

2. Dr. Feng(1944-), Ph.D, professor. He focuses on the silicothermic and aluminothermic processes. He proposed a novel internal heating silicothermic process. He is in charge of the projects "Key industrial project of Liaoning Province: study on advanced magnesium production technology".



## Novel therapeutic potential of the anti-cancer drug **BIBR1532** in ischemic stroke

**C.K. Tsang<sup>1</sup>, Guangpu Su<sup>1,2</sup>, Siwei Luo<sup>1,2</sup> and Xuemin Xie<sup>1,2</sup>**

<sup>1</sup>*Clinical Neuroscience Institute, The First Affiliated Hospital of Jinan University, China*

<sup>2</sup>*Department of Neurology, The First Clinical Medical School of Jinan University, China*

**T**elomerase reverse transcriptase (TERT) plays a crucial role in maintaining telomeric DNA integrity as well as non-telomeric functions. It is also a major target in cancer therapeutics as demonstrated by using the specific TERT inhibitor BIBR1532. However, its role in the neuronal cells remains unclear. Our previous transcriptomics study has implied that TERT is associated with ischemic preconditioning (IPC)-mediated tolerance. In this study, we used the oxygen-glucose deprivation (OGD)-induced ischemic stroke model to demonstrate that BIBR1532 conferred ischemic tolerance in neurons. We further used the Cleavage-Under-Targets-And-Tagmentation approach, a recently developed method with superior signal-to-noise ratio, to comprehensively map the genomic binding sites of TERT in primary neurons, and showed that more than 50% of TERT-binding sites were located at the promoter regions. Mechanistically, we demonstrated that under normal conditions TERT physically bound to many previously unknown genomic loci in neurons, whereas BIBR1532 preconditioning significantly altered TERT-chromatin binding profile. Intriguingly, we found that BIBR1532-

preconditioned neurons showed significant up-regulation of promoter binding of TERT to the mitochondrial anti-oxidant genes, which were correlated with their elevated expression. Functional analysis further indicated that BIBR1532-preconditioning significantly reduced ROS levels and enhanced tolerance to severe ischemia-induced mitochondrial oxidative stress in neurons in a TERT-dependent manner. Therefore, we found that TERT plays a previously unknown direct transcription regulatory role in neurons. We further discover that BIBR1532 exhibits promising potential to be a novel pharmacological preconditioning drug for protecting neuronal cells against subsequent ischemic stroke. Being a lead compound among TERT inhibitors, BIBR1532 has been extensively studied as an anti-cancer drug candidate. Its effect on neuron has not been fully characterized. Thus, our findings reveal the translational potential of BIBR1532 and may open a new avenue for the development of therapeutic strategies for preventing ischemic injury resulted from stroke and other neurological disorders.

## Biography

Dr. Chi Kwan Tsang obtained his Bachelor and Master degrees in Biology from the Hong Kong University of Science and Technology, and Ph.D. in Applied Biochemistry and Neuropharmacology from Kagoshima University. After graduation, he went on to have his postdoctoral training in the School of Medicine at Washington University in St. Louis. In 2004, Dr. Tsang was appointed as the Research Teaching Specialist in the University of Medicine and Dentistry of New Jersey. In 2009, he joined the faculty in the Department of Pharmacology at Rutgers University. In 2016, Dr. Tsang was recruited as a full professor in the Clinical Neuroscience Institute of Jinan University. His research interests focus on neurochemistry and stroke treatment. By far, Dr. Tsang has published over 40 original articles in journals including Nature, Molecular Cell, Circulation Research, Nature Communications, Molecular Therapy and EMBO Journal.



## Recent advances of magnetic gold hybrids and nanocomposites, and their potential biological applications

**Mirza Muhammad Faran Ashraf Baig**

*The Hong Kong University of Science and Technology, China*

**M**agnetic gold nanoparticles (mGNP) have become a great interest of research for nanomaterial scientists because of their significant magnetic and plasmonic properties applicable in biomedical applications. Various synthetic approaches and surface modification techniques have been used for mGNP including the most common being the coprecipitation, thermal decomposition, and microemulsion methods in addition to the Brust Schiffrin technique, which involves the reduction of metal precursors in a two-phase system (water and toluene) in the presence of alkanethiol.

The hybrid magnetic–plasmonic nanoparticles based on iron core and gold shell are being considered as potential theragnostic agents. Herein, in addition to future works, we will discuss recent developments for synthesis and surface modification of mGNP with their applications in modern biomedical science such as drug and gene delivery, bioimaging, biosensing, and neuro-regenerative disorders. I shall also discuss the techniques based on my research related to the biological applications of mGNP.

### Biography

My research work mainly focuses on the construction and function of DNA nanomachines, which are cutting-edge and challenging topics. I designed and constructed unique DNA motifs using a short circular DNA nanotechnology technique and functionalized these probes with fluorophores, gold nanoparticles, small molecular drugs, and peptide ligands. To achieve plasmon resonance effects, I achieved nano-specific precision in organizing plasmonic nanoparticles on the nano DNA frameworks. My work on the DNA nanomachines provided an efficient fluorescence resonance energy transfer mechanism that realizes the bio-imaging, detection of biological events, and functions of the biomolecules. I have also been working on multilayered hybrid magnetic nanoparticles for applications in nanomedicine for the last three years.



## Free of cost energy conservation through behavioural training: An Indian perspective

**Ali Shaikh Shamsar**

*Energy Conservation Project Management, India*

**I**mpact of an effective Transfer of Training in many applications is a proven fact but strongly recommended by previous studies on energy conservation due to a dearth of literature on this application. Energy conservation measures use less energy to reduce operating costs and the environmental impact without compromising the consumer's operational output. No-Cost or Low-cost energy conservation measures play a significant role in energy saving leading to the reduction in operational cost. This study was undertaken in the Indian context for commercial buildings application to establish the fact that there will not be any slip between an intention to conserve energy after the training and an actual application of the learning much after the training. If the Transfer of Training actually happens for Energy Conservation by influencing human behaviour through a tailor-made energy conservation training program, then the outcome will always be positive.

The study compares two different facilities using air-conditioning applications to study

the impacts of low-cost energy conservation measures (LCECM) in real-time operations. The effect was recorded at both facilities by lowering the air-conditioning running time and increasing its set temperature ensuring that there was no compromise in occupants' comfort level. Measured data was analyzed as per international performance measurement and verification (IPMV) Protocol A using pre- and post-training readings. IPMVP output was analyzed further by running a t-Test in the SPSS software and compared with the result of same t-Test of the feedback from the participants after the training. Results indicated energy conservation with a cumulative impact on carbon footprint, environment, and cost of importing fossil fuel. Thus, the Transfer of Training and the intention to apply the learning from the training at a later time were proven by scientific analysis of the feedback collected from the participants after the training as stated above. The actual application of the learnings on energy usage was measured at two different facilities in air-conditioning application for 90 working days each.

### Biography

Senior techno-commercial professional having 40 years of hands-on varied experience with international exposure in business leadership, project management, stakeholder management, operations and maintenance, manufacturing, energy conservation, concept selling, marketing, training, and team building. Certified Professional Engineer (2000, UK), Certified Energy Manager (2005, Govt. of India), Certified Energy Auditor (2008, Govt. of India), Certified Project Manager (2012, PMI), BE in Electrical Engineering (1982), MBA in Operations Management (1987) and PhD in Energy Management (2020).

## Autoclave and pulsed low frequency ultrasound cavitation based thermal activation of persulfate for regeneration of hydrogen titanate nanotubes as recyclable dye adsorbent

**Satyajit Shukla**

*CSIR-National Institute for Interdisciplinary Science and Technology (NIIST), Council of Scientific and Industrial Research (CSIR), India*

In the dye removal application, the regeneration of hydrogen titanate (HTN,  $\text{H}_2\text{Ti}_3\text{O}_7$ ) nanotubes has been achieved via the thermal activation of persulfate anion ( $\text{PS}$ ,  $\text{S}_2\text{O}_8^{2-}$ ) by using the conventional hot plate technique which has limitations from the commercial perspective since it does not provide any precise control over the thermal generation process typically during the scale-up operation. To overcome this drawback, HTN have been synthesized via the hydrothermal process which exhibit the methylene blue (MB) adsorption of 93% at the initial dye concentration and initial solution pH of 90  $\mu\text{M}$  and 10 respectively. HTN have been regenerated via the thermal activation of PS by varying its initial concentration and regeneration temperature, within the range of 0.27-1 wt% and 40-80°C, under the thermal conditions set by the autoclave and pulsed ultrasound (US) cavitation process. The results of recycling experiments suggest that

the optimum values of initial PS concentration and temperature, for the regeneration of HTN under the autoclave conditions, are 1 wt% and 70°C with the maximum MB adsorption of 92%; while, the corresponding values for the pulsed US cavitation process are 1 wt%, 80°C, and 91% respectively. Thus, the regeneration and recycling of HTN have been successfully demonstrated by using the autoclave and pulsed US cavitation process. The mechanism of regeneration of HTN has been examined via the radical trapping and scavenging experiments. The combination of various processes and reaction pathways such as the US cavitation, classic Haber-Weiss reaction,  $\text{O}_2$  degassing, and quenching by PS are typically noted to govern the dynamics of the formation of hydroxyl radicals ( $\bullet\text{OH}$ ) depending on the test conditions. Under the optimum conditions, the MB degradation primarily involves the generation and attack of sulfate radical ( $\text{SO}_4\bullet^-$ ) for both the thermal generation techniques.

### Biography

Satyajit Vishnu Shukla obtained his Ph.D. from the University of Central Florida (UCF), Orlando, Florida, U.S.A in 2002. During his Post-Doctoral research at UCF during 2002-2006, he worked in the area of hydrogen technology funded by NASA, Glenn, U.S.A. in collaboration with the Kennedy Space Center (KSC), Titusville, Florida, U.S.A.. He joined CSIR-NIIST, Thiruvananthapuram, Kerala, India in 2006 and presently he is working as a Principal Scientist. He visited Argonne National Laboratory (ANL), Argonne, U.S.A. in 2009-2010 as an Indo-US Science and Technology Forum (IUSSTF) Research Fellow. His current areas of research include the textile wastewater treatment via the advanced oxidation processes (AOPs) and the development of hydrogen leak detectors. He has published 78 research articles, 5 book chapters, and holds 5 U.S. patents. He is a life-member of Society for Environmental Chemistry and Allied Sciences (SECAS), India. His Goolge Scholar Citation h-index and total citations are 30 and > 4000.

## Anticancer potency of N(4)-ring incorporated-5-methoxyisatin thiosemicarbazones

P. N. Yadav<sup>1</sup>, U. Chaudhary<sup>1</sup>, D. Dawa<sup>2</sup>, I. Banerjee<sup>2</sup>, S. Sharma<sup>2</sup>, K. Mahiya<sup>3</sup>, A. Rauf<sup>4</sup> and Y. R. Pokharel<sup>2</sup>

<sup>1</sup>Central Department of Chemistry, Tribhuvan University, Nepal

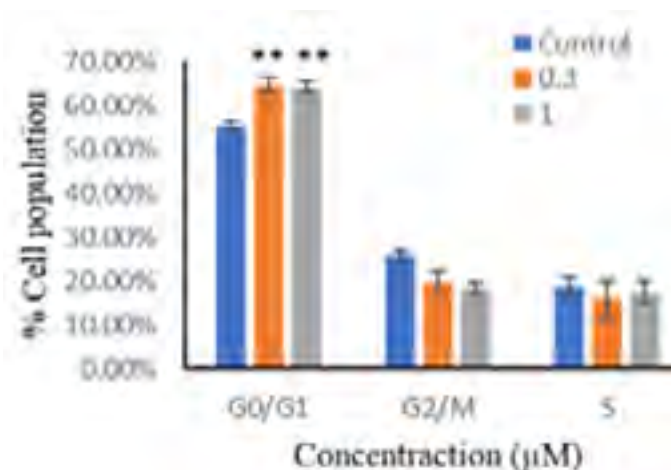
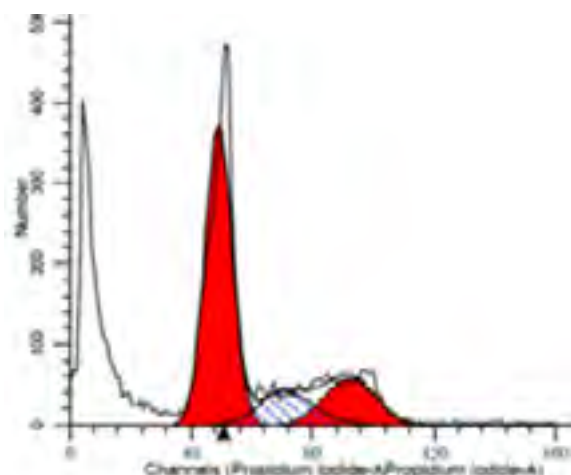
<sup>2</sup>Faculty of Life Science and Biotechnology, South Asian University, India

<sup>3</sup>Department of Chemistry, F G M Government College, India

<sup>4</sup>Department of Chemistry, University of Swabi, Pakistan

(Z)-N'-(5-methoxy-2-oxoindolin-3-ylidene) thiomorpholine-4-carbothiohydrazide (MeOIstTmor), (Z)-N'-(5-methoxy-2-oxoindolin-3-ylidene)-2,6-dimethylmorpholine-4-carbothiohydrazide (MeOIstDmMor), (Z)-N'-(5-methoxy-2-oxoindolin-3-ylidene) morpholine-4-carbothiohydrazide (MeOIstMor) and (Z)-2-(5-methoxy-2-oxoindolin-3-ylidene)-N,N-dimethylhydrazine-1-carbothioamide (MeOIstDm) are synthesized through the condensation of 5-methoxyisatin with carbazides. The new compounds were characterized by elemental analysis, FT-IR, <sup>1</sup>H NMR, <sup>13</sup>C NMR, UV-Vis, ESI-HRMS as well as single crystal X-ray analysis. The compound MeOIstDm and MeOIstDmMor crystallizes in monoclinic space group P2<sub>1</sub>/c and in orthorhombic Pna2<sub>1</sub> space group respectively. Compound, MeOIstDmMor crystallized with two molecule of compound and two lattice water molecules in the asymmetric unit. Strong interaction of MeOIstDmMor with VEGFR2 via hydrogen bonding was established from molecular docking study. MeOIstDmMor forms hydrogen bonds interactions with Ile1025

and Arg1027 and binding energy value was -6.3185 Kcal mol<sup>-1</sup>. The compounds were screened for their anticancer activity against breast cancer (MCF-7), skin cancer (A431), and lung cancer (A549) and exhibited anticancer potency in micromolar concentration (IC<sub>50</sub>, 2.52-7.41 μM). Compound, MeOIstDmMor effectively influenced the cell cycle profile with an increase in G<sub>0</sub>/G<sub>1</sub> cell population and decline in G<sub>2</sub>/M and S cell population. Arrest of cells in S phase must be attributed to irreparable damage of DNA. Further the compound MeOIstDmMor induced cytotoxic activity through the inhibition of β-catenin, C-Jun and Akt expression. These components have critical role in the cell proliferation, migration and apoptosis in cancer. As well as Agarose gel of compound MeOIstDmMor in A431 cells showed the fragmentation of DNA. Among the synthesized compounds, MeOIstDmMor was more potent as anticancer agent in A549 (IC<sub>50</sub>, 2.52 μM) while MeOIstMor exhibited high anticancer activity in MCF-7 of IC<sub>50</sub>; 2.93 μM.



## Biography

Paras Nath Yadav obtained his M. Sc. from Tribhuvan University, Nepal and his Ph.D. from University of Ioannina, Greece in 2002. He was postdoc fellow at Acadia University, Canada (2003-2005), Academia Sinica, Taiwan (2008) and Research Professor at Ewha Womans University, South Korea (2012-2013). He is Academician and senator at Nepal Academy of Science and Technology (NAST), and currently serving as Professor and Executive Director of Curriculum Development Centre, Tribhuvan University, Nepal. Dr Yadav has (co)authored 60+ research papers in peer reviewed journals and six books of chemistry. Currently he is supervising eight Ph.D. scholars. He is serving as; Theme Editor: Frontiers in Molecular Biosciences, UK, (2021), Editorial Board Member: Current Indian Science, Bentham Science, Publishers, Sharjah, U.A.E. (2021) and Editorial Board Member: Nepal Journal of Science and Technology, Nepal Academy of Science and Technology (NAST). He is a recipient of several scientific awards and his research interests are centered on the coordination chemistry, bioinorganic chemistry, synthetic chemistry and the design of novel therapeutic agents.



## Simulations of liquid chromatography using two-dimensional non-equilibrium lumped kinetic model with Bi-Langmuir Isotherm

S. Perveen<sup>1</sup>, A. Khan<sup>1,2</sup>, A. Iqbal<sup>1</sup> and S. Qammar<sup>2</sup>

<sup>1</sup>Air University, Pakistan

<sup>2</sup>COMSATS University Islamabad, Pakistan

A two-dimensional non-equilibrium and non-linear lumped kinetic model of liquid chromatography is formulated and numerically approximated to simulate the separation of multi-component mixtures in a packed fixed bed cylindrical column operating under isothermal conditions. The model equations incorporate the Bi-Langmuir adsorption thermo-dynamics as well as the radial and axial variations of concentration. By introducing distinct regions of injection at the column inlet, radial concentration gradients are generated to intensify the effect of mass transfer rate in the radial-direction, inside the column. The mathematical model is developed by a system of non-linear convection-diffusion

partial differential equations for mass balance in the mobile phase, coupled with differential equation for mass balance in the stationary phase and algebraic equations for adsorption isotherm. In this study, a high-resolution, semi-discrete, finite-volume technique is formulated and applied to gain the numerical solution of the governing non-linear-model equations. A few numerical case studies are performed to investigate the effects of the various critical parameters on the process performance. The developed numerical algorithm provide an efficacious mechanism for investigating the retention behavior, systematic monitoring and efficient operation of non-equilibrium, liquid chromatographic processes.

### Biography

I am a mathematician, who completed MSc in applied mathematics from the Quaid-i-Azam University, Islamabad, Pakistan, M-Phil in applied mathematics from the Quaid-i-Azam University, Islamabad, Pakistan and PhD in applied mathematics with specialization in the numerical solutions of liquid chromatographic models, from the COMSATS University, Islamabad, Pakistan.

I have been engaged in teaching mathematics to undergraduate and graduate students across the last 15 years as a full time and visiting faculty members across various prestigious institutes such as the Quaid-i-Azam University Islamabad, Comsats University Islamabad, Air University Islamabad and the Bahria University Islamabad. My research and work areas are mathematical modeling and simulation of liquid chromatographic models. In addition to pedagogic teaching, I have been involved in supervision of undergraduate and graduate students during my current placement as Assistant Professor at the Air University, Islamabad. During this work tenure, I have been engaged in various research activities, and have been able to publish my work during the last decade in significant and internationally well reputed peer reviewed chromatography and engineering sciences journals.



## Electrochemical sensing by novel copper oxide nanostructures

**Rupali Nagar and Abha Mahajan**

*Nanomaterials for Energy Applications Lab, Applied Sciences  
Department, Symbiosis Institute of Technology, India*

Sensors, in various aspects, have become an integral part of routine activities as either safety installations or health/motion detectors, warning systems, etc. Automation in different technological areas, in near future, will be heavily dependent on sensors. Thus, their response, sensitivity, reproducibility, reliability, material safety, economics, etc. are many fronts where innovation is required. Health sector is no exception in this regard. One of the very common ailments that affects the global population is diabetes. Early detection and preventive steps can help a large fraction of the population that suffer not only from diabetes but also from other health complications that need to be dealt with along with diabetes. Recently, a term type 3 diabetes is being coined for Alzheimer's disease due to a close relation between insulin resistance and dementia. With the objective of easy glucose detection,

there is a high chance to curb the condition at an early stage and improve the quality of life. Thus, a reliable, sensitive and affordable sensor is required. In this regard, copper oxide nanostructures have been synthesized using liquid-liquid phase separation technique. Copper oxide nanostructures synthesized in this work carry benefits of being eco-friendly material, economical as well as do not carry harmful effects of nano-toxicity when released in the environment. The reason for the latter is that these structures have high aspect ratios and can be filtered using membranes of appropriate pore sizes. The results of electrochemical sensing show that the synthesized nanostructures are able to detect glucose levels as low as 2 $\mu$ M. Thus, monotonically rising levels of glucose sensed via electrochemical sensors can be read as a warning sign in patients and provide timely medical intervention to them.

### Biography

Dr. Rupali Nagar is working at Symbiosis Institute of Technology (SIT), Pune, India as an Assistant Professor in the Department of Applied Sciences and is the Group Leader of Nanomaterials for Energy Applications Lab at SIT. She completed her Ph.D. from Indian Institute of Technology Delhi (IIT D) and continued her research while working at Indian Institute of Technology Madras (IIT M) as Project Officer till 2012. Her research interests include studying nanomaterials for energy and gas sensing applications. She has co-authored 20+ research publications, presented research work at multiple conferences, has two patents, two book chapters, three research funding projects till date to her credit.



## Safety culture in Sri Lankan industrial chemical laboratories

**Udaya K Jayasundara, Ashen I Samaranayake  
and Sajani Nishadya**

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Chemistry Ceylon, Sri Lanka*

Chemical safety should be an integral part of safety education as accidents happen during the handling of chemicals. A laboratory is a specific room where chemicals are handled on a large, medium, or small scale. Therefore, the area can be considered a hazardous environment and hence prudent practices should be strictly followed by anyone who is using or working in the area. The main reason for the deadly accidents and incidents is the lack of safety practices and poor safety culture. The purpose of this study is to gather data from local industrial settings and analyze the existing safety culture in the Western Province of Sri Lanka. A survey questionnaire was administered in the academic year 2018/2019. Even though 80 surveys were

distributed among prospective participants, only 46 surveys were submitted which is 58 % of response rate. Majority of the participants were females below 35 years old. Regardless of the working experience of the participants, 80 % of them continued in the same workplace with moderate self-perceived risks. Almost all participants believed that safety is an important factor which needs further improvement in their respective organizations. Although each participant demonstrated some knowledge on safety culture, it can be concluded that proper education must be provided to enhance their awareness. The tailor-made training programs and hands on experience with demonstrations would make the employees better prepared to address emergency situations.

### Biography

Dr Udaya K Jayasundara received his BSc (Hons) Chemistry from the University of Peradeniya in 2004 and PhD in Chemistry from the University of Nevada Reno, Reno NV USA in 2011. After his doctoral study he served as an adjunct professor and as a scientist at a Pharmaceutical Contract Research Organization. During that time, he has received extensive training in Occupational Health and Safety, Environmental Health and Safety, Good Laboratory Practices, and Safe Handling of Chemicals in addition to his main role as a lead scientist in Analytical Chemistry. He is currently serving as a senior lecturer at the Institute of Chemistry Ceylon (ICChemC) in Sri Lanka. In addition, he is a visiting lecturer at the National Institute of Occupational Safety and Health, and at Post Graduate Institute of Science, University of Peradeniya Sri Lanka. Further he has been practicing as a Laboratory Safety and Chemical Safety Consultant since 2016.



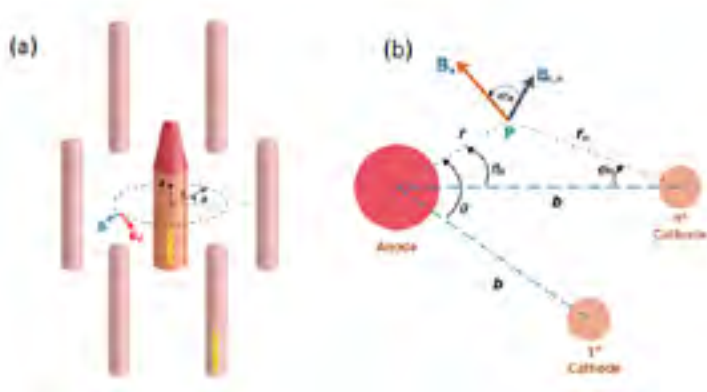
## Soft X-ray emission in plasma focus device

**Hadi Barati**

*Department of Energy Engineering and Physics, Amirkabir University of Technology, Iran*

A dense plasma focus (DPF) device can generate a very-dense very-hot column of a gas plasma by electromagnetic forces. This extremely compressed plasma column is called pinch. The pinch column is the sources of multiple type emissions. These emissions include soft x-ray radiation (SXR), hard x-ray radiation (HXR), electron beam (EB) emission, ion beam (IB) emission, etc. These copious emissions provide various applications in various fields of science such as material science which is very important, for example, in investigating the blanket materials for the future fusion-power tokamaks. Here, the SXR emission is under attention. The SXR emission takes place through three mechanisms in the pinch: Bremsstrahlung, line, and radiative recombination. To calculate the SXR power, the DPF operation is modelled in 5 consecutive phases which is known as the Lee model. In one of our recent papers, the scaling curves of the argon SXR for the Amirkabir plasma focus (APF) device have been investigated by

the modified Lee model. In this modification, the method of calculation of the magnetic field produced by the electrodes has been enhanced in such a way that has brought much more flexibility in simulations of the DPF device by the Lee model (see figure). Some results of the model have been compared with experimental results and a good agreement has been observed. The relation between the pressure and the charging voltage for an optimum(maximum) argon SXR has been obtained as  $P_0$  (Torr) =  $0.032 \times V_0$  (kV) - 0.13. It has also been found that the argon SXR yield has a linear relation with the pinch current as  $Y_{SXR}$  (J) =  $0.016 \times I_p$  (kA) - 1.1. In addition, the effect of the non-equal currents of the cathodes on the device inductance and SXR has been investigated by assigning random current distribution for the cathodes. The results have shown that non-uniformity of the cathodes' currents causes in increase of the growth-rate of the axial-phase inductance and consequently in reduction of the pinch-phase soft x-ray radiation.



**Fig. (a) The schematic of the APF electrode system. (b) The geometrical model used for vector calculations of the magnetic field in the modified Lee model.**

## Biography

Hadi Barati received the Ph.D. degree in nuclear fusion engineering from Amirkabir University of Technology (former Tehran Polytechnics), Tehran, Iran in 2019. He is currently a Research Advisor of nuclear fusion and plasma sciences in the Department of Energy Engineering and Physics, Amirkabir University of Technology. He has also been as a co-advisor for MSc students at this department. His current research interests include the applications of the Vlasov–Maxwell as well as the magnetohydrodynamic (MHD) equations to study the physics of the plasma phenomena in plasma devices, such as dense plasma focus and tokamak, and investigating the effect of magnetizing materials like ferrites on the electrical behavior of the plasma confinement device and its plasma pinch formation process.



## A new ant algorithmic approach for solving PFSP

**S. Farahmand Rad**

*Department of Mathematics, Payame Noor University, Iran*

In this paper, a new ant algorithmic approach is presented for solving n-job, m-machine permutation flow shop scheduling problem. The main objective is to find a permutation of n given jobs, i.e.,  $\sigma: \{1, 2, \dots, n\} \rightarrow \{1, 2, \dots, n\}$ . This permutation minimizes the maximum completion time of the schedule arising from  $\sigma$ . An illustration of using the presented heuristic algorithm for finding a good initial sequence of jobs is given. The proposed method is an ant-based approach to permutation flow shop scheduling problem by the behavior of real ants,


but it is different with the pheromone trail concept. The presented model is compared against the one by NEH which has been considered the best constructive algorithm so far. Regarding the quality of results, the superiority of the proposed method over NEH is demonstrated by computational evaluation. The comparison is produced on generated random test problems. This comparison is drawn in domain of feasible instances. It is easy to implement the produced method as a metaheuristic.

### Biography

Born and raised in Iran, Shahriar Farahmand Rad obtained his B.Sc. in mathematics from Kharazmi University and received his M.Sc. in mathematics from the University of Tehran, where his research area was ergodic theory. He then moved to Payam-e Noor University and joined the faculty of fundamental sciences in 1994 before completing a Ph.D. in pure mathematics at Amirkabir University of Technology (Tehran Polytechnic).

His books include "Calculus 1", "Calculus 2" and "Foundations of Combinatorics" as the author and "Foundations of Matrices and Linear Algebra" as the co-author, all of which are taught in Iranian universities as textbooks. One of his papers, namely "New high performing heuristics for minimizing makespan in permutation flowshops", has been published in Omega Journal.

Recently, Dr. Farahmand Rad has become a member of the education committee in Prof. Maryam Mirzakhani Foundation, where professors Ebadollah S. Mahmoodian and Yahya Tabesh are other members of this committee



## **Application of nanotechnology to monitor agricultural parameters that promote health and nutritional crop growth in order to provide sustainable economic growth in Aatma Nirbhar Bharat**

**Sumanta Bhattacharya**

*Maulana Abul Kalam Azad University of Technology, India*

A new area called nanobioremediation focuses on using nanotechnology to stop environmental deterioration. The traditional way of agriculture degrades the quality of farming land by the intensive use of chemical fertilizers and pesticides, which lowers agricultural output and lowers the quality of food grains. Consuming contaminated food also increases the risk of contracting acute illnesses including cancer and a number of genetic problems. By improving plant nutrition, precision farming, increasing plants' ability to absorb water and nutrients, and shielding crops from pests and diseases, nanotechnology

has been shown to be an effective way to stop the degradation of agricultural land. This also increases crop growth, soil health, and productivity of agricultural land. By estimating pollutants in the agricultural field both qualitatively and quantitatively, nanosensors are also employed to monitor the condition of the soil. In addition to providing more oxygen to India's primary sector economy with sustainable growth and the SDGs that will usher in the initiative, this article evaluates the spectrum of applications of nanotechnology to increase agricultural productivity sustainably and achieve an Aatma Nirbhar Bharat.

### **Biography**

Dr Sumanta Bhattacharya is a research scholar at Maulana Abul Kalam Azad University of Technology, West Bengal, India and a policy Analyst. He completed his B.Tech, M.Tech in Textile Technology and currently pursuing his Ph.d (2) in Tech, along with that he has MA in Development studies, LLB, MA in security and defence law, Post Graduate Diploma in Environment and Sustainable Development, Diploma in International Affairs and Diplomacy, Diploma in Government and Governance studies, MPI (Oxford University). Being a research scholar he has 197 research papers published in International and Scopus index journal, Wiley, Springer, Hindawi in various sectors like law, economic, Development studies, Textiles, Climate Change, SDGs, Public policy, Nanotechnology, Biotechnology, cancer, environment studies, 38 Book chapters published, 44 patents International and National, 4 copyrights, attended 70 International and National conference and presented papers and won 18 awards for his excellent in education, policy making and innovation.



## Absorption spectra of dissolved oxygen molecules in aerated solvents. A review of laser activation experiments

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 Russian Federation*


**M**olecular oxygen has the triplet ground state and two low-lying singlet states. The triplet-singlet transitions in oxygen molecules are strictly forbidden. Therefore, corresponding absorption bands are extremely weak. In the gas phase at low pressure, the main absorption bands of oxygen molecules had been revealed at 688, 762, 1067 and 1268 nm using multipass spectroscopic cells. The absorption coefficient of the oxygen band at 1270 nm increased 1000-fold at oxygen pressure 100-150 atm due to dimerization of oxygen molecules. Simultaneously, the absorption bands of comparable intensity appear at 1063 nm and also in violet, blue, green and red regions. Thus, the absorption properties of oxygen are radically different at low and high pressure. For a long time, there was no information on the oxygen absorption

properties in organic and aqueous media saturated with air at normal temperature and pressure. Nevertheless, an idea that light absorption by oxygen causes biological and therapeutic action of laser and LED radiation is very popular in biomedical community. Knowledge of the absorption properties of dissolved oxygen under normal conditions is of crucial importance for verification of this idea. More than 15 years ago our group started a project, which allowed us to find a solution of this problem. The success was reached due to studies of oxygen activation by laser radiation using chemical trapping and phosphorescence of dissolved singlet oxygen under ambient conditions. The present paper is aimed to review the most recent results and biomedical importance of the data obtained.

### Biography

Alexander Krasnovsky, Doctor of Science and Professor of Biophysics, Principal research scientist, head of the research group on singlet oxygen biochemistry at Federal Biotechnology Centre Russian Academy of Science, Moscow, an author in more than 200 papers in peer-reviewed journals, Past-President of the Russian Society for Photobiology, editorial member and reviewer of several scientific journals, worked as researcher and lecturer at Moscow State University Moscow, Arizona State University, Tempe, University of California, Los Angeles, Bowling Green State University in USA, Max Plank Institute in Mulheim at Ruhr (Germany), Strasbourg University (France) and other organizations, specialist in biophotonics of plant pigments and oxygen and related problems, frequent invited speaker at National and International Symposia.





## Locus of chemical reactions domains in the freely falling drop impact flow

**Yuli D. Chashechkin**

*Ishlinsky Institute for Problems in Mechanics RAS, Russia*

Heterogeneous fluids are characterized by complex spatial distributions of the Gibbs potential and density [1]. In fresh experimental studies, a fine spatial structure of flows of heterogeneous fluids, including thin fibers and interfaces, has been identified [2]. Among the solutions of the system of fundamental equations thin flows are described by singularly perturbed functions [3]. The transverse scale of fine components is determined by the values of dissipative coefficients and the characteristic flow parameter that are frequency for a periodic flow, velocity – for uniform current, or the time for a non-stationary process. The direct transfer of energy to fine components ensures by fast processes of internal energy conversion during chemical reactions or elimination of the free surface. The influence of internal energy conversion processes on the flow dynamics is manifested in the patterns of drop impact flows. Boundary of the contact area during the merging of chemically inert and reacting substances is ruptured by fine jets [4, 5]. The fine structure of

the flows formed when a drop of ferric chloride solution merges with an ammonium thiocyanate solution in the impact mode was visualized [6]. The high density of the transferred energy ensures the disintegration of a continuous drop into individual fibers that form linear and mesh structures (reticular formations). At the initial stage of coalescence, the bottom of the cavity is pierced by thin normal fibers creating a characteristic "mossy" structure. Over time, diffusion processes equalize large density gradients, and a layer of intermediate density material appears at the cavity boundary. At the same time, the liquid that flows along the fibers collects at the grid nodes and begins to invade the environment in the form of thin jets with a vortex tip. Vortices are drawn out by secondary flows and form a rapidly evolving system of loops and fibers. At the final stage, the fibrous structures are washed out by the dominant diffusion processes. The work was supported RSF (grant 19-19-00598-P).

### Biography

Yuli D. Chashechkin graduated from the full course in 1964 with a degree in Theoretical Nuclear Physics and started working at the All-Union Institute for Physics- and Radiotechniques Measurements. He defended his thesis for the degree of candidate in 1973 and for the doctor of physical and mathematical sciences in 1981. Then he started to work at the Institute for Problems of Mechanics of the AS USSR as head of the laboratory of fluid mechanics. The range of scientific interests includes theoretical and experimental studies of flows, wakes, vortices, waves, and ligaments. He develops methods of optical and acoustic visualization of flows. He is the author of over 400 articles, preprints, and reports.

## The relationship between the efficiency of energy conversion, fertility and the presence of branched ears as indicators for the determination of the optimal dosage for disease resistance mutation breeding when gamma irradiation is applied to kernels of *Triticum aestivum* L.

**Eben von Well**

*ARC-Small Grain Institute, An institute of the Field Crops Division,  
South Africa*

This study was conducted to determine whether the efficiency of energy conversion into growth, branched ears and fertility could be used as indicators of optimal gamma irradiation dosage for mutation breeding in connection with resistance against stem rust (Ug99). A 50% seedling growth reduction (GR50) is normally used for the determination of the optimal gamma irradiation dosage for mutation breeding, but recent studies indicated that it predicts a dosage that is too high. Kernels of two wheat cultivars, Ratel and Kwartel, were given gamma irradiation. GR50 was determined by planting the control and irradiated kernels (50, 150, 250, 350 Gy) in sowing trays and measuring seedling height at 14 days after planting. The efficiency of energy conversion into growth was determined by placing the control and irradiated kernels (150, 200 and 250 Gy) in germination paper in an incubator at 25°C in the dark for 132 hours.

Seedlings were removed every 12 hours from 60 hours after the onset of imbibition and placed in an oven to dry at 108°C for two days to record shoot, root and caryopsis dry weight to determine the efficiency of energy conversion into growth. Fertility and branched ears were determined by planting the control and irradiated kernels (150, 200 and 250 Gy) in pots in a glasshouse. Fertility was calculated as the number of seeds per length of the ear. M2 seed of both cultivars were sent to Kenya for resistance evaluation against Ug99. The efficiency of energy conversion into growth and fertility/sterility displayed a good relationship, while both differed from GR50 significantly. Ratel displayed significantly higher resistance to gamma irradiation in comparison to Kwartel as well as a broader gamma irradiation interval for optimal mutation breeding as observed in resistance changes against Ug99 and appearance of branched ears.

### Biography

Presently I am the curator of the Small Grain Germplasm Collection, mutation and winter / facultative wheat breeder at the Agricultural Research Council – Small Grain at Bethlehem, Free State, South Africa. I also have six years' experience as a leukemia cancer chromosomal analyzer. I have seven articles in peer reviewed journals and two manuscripts that are under consideration. I presented ten poster and four oral presentations at congresses. I am an editor for one peer review journal and reviewer for six international journals. I have been involved in two international collaborative projects of the IAEA. I am also involved in basic mutation breeding research for the determination of the optimal gamma irradiation dosage for mutation breeding as well as the mechanism behind the effect of storage time.



## Spectroscopic features of NH-tautomers of the free base corroles

**Yousef H. Ajeeb<sup>1</sup> and Mikalai M. Kruk<sup>2</sup>**

<sup>1</sup>Modern University for Business and Science, Lebanon

<sup>2</sup>Belarusian State Technological University, Belarus

Free base corroles possess special spectral and photophysical features due to lack of one of the meso-carbons due to ultimate formation of the nonplanar macrocycle conformation and two possibilities for pyrrolic protons to reside in the macrocycle core. Thus, the free base corroles was proven to exist as NH-tautomers [1,2].

In this talk we aim to report our recent results on the role of NH-tautomerization in the lowest excited singlet S<sub>1</sub> state on the pathways of the excitation energy deactivation and on the relationship of the architecture of the macrocycle peripheral substitution with both absorption and luminescence spectra [3,4]. It was shown

that the efficiency of NH-tautomerization of alkylated corrole derivatives is controlled by the architecture of the peripheral substitution of the macrocycle. The interpretation of the electronic absorption and fluorescence spectra of alkylated corroles was performed for the first time and the individual absorption and fluorescence spectra of NH-tautomers were identified and the features of the formation of absorption spectra in comparison with derivatives of corroles bearing substituents at the methine bridges are established. The mechanism of thermochromic effects in the ethanol solutions of 5,10,15-triarylcorrols has been proposed.

### Biography

Dr. Ajeeb has more than 15 years' experience in higher education level in Lebanon and abroad with a PhD in Applied Mathematics in 2007 from USA and a Doctor of Science from the National Academy of Science of Belarus in 2021. Throughout his university career he held many positions as chairman, coordinator, assistant to the president and currently as director of development. Dr. Ajeeb's most recent research interest is in Mathematical Physics and Chemistry mainly in the field of spectroscopy, studying the optical features of tetrapyrrolic compounds such as Porphyrins and free base Corrole. He is an author and co-author of more than 20 scientific papers in journals, conference proceedings and abstract contribution. He has joined many international conferences worldwide in USA, Germany, Russia, Belarus, Lebanon. Dr. Ajeeb is a member of a number of international organizations including the American Mathematical Society - USA, European Physical Society - France, Society of Porphyrins and Phthalocyanines - France, etc.



## High-temperature hydrogen attack on 2.25Cr-1Mo Steel: The roles of residual carbon, initial microstructure and carbide stability

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G. El-fallah<sup>5</sup> and H.K.D.H. Bhadeshia<sup>2,6</sup>

<sup>1</sup>Saudi Aramco Research and Development Centre, Saudi Arabia

<sup>2</sup>Materials Science and Metallurgy, University of Cambridge, UK

<sup>3</sup>Ovako Corporate R&D, Maxwell Centre, University of Cambridge, UK

<sup>4</sup>Department of Physics, Chalmers University of Technology, Sweden

<sup>5</sup>School of Engineering, University of Leicester, UK

<sup>6</sup>School of Engineering and Materials Science, Queen Mary University of London, UK

High temperature hydrogen attack is a damage mechanism that occurs in critical steel components in petrochemical plants and refineries when the hydrogen penetrates the steel and reacts with the carbides within to produce pores containing methane. With the motivation of understanding the role of carbide stability on the reaction with hydrogen, samples of a classic 2.25Cr-1Mo steel were subjected to a variety of heat treatments that generate a corresponding variety of precipitates, prior

to exposure to high-pressure hydrogen in an autoclave. Using quantitative carbide, porosity and microstructural characterisation, it has been possible to demonstrate the roles of four variables: (a) the carbon residue present in the ferrite; (b) the non-equilibrium chemical composition of carbide; (c) the fraction of the carbide that is closest to the thermodynamic equilibrium state and (d) the initial microstructural state, i.e., whether it is martensitic or bainitic prior to heat treatment.

### Biography

Mohammed is a Materials Science PhD holder from the University of Cambridge. His work was focused on understanding and mitigating the mechanism of high-temperature hydrogen attack in commercial steels. He currently works in the modelling & prediction team in the research centre in Saudi Aramco in Saudi Arabia. His work is focused on the integrity of Saudi Aramco assets, which includes studying and predicting corrosion mechanisms to allow the deployment of digital twins in the company.



## **Economic performance of certified cocoa-based agro-forestry systems in Cameroon**

**Ngoucheme Rene**

*Institute of Agricultural Research for Development (IRAD), Cameroon*

Several studies exist today on the adoption of innovations (certification) in the cocoa value chain in Africa's largest cocoa-producing countries (Ivory Coast and Ghana). Despite the importance of the cocoa sector in Cameroon's economy and as a source of income to the majority of its farmers, similar studies are few. In view of the above, this article evaluates the impact of certification on the economic performance of cocoa-based agroforestry systems in Cameroon's main production basins (the Center and South West Regions). Primary data, from 506 identified farmers, were complemented by those from field observations and a survey of key resource persons of the cocoa sector. The evaluation

was carried out using the quasi-experimental method. The endogenous switching regression (ESR) treatment effects complemented with a binary propensity score matching (PSM) methods were adopted to test their robustness and reduced selection bias from both observed and unobserved characteristics. Obtained results showed that the adoption of certification significantly and positively impacted the economic performance of cocoa producers, in yield (at about 87 kg/ha) and value (~ 200 USD). Hence, government and private developmental partners should jointly finance and organize the cocoa sector and facilitate small farmers' access to certification norms.

## Carbon and nutrient cycling in tree plantations vs. natural forests: Implication for an efficient cocoa agroforestry system in West Africa

Michel K. Yao<sup>1</sup>, Armand W. Koné<sup>2</sup>, Abigael N. Otinga<sup>3</sup>, Emmanuel K. Kassin<sup>4</sup> and Yao Tano<sup>5</sup>

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<sup>2</sup>UFR Sciences de la Nature, UR Gestion Durable des Sols, Université Nangui Abrogoua, Côte d'Ivoire

<sup>3</sup>Department of Soil Science, School of Agriculture and Biotechnology, University of Eldoret, Kenya

<sup>4</sup>Centre National de Recherche Agronomique, Côte d'Ivoire

<sup>5</sup>UFR Biosciences, Laboratoire de Zoologie, Université Félix Houphouët-Boigny de Cocody, Côte d'Ivoire

Nutrient cycling has been widely studied in tree plantations. However, studies on the observed negative changes relative to natural vegetations and how these could be capitalized toward setting up ecofriendly agroecosystems are rare. This study was conducted in Central-West Côte d'Ivoire to establish the changes in carbon and macronutrient cycling occurring in full-sun cocoa (*Theobroma cacao* L.) and Teak (*Tectona grandis*) relative to primary forest and subsequently make cocoa agroforestry-based recommendations. Leaf litterfall and associated carbon and macronutrient inputs, rates of leaf litter decomposition, and macronutrient release were assessed. In addition, soil (0–10 cm depth) chemical and microbial parameters were evaluated. Litterfall yields were  $10.6 \pm 2.0$ ,  $9.3 \pm 0.8$ , and  $10.1 \pm 0.4$  Mg dry mass ha<sup>-1</sup> year<sup>-1</sup> in forest, cocoa, and teak, respectively. Compared to the forest, the cocoa plantation supplied lower inputs of C (–736 kg ha<sup>-1</sup> year<sup>-1</sup> or –15.5%) and N (–75 kg ha<sup>-1</sup> year<sup>-1</sup> or –27%), similar P, but greater K. Similar quantities of C and N were recorded in the teak plantations and the forest. However, the teak

plantation supplied lower K but higher P inputs than the forest. Cocoa leaf litters decomposed at the same rate as those of the forest ( $k = 0.3$  month<sup>-1</sup>) but faster than the teak's, the initial leaf litter N:P ratio being the most influencing factor. Except for P, the macronutrient release from cocoa and forest litters exhibited similar patterns and rates, which were significantly different from those observed in the teak leaf litter. Soil C mineralization rate and mineral N concentration drastically declined in both tree plantations, the greatest gap occurring in cocoa (Cmin: –40%, mineral N: –54.2%) due to lower litter Ca input and soil acidity. Teak appears to be a good candidate for shade as it may compensate for the deficit in litter C (and N, to a lesser extent) supply exhibited by cocoa relative to the forest. The trends in microbial activity underscore the need to grow cocoa in association with trees that provide quality litter materials, for improved cocoa nutrient availability and faster C storage in soil. In line with this, some suggestions were made and discussed. This study can be used in support of developing an efficient cocoa agroforestry system in West Africa.

## Biography

- Researcher, UFR Sciences et Gestion de l'Environnement, UR Gestion Durable des Sols, Université Nandjui Abrogoua.
- Senior Environmental Consultant
- HSE Manager for PORTEO BTP, Road Construction Company, based in Côte d'Ivoire
- Former HSE Manager for PERSEUS MINING YAOURE Sarl, based in Côte d'Ivoire
- Former Regional Environmental Manager (West Africa) for CLUFF GOLD WEST AFRICA and AMARA MINING (Burkina Faso, Sierra Leone, Côte d'Ivoire)
- Former Environnement Consultant for SGS Environnement, Accra, Ghana
- Master of Environmental Management Sciences
- Bachelor in Earth Sciences
- Environmental Lead Auditor, ISO14001, IRCA Certification
- NEBOSH, IGC1 and GC3 Certification



## Phosphogypsum as secondary resource in the circular economy

**K. Kiegiel<sup>1</sup>, L. Maina<sup>1</sup>, G. Zakrzewska-Kołtuniewicz<sup>1</sup>,  
 A. Pryzowicz<sup>2</sup> and K. Dziarczykowski<sup>2</sup>**

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The group of rare earth elements (REE) is considered to be an important raw material important for the economy and is on the EU critical raw materials (CRMs) 2020 list. As REE are widely used in industry, the demand for these metals is very high nowadays. Among others, these elements are the most important component of magnets used in mobile computers, mobile phones, cameras, electric motors, hybrid cars, magnetic resonance devices, batteries of hybrid vehicles and hydrogen-absorbing alloys. In Poland, the occurrence of REE in minerals is low, so the impact of these resources on the national economy is small. Potential sources of these metals are also secondary materials among them phosphogypsum [1]. Phosphogypsum is a problematic waste generated in the production of mineral fertilizers from phosphate rocks.

It is estimated that 2.2 to 2.6 million tonnes of phosphogypsum per year are produced in Poland alone. When properly managed, phosphogypsum does not have to be necessary considered as a waste material [2]. The 200 million tons of phosphogypsum produced annually accounts for almost 95% of the worldwide REE demand [3]. The application of innovative process for REE recovery from phosphogypsum and the way of using the remaining gypsum matrix will be presented.

### **Acknowledgement:**

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## Biography

Katarzyna Kiegiel, PhD in chemistry, University of Warsaw Warsaw, Poland (1998); Scientific assistant, University of Warsaw, The Faculty of Chemistry (1998-2000);

Postdoctoral position, University of Kentucky, Department of Molecular and Cellular Biochemistry, Lexington, KY USA (2000-2001);

Senior researcher at Institute of Nuclear Chemistry and Technology, Warsaw since 2011.

The specialist in organic chemistry (PhD work). Presently, chemist working in the field of uranium chemistry and new extracting agents for actinides. The main area of expertise is the recovery of uranium and other valuable metals from uranium ores and from the secondary raw materials.

Katarzyna Kiegiel is a specialist in separation process like liquid-liquid extraction and solid-liquid extraction. She is an author of numerous publications concerning this topic.

Her scientific activity has a strong basis in the international cooperation. She actively participate in the implementation of the Polish Nuclear Power Program.

Katarzyna Kiegielis is co-author of over 25 scientific papers, numerous conference presentations; has over 230 citations of her research papers.



## Tunable polycationic organohalloysite electrocatalyst

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 Evgenia Dmitrieva<sup>1</sup>, Susanne Boye<sup>3</sup>, Giscard Doungmo<sup>4</sup>,  
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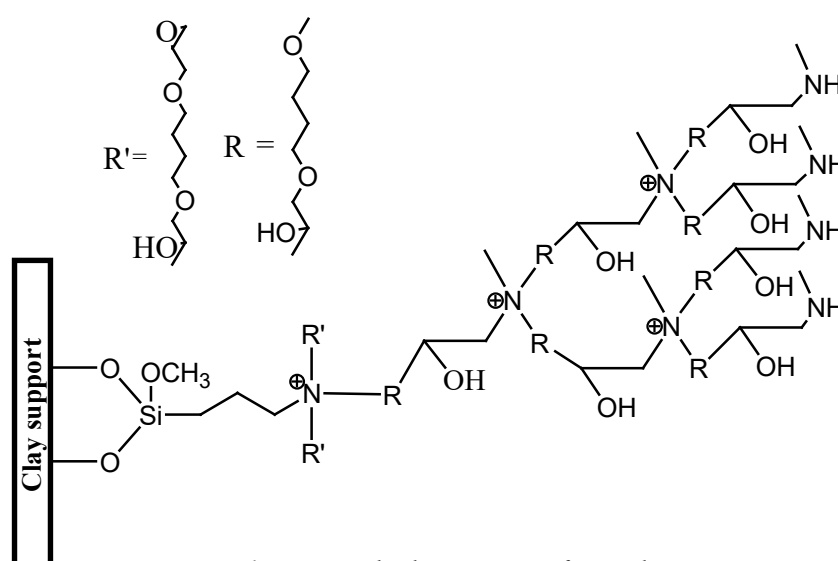
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In a sequential manner, a quaternary ammonium polyelectrocatalyst was built from the surface of an aminosilane-grafted halloysite. The as obtained material was characterised by scanning electron microscopy (SEM), X-ray diffraction (XRD), nitrogen adsorption/desorption isotherms (BET method), elemental analysis (EA), Fourier-transform infrared spectroscopy (FTIR) and thermogravimetric analysis (TGA). XRD

analysis showed that the pristine halloysite was in a partial dehydrated state with a d001 value of 0.74 nm. Not only was the success of the grafting process ascertained but also the tubular nature of the used halloysite sample as seen on the SEM micrographs. The significant increase in the d value of the modified clay (H-polyQ<sub>22</sub>, Scheme 1) suggested interlayer grafting. FTIR results showed that grafting was through OH groups, certainly interlayer, lumen



*Scheme 1: Ideal structure of H-polyQ<sub>22</sub>.*

and edge aluminol groups as well as defect site silanol groups. The electron transfer enhancing properties of the prepared polyelectrolyte were investigated by electrochemical impedance spectroscopy (EIS). The charge transfer resistance dropped significantly when

H-polyQ<sub>22</sub> was used as electrode modifier. The electrocatalytic behaviour of the H-polyQ<sub>22</sub> modified electrode was further investigated using [Fe(CN)<sub>6</sub>]<sup>3-</sup> as anionic target. The halloysite polymer nanocomposite proved to be a good candidate for electrocatalysis.

## Biography

Dr Francis Merlin Tchieno Melataguia received a B.Sc. in Chemistry and M.Sc. in Inorganic Chemistry from the University of Dschang, Cameroon, in 2008 and 2011 respectively. He equally received a PhD degree in Inorganic Chemistry/Analytical Chemistry/Electroanalysis from the same university in 2016. From 2020-2022, he was an Alexander von Humboldt postdoctoral research fellow to the Leibniz Institute for Solid State and Materials Research (IFW) Dresden. His research interests focus on the development of new electrode modifiers and their application to the electroanalytical determination of organic molecules both of medicinal interest and hazardous types. His future interest is in the elucidation of the redox mechanism of organic molecules by in situ spectroelectrochemical techniques and in the synthesis of new electrode materials.



## Optimization of essential oils yield extracted from *Curcuma longa* residue through solid state fermentation

**S. Nguikwie Kwanga<sup>1</sup>, D. Djuffo Tegoundio<sup>2</sup>,  
 PM. Jazet Dongmo<sup>1</sup> and AT. Boum<sup>2</sup>**

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<sup>2</sup>Laboratory of Process Engineering, National High School of Technical Study, University of Douala, Cameroon

The solid waste of *Curcuma longa* rhizomes generated after cold juice extraction is mostly unused and discarded even though they can contain essential oil. Conventional techniques such as hydrodistillation can be used to extract essential oil, but this generally results in low essential oil yield and inefficient extraction time. Solid-state fermentation as a pretreatment of distillation could improve the yield of essential oil. In this study, we evaluated the effect of solid-state fermentation on the yield of extraction of *Curcuma longa* solid wastes essential oil. The solid-state fermentation was carried out naturally without any addition of inoculum and the extraction was performed by hydrodistillation. Under experimental conditions at room temperature (25°C) with a moisture

content of 44% and anaerobically in the dark, the treatment of 7 days of solid-state fermentation followed by 2h of hydrodistillation provided the highest yield of 1.21% as compared to non-fermented of 0.35% and of 0.96% relative to the raw plant material representing an increase of 71% and 21% respectively. A set of experiments was then carried out by a Doehlert matrix to optimize the yield of extraction. Two independent variables, namely the distillation time and the fermentation time, were studied. Under optimal experimental conditions of 10 days and 4 hours, a yield of 1.96% was obtained validating the statistical model. The solid-state fermentation applied before the hydrodistillation step has been successful and proves its potential to improve the efficiency of essential oil extraction.

### Biography

I'm a lecturer at the Biochemistry Department of the Faculty of Sciences, at the University of Douala since 2006. My research interest deal with volatiles components from essential oils of aromatic and medicinals plant from Cameroon, and theirs potential properties as follow:

Axe 1	Study of the antioxidant and antimicrobial potential of essential oils extracted from Cameroonian <i>Aframomum</i> fruits
Axe 2	Research into synergies of potentially antioxidant and antimicrobial essential oils for their applications as natural preservatives in food, pharmaceuticals and cosmetics
Axe 3	Development of new extraction processes for functional biomolecules from natural sources and their optimization (biotechnologies)



## Improved surface morphology and corrosion resistance performance of 2205 duplex stainless steel by low temperature gas nitriding

**Nsikan Etim Dan**

*Department of Materials and Metallurgical Engineering, Federal University of Technology Owerri, Nigeria*

This paper investigates the effect of low temperature gas nitriding on surface properties of 2205 duplex stainless steel performed at 400 °C with variation of holding time of 5 h, 10 h and 15 h. Thickness of as-developed nitrided layer increased with time reaching a maximum value of 13.29  $\mu\text{m}$  having 4.68 wt% nitrogen content. Phase analysis established formation of expanded austenite ( $\alpha\text{N}$ ),  $\text{Fe}_4\text{N}$  and  $\text{Fe}_3\text{N}$  phases for all nitrided samples while un-nitrided DSS constituted only  $\alpha$  (ferrite) and  $\gamma$  (austenite). X-ray photoelectron spectroscopy revealed

that diffused  $\text{N}_2$  preferably bonded with Fe thereby suppressing the formation of  $\text{Cr}_2\text{N}$  and  $\text{CrN}$ . Hence, absence of brittle intermetallics helped in retaining inherent ductility of duplex stainless steel. Topographical analysis depicted that nitriding resulted in surface modification, increasing roughness of the treated samples. Polarization analysis test analysis under sour environment recorded 8 times improved corrosion resistance while in a combined sour and sweet environment had 3.7 times better corrosion resistance property than non-nitrided DSS.

## Healthy humans can be a source of antibodies countering COVID-19

Antonietta M. Lillo<sup>1</sup>, Nileena Velappan<sup>1</sup>, Hau B. Nguyen<sup>1</sup>, Sofiya Micheva-Viteva<sup>1</sup>, Daniel Bedinger<sup>1</sup>, Chunyan Ye<sup>3</sup>, Betty Mangadu<sup>4</sup>, Austin J. Watts, Robert Meagher<sup>4</sup>, Steven Bradfute<sup>3</sup>, Bin Hu<sup>1</sup> and Geoffrey S. Waldo<sup>1</sup>

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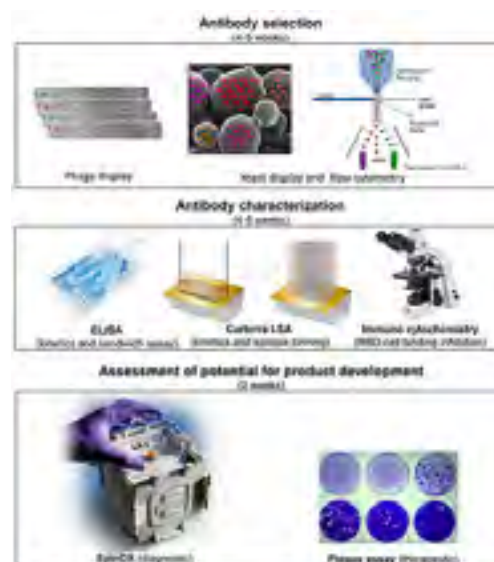
<sup>2</sup>Experimental Division, Carterra Inc., USA

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<sup>4</sup>Biotechnology and Bioengineering Department, Sandia National Laboratories, USA

Here, we describe the isolation of 18 unique anti SARS-CoV-2 human single-chain antibodies from an antibody library derived from healthy donors. The selection used a combination of phage and yeast display technologies and included counter-selection strategies meant to direct the selection to the receptor-binding motif (RBM) of SARS-CoV-2 spike protein's receptor binding domain (RBD2). Selected antibodies were characterized in various formats including IgG, using flow cytometry, ELISA, high throughput SPR, and fluorescence microscopy. We report antibodies' RBD2 recognition specificity, binding affinity, and epitope diversity, as well as ability to block RBD2 binding to the human receptor angiotensin-converting enzyme 2 (ACE2) and to neutralize authentic SARS-CoV-2 virus infection in vitro. We present evidence supporting that: 1) most of our antibodies (16 out of 18) selectively recognize RBD2; 2) the best performing 8 antibodies target eight different epitopes of RBD2; 3) one of the pairs tested in sandwich assays detects RBD2 with sub-picomolar sensitivity; and 4) two antibody pairs inhibit SARS-CoV-2 infection at low nanomolar half neutralization titers. Based on these results, we conclude that our antibodies

have high potential for therapeutic and diagnostic applications. Importantly, our results indicate that readily available non immune (naïve) antibody libraries obtained from healthy donors can be used to select high-quality monoclonal antibodies, bypassing the need for blood of infected patients, and offering a widely accessible and low-cost alternative to more sophisticated and expensive antibody selection approaches (e.g. single B cell analysis and natural evolution in humanized mice).






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## Biography

Dr. Lillo received her PhD in Chemistry from Brown University (Providence, RI, USA). She continued her education as a post-doctoral fellow at The Scripps Research Institute (San Diego, CA, USA) and at the Los Alamos National laboratory (LANL, Los Alamos, NM, USA), where she became an expert in display technologies and antibody discovery. Currently she is scientist at LANL, where she leads the antibody discovery team. Notable recent work includes using phage and yeast display to generate ML training data sets for computational prediction of protein-protein interactions, and antibody manufacturability and toxicity.



## Peukert generalized equations with due consideration of internal resistance of automotive-grade lithium-ion batteries for their capacity evaluation

**N. Yazvinskaya**

*Laboratory of Electrochemical and Hydrogen Energy,  
 Don State Technical University, Russia*

In this paper, the applicability of the Peukert equation and its generalizations were investigated for capacity evaluation of automotive-grade lithium-ion batteries. It is proved that the classical Peukert equation is applicable within the range of the discharge currents from  $0.2C_n$  to  $2C_n$  ( $C_n$  is the nominal battery capacity). As a rule, the operating currents of many automotive-grade lithium-ion batteries are exactly within this range of the discharge currents. That is why, successfully, the classical Peukert equation is used in many analytical models developed for these batteries. The generalized Peukert equation  $C=C_m/(1+(i/i_0)^n)$  is applicable within the discharge currents range from zero to approximately  $10C_n$ . All

kinds of operating discharge currents (including both very small ones and powerful short-term bursts) fall into these discharge currents range. The modified Peukert equation  $C=C_m(1-i/i_1)/((1-i/i_1)+(i/i_0)^n)$  is applicable at any discharge currents. This equation takes into account the battery's internal resistance and has the smallest error of experimental data approximation. That is why the discussed modified Peukert equation is most preferable for use in analytical models of automotive-grade lithium-ion batteries. The paper shows that all the parameters of the generalized Peukert equations have a clear electrochemical meaning in contrast to the classical Peukert equation, where all the parameters are just empirical constants.

### Biography

Dr. Nataliya Yazvinskaya is an associate professor at Don State Technical University, Russia. She is a senior researcher of laboratory "Electrochemical and hydrogen energy". She received Dr. in Engineering from the South-Russian State Polytechnical University in 2006. Her research interests include:

Firstly, the modeling of processes in electrochemical batteries to develop battery models suitable for practical use in electric vehicles.

Secondly, the study of the processes of thermal runaway in alkaline, acid and lithium-ion batteries.

Thirdly, she is an active participant in the development of hydrogen storage systems, high-capacity meeting the criteria for on-board hydrogen storage systems that have been defined by the US Department of Energy.





## Quantum-classical mechanics: Principles, applications and prospects

**Vladimir V. Egorov**

*FSRC Crystallography and Photonics, Russia*

In quantum mechanics, the theory of quantum transitions is grounded on the convergence of a series of time-dependent perturbation theory. In nuclear and atomic physics, this series converges because the dynamics of quantum transitions are absent by definition. In molecular and chemical physics, the dynamics of "quantum" transitions, being determined by the joint motion of a light electron (or electrons) and very heavy nuclei, are present by definition, and this series becomes singular. An exception is the dynamic problem for stationary states in the Born-Oppenheimer adiabatic approximation, when the electronic subsystem turns out to be "off" from the general dynamic process and therefore is not dynamically full-fledged: it only forms an electric potential in which the nuclei oscillate. Removing the aforementioned singularity can be accomplished in two ways. The first method consisted of introducing an additional postulate in the form of the Franck-Condon principle into molecular quantum mechanics, in which the adiabatic approximation is used. The second method was proposed by the author and consisted of damping the singular dynamics of the joint motion of an electron and nuclei in the transient state of molecular "quantum" transitions by introducing chaos. This chaos arises only during molecular quantum transitions and is called dozy chaos. Dozy chaos leads to the continuity of the energy spectrum in the molecular transient state, which is a sign of classical mechanics. Meanwhile, the initial and

final states of the molecule obey quantum mechanics in the adiabatic approximation. Molecular quantum mechanics, which takes into account the chaotic dynamics of the transient state of molecular "quantum" transitions, can be called quantum-classical mechanics (QCM). The efficacy of the damping for the aforementioned singularity is shown by different QCM applications, in particular, by applications of the so-called Egorov resonance to optical spectra in polymethine dyes and J-aggregates both for single-photon and two-photon processes, which, in particular, are rationalizing experimental studies in the field of bioimaging and photodynamic therapy. Prospects for further developments in QCM and their applications to problems of cancer and viral infections are discussed. Applied development of the theory will also be associated with the complication of a quantum-classical system by organizing various molecular aggregates in order to find the "molecule of life", that is, that rather complex, but "minimal" structural configuration, in which there are clear elements of self-organization, both structural and dynamic. Note that the "atom of life" is the quantum-classical electron itself, which provokes dozy chaos. Of particular interest are experimental studies on the search and synthesis of the "molecule of life".

**Funding:** This work was supported by the Ministry of Science and Higher Education within the State assignment Federal Scientific Research Center "Crystallography and Photonics" Russian Academy of Sciences.

## Biography

Prof Dr Vladimir Valentinovich Egorov has his expertise in theoretical molecular and chemical physics. Education: National Research Nuclear University MEPhI, Faculty of Theoretical and Experimental Physics (1966 – 1972), Moscow, USSR. He has completed his PhD from Theoretical Department of Institute of Chemical Physics, USSR Academy of Sciences (1981), and he has completed his Dr Phys&Math Sci degree from Institute of Physical Chemistry, Russian Academy of Sciences (2004). He is leading researcher at FSRC “Crystallography and Photonics”, Russian Academy of Sciences, Moscow, Russia. Prof Egorov is working on the development of a fundamentally new physical theory – quantum-classical mechanics and its applications in physics, chemistry, biology and biomedicine.

## Quantification of kinetic rate constants of oxygen reduction reaction pathways over Pt-free electrocatalysts and its application in Tafel slope evaluation

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<sup>2</sup>Indian Institute of Science Education and Research, India

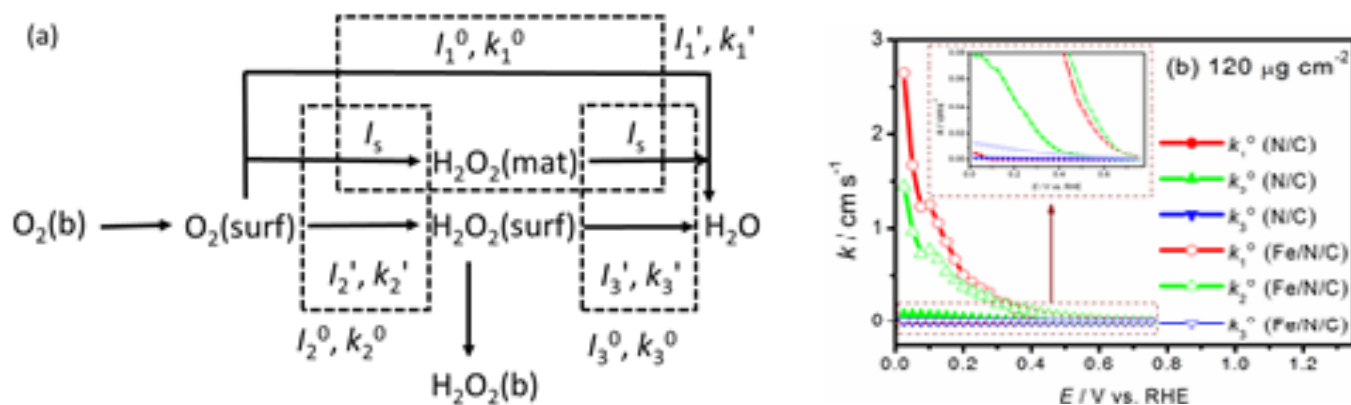
<sup>3</sup>Department of Materials Science and Engineering, Tokyo Institute of Technology, Japan

Oxygen reduction reaction (ORR) plays an important role in proton exchange membrane fuel cell [1, 2] and electrochemical synthesis of hydrogen peroxide based on fuel cell setup [3]. Recently, much attention was focused on developing new ORR non-precious-metal catalysts, nitrogen-doped carbon (N/C) and Fe-containing nitrogen doped carbon (Fe/N/C) catalysts [4-6]. Over these catalysts, there are maybe different pathways for ORR. (1) Oxygen could be directly reduced to water by 4-electron-reduction pathway and the corresponding active sites or catalyst is desirable for PEMFC application; (2) oxygen is reduced to hydrogen peroxide by 2-electron-reduction pathway and the corresponding active sites or catalyst is expected for electrochemical synthesis of hydrogen peroxide; (3) And the produced hydrogen peroxide could be further reduced to water by (2+2)-electron-reduction pathway. Therefore, it is of great significance to clarify the real ORR pathway over Fe/N/C and N/C catalysts. In the present study, we tried

to investigate the mechanistic pathway of the ORR over Fe/N/C and N/C catalysts prepared from the pyrolysis of polyimide particles at high temperatures in the presence and the absence of Fe(acac)<sub>3</sub>, in acidic media based on the model with loading correction which, in order for concision, was denoted as Nabae model [7] (Figure 1(a)). It demonstrated that Fe/N/C catalyst facilitates the oxygen reduction to water (dominant 4-electron-pathway) for PEMFC generating power, and N/C catalyst is promising to the selective electrochemical production of hydrogen peroxide (dominant 2-electron-reduction pathway) based on fuel cell setup (Figure 1(b)) [8-11]. Tafel slopes of different ORR pathways are further evaluated separately through calculations of

$$\left(\frac{\partial E}{\partial \log k_1}\right) \text{ and } \left(\frac{\partial E}{\partial \log k_2}\right)$$

for Fe/N/C and N/C catalysts in acidic and alkaline media to study ORR mechanisms over catalysts [12].



**Figure 1.** (a) Nabae model, which consider  $\text{H}_2\text{O}_2$  to be further reduced to  $\text{H}_2\text{O}$  in the catalyst layer matrix,  $\text{H}_2\text{O}_2(\text{mat})$ .  $I_1'$ ,  $I_2'$ ,  $I_3'$ ,  $k_1'$ ,  $k_2'$  and  $k_3'$  are the individual currents and kinetic constants based on the Damjanovic model with a modified mathematical approach.  $I_1^0$ ,  $I_2^0$ ,  $I_3^0$ ,  $k_1^0$ ,  $k_2^0$  and  $k_3^0$  are those based on the correction for the quasi-four-electron reduction.  $I_s$  is the current via the series reaction in the catalyst layer matrix. (b) Comparison of individual rate constants based on Nabae model for  $120 \mu\text{g cm}^{-2}$  of the N/C and Fe/N/C catalysts.

## Biography

Yun Wu, lecturer of Department of Material Science and Engineering, Guangdong University of Petrochemical Technology (GDUPT), China. He completed his PhD degree with Takeo Ohsaka at Tokyo Institute of Technology in Tokyo, Japan in 2013 and was a postdoctoral research associate with Yuta Nabae at Tokyo Institute of Technology. He joined GDUPT in 2019 as Advanced Talent program. He is a member of ISE and CCS Chemistry. His research is focused on Nanomaterial for energy storage and conversion (Nanoporous alloy and N-doped Nano-carbon materials), Battery chemistry (Fuel cell and lithium-ion battery), Electrochemical redox of water, Electrochemical reduction of  $\text{CO}_2$ , Electrochemical reaction interface, Homogeneous and heterogeneous catalysis, and kinetics over oxygen reduction reaction catalysts.

## Mercury prediction in groundwater of Naameh Landfill (Lebanon) using an Artificial Neural Network (ANN) model

**F. Kanj<sup>1</sup>, R. Sawaya<sup>2</sup>, J. Halwani<sup>2</sup> and N. Nehme<sup>1</sup>**

<sup>1</sup>*Lebanese University, Faculty of Agriculture Engineering and Veterinary Sciences, Lebanon*

<sup>2</sup>*Lebanese University, Water & Environment Science Lab, Lebanon*

**N**aameh Municipal solid waste landfill located in Chouf Caza (Lebanon) is the biggest landfill in the country and it operated for almost 18 years whereby it received baled wastes from 51% of the Lebanese regions. Mercury is a highly poisonous metal which is mostly found in the environment. The mercury is at the top of the parameters of water quality that requires investigations for planning and management. In order to assess the status of mercury in the groundwater of Naameh landfill, Artificial Neural Network (ANN) models were used as indicators of water quality and for the prediction of mercury. Two types of feedforward networks have been used including multilayer perceptron (MLP) and radial basis function (RBF). A number of different MLP neural networks algorithms and RBF networks trained and

developed with reference to pH, EC, TDS, TON, calcium and magnesium to predict mercury concentrations in groundwater. Six scenarios were used to train MLP and RBF networks for choosing the best model for predicting water quality parameters in groundwater of Naameh Landfill. The performances of MLP and RBF models were evaluated by utilizing the coefficient of determination ( $R^2$ ). The results showed that the computed values of  $R^2$  for MLP and RBF were 0.791 and 0.881, respectively. In addition, the prediction results showed that both types of networks are very good for predicting mercury concentrations in the groundwater of our study area. Moreover, the results reveal that mercury residues will persist for an additional two years although the landfill's operation ended year 2016.

### Biography

I graduated with a PhD Degree in Environmental, Geography and spatial planning from 2018 and agricultural engineer from 2013. I am an Environmental and territorial management specialist with experience in water quality testing and treatment. Proven ability to collect and analyze data, develop solutions, and lead teams in a safe and efficient manner. Passionate about protecting the environment and promoting sustainability.

In addition, I am a scientific researcher and lecturer at the faculty of Agronomy - Lebanese University. I have work in several environmental and rural development project as a consultant. I also work with several NGO as a field coordinator, socio-economic expert that I have tasks to prepare a business plan and marketing plan for agriculture product, to prepare a market based assessment.



***ACCEPTED  
ABSTRACTS***

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**ADV. CHEMISTRY 2023**



**Study of electrical conductivity in metallic n-type InP semiconductor at low temperature in presence of strong magnetic field**



**A. El Kaaouachi<sup>1</sup>, A. El Oujdi<sup>2</sup> and A. Echchelh<sup>2</sup>**

<sup>1</sup>MPAC group, Faculty of Sciences, Morocco

<sup>2</sup>Laboratory of Energetic Engineering and Materials, Faculty of Sciences Ibn Tofail, Morocco

**W**e have studied the transport properties in metallic n-type InP semiconductor. We show that the dependence on temperature of metallic electrical conductivity obey to the law  $\sigma(T) = \sigma(T=0) + mT^{(1/2)}$ . We have found that the coefficient of thermal variation  $m$  changes

sign when the magnetic field increases. We have proposed several complex theories to provide a physical explanation for this sign change such as the Zeeman effect, the effects of weak localization and the effects of electron-electron interactions.



## **Environmental monitoring of heavy metals distribution in the agricultural soil profile and soil column irrigated with wastewater from the Day River, Beni Mellal City (Morocco)**



**A. Hilali and M. El Baghdadi**

*Geomatics, Georesources and Environment Laboratory, Departement of Earth Sciences, Faculty of Sciences and Techniques, Sultan My Slimane University, Morocco*

This study examines the vertical distribution of heavy metals (As, Cr, Cu, Cd, Pb, Zn, and Fe) in the soil profiles irrigated with wastewater from Day River and explores the impact that this wastewater has on agricultural soil profile. To this end, three soil profile samples were taken from three unirrigated sites except for rain, and three soil profile samples are collected from wastewater-irrigated sites in June 2017. Each soil profile is divided into three horizons H1, H2, and H3 at the depth of 0-30, 30-60, and 60-90 cm respectively. The results of the physio-chemical characteristics of the soil show that excessive irrigation with wastewater increases organic matter, electrical conductivity, pH, carbonates, and the concentration of all evaluated heavy metals in the soil. In addition, the concentration of all evaluated heavy metals stayed within

permissible limits proposed by the World Health Organization for all soil profiles except for Cd, Pb, and As in the irrigated soil profiles. The vertical distribution of heavy metals demonstrates that the concentration of As, Cr, and Fe increases with the depth, while Pb and Cu decrease downward. In addition, the Cd and Zn have a random distribution. The concentration of heavy metals in the discharged water reveals that the Cd, Pb, and As are gradually decreasing with the depth which confirms that the studied soil retains the heavy metals. The study concludes that wastewater irrigation from the Day River contributes to the accumulation of heavy metals and has a dangerous impact on agricultural soil. It is then advisable that local authorities come up with an action plan to treat all wastewater before discharging it into the Day River.





## Influence of magnetic field on transport phenomena and scale laws in metallic n-type InP



**A. Echchelh<sup>1</sup>, A. El Kaaouachi<sup>2</sup> and A. El Oujdi<sup>2</sup>**

<sup>1</sup>Laboratory of Energetic Engineering and Materials, Faculty of Sciences Ibn Tofail, Morocco

<sup>2</sup>MPAC group, Faculty of Sciences, Morocco

**W**e have studied the transport properties in metallic n-type InP semiconductor. We show that the dependence on temperature of metallic electrical conductivity obey to the law  $\sigma = \sigma(T=0) + mT^{(1/2)}$ . We highlight the absence of a minimum electrical

conductivity  $\sigma_{\min}$  proposed by Mott at the metal insulator transition (MIT). We show that the conductivity at temperature  $T = 0K$ , ( $T=0$ ), follows a scaling law as a function of the effective parallel and perpendicular Bohr radii  $a_{\parallel}$  and  $a_{\perp}$ .



## Determination of number density and void fraction of active bubbles for a maximum sonochemical efficiency



**Aissa Dehane<sup>1</sup>, Atef Chibani<sup>2</sup> and Slimane Merouani<sup>1</sup>**

<sup>1</sup>Laboratory of Environmental Process Engineering, Department of Chemical Engineering, Faculty of Process Engineering, University Salah Boubnider Constantine 3, Algeria

<sup>2</sup>Department of Mechanical Engineering, Faculty of Technology, University of Mostefa Ben Boulaid, Algeria

Tiny gas bubbles oscillate as a result of the ultrasound perturbation transported throughout an irradiated solution. The thermal breakdown of gas molecules like water vapor and volatile solutes that are present in the gas bubbles causes free radicals and active species to be created during the adiabatic compression phase (several thousand Kelvin and hundreds of bars) of bubbles. Oxidative species (OH, H<sub>2</sub>O<sub>2</sub>, O, HO<sub>2</sub>, etc.) are regarded as potent tools for water treatment (degradation of the different pollutants). Additionally, hydroxyl radicals (OH, E°=2.8 V vs NHE) are one of the primary species produced during bubble collapse. Despite the promising advancements of the sonochemical process, its efficiency still unsatisfying. Therefore, innovative solutions, such as

the use of additives and the integration of the sono-process with other techniques, are needed. Moreover, our understanding of the sonochemical process should be improved for its better reliability. In the present work, our recently developed methods for the evaluation of the number density and void fraction are discussed in light of those available in literature. In addition, future perspectives and plausible solutions are analyzed. It should be noted that an accurate determination of bubbles population allows the evaluation of their sonochemical behavior (oxidants production, hydrogen yield, conversion of pollutants...), thus, sonoactivity of the irradiated medium can be enhanced.



**Design, synthesis,  
biological evaluation  
and molecular docking  
of novel quinazolinone  
EGFR inhibitors as  
targeted anticancer  
agents**



**Alaadin E. Sarhan, Zinab M. Nofala, Kamelia M. Amin, Hanaa S. Mohameda,  
Ahmed M. El-Kerdawy, Magdy S. Alyc and Basma S. Habiba**

*The Department of Therapeutic Chemistry, Pharmaceutical and Drug Industries Research Institute,  
National Research Center, Egypt*

**A** novel series of 2-methyl-3-phenylquinazolin-4-one derivatives were synthesised and biologically evaluated for their cytotoxic potential towards MCF-7, HepG2 and PC-3 cancer cells. Most of the tested compounds showed reasonable safety in the normal human skin melanocyte HFB4 cell line. Compound 4 showed promising cytotoxic activity on all the tested cell lines, while compound 9 showed potent cytotoxicity on the MCF-7 cell line, whereas compounds 10 and 12 showed potent cytotoxicity on

Hep-G2 cell lines using 5-fluorouracil as a reference standard. Cell division analysis on the tested cell lines revealed that compounds 4, 9, 10, and 12 have potent antiproliferative properties. An in vitro enzymatic inhibition assay against EGFR-TK confirmed that those compounds have potent EGFR inhibitory activity. The target compounds arrested the cell cycle at the pre-G1 and G2/M phases. Molecular docking simulations showed that all the target compounds possess a common binding pattern like that of Erlotinib.



## **Characterization and quality evaluation of cement raw materials and their possible substitutes in Yemen**



**Ahmed Mohammed Al-Anweh<sup>1</sup>, Mohamed Mahmoud Abu-Zeid<sup>2</sup>, Mohammed Ibrahim El-Anbaawy<sup>3</sup> and Ibrahim Abdulhamid Al-Akhaly<sup>4</sup>**

*<sup>1</sup>Faculty of Sciences and Literatures, Amran University and Amran Cement Factory, Yemen*

*<sup>2</sup>Geology Department, Ain Shams University, Egypt*

*<sup>3</sup>Geology Department, Cairo University, Egypt*

*<sup>4</sup>Department of Earth Sciences, Faculty of Petroleum and Natural Resources, Sana'a University, Yemen*

Combined geologic, lithologic, petrographic, mineral, and chemical investigations were conducted on the natural cement raw materials that are presently used by the six main cement plants in Yemen. The results of investigations were implemented to precisely characterize those materials. This permitted the determination of the relative suitability of the carbonates exploited from the various quarries to produce Portland cement either as natural cement rocks or by using correctives to modify their

composition. This study involved also the determination of the types and composition of the correctives that can produce cements with highest quality. Moreover, an attempt has been made to assess the available natural substitutes for the presently used correctives and additives. This is most importance to deal with the progressive decrease in their reserves and to avoid getting the sand and clay raw materials by excavating the valuable agricultural and reclaimed lands.



## Plasma-assisted modifications of polypropylene fabric for improved performance and comfort attributes



**Amira Saed, Marwa Abou Taleb, Salwa Mowafi and Hosam El-Sayed**

*Proteinic and Man-made Fibres Department, Textile Technology Research Institute, National Research Centre, Egypt*

Some polymeric materials, such as polypropylene, exhibit excellent properties of specific strength (lightness combined with good mechanical strength) with chemical inertia. Polypropylene is one of the most difficult polymeric materials to treat because it has poor adhesive properties and high chemical barrier responses. This work aims to adopt an easy applicable eco-friendly method to render polypropylene certain desired properties and functions suitable for clothing and applications. Activation of polypropylene surface was carried out using plasma discharge (oxygen or nitrogen). Two eco-friendly biopolymers; namely keratin or sericin, were extracted in our laboratory from their renewable natural resources. The said biopolymers were applied to the plasma-pretreated polypropylene fabrics using pad-dry-cure or exhaustion method. Plasma/biopolymers-finished polypropylene fabrics exhibited multifunctional properties including antimicrobial and ultraviolet protection that make it suitable for packaging. Moreover,

the hydrophilicity and comfortability of polypropylene fabrics were enhanced which make it more appropriate for clothing field. The dyeability of the treated fabrics with acid, reactive and basic dyes was investigated. The alteration in the chemical composition of the treated polypropylene fabric was assigned using FTIR, EDX, and <sup>13</sup>C-NMR.

The work has ecological, commercial and socioeconomic positive impacts. The use of eco-friendly method for activation of polypropylene surface, without need of aggressive chemicals, and the use of biopolymers (keratin and sericin) which are available as byproducts from textile industry (ecological demand). Obtaining polypropylene with multifunction properties will make it suitable for packaging and textile applications (commercial and socio-economical demand). Applying plasma technology in treatment of textiles will save large amounts of water and energy which is traditionally used in textile wet processing.



## Relative Abundance of PGRs in the Liquid Endosperm of Young Nuts of *Cocos nucifera* L. Parental Cultivars and their Reciprocal Hybrids



**Amritha V. V and Dr. K.G Ajith Kumar**

*Department of Botany and Research Center, Govt. College for Women, India*

Coconut water (*Cocos nucifera* L.), the semi-clear liquid endosperm obtained from immature coconut is a refreshing, nutritious beverage having beneficial health properties, used as an important alternative for oral rehydration and even for patient intravenous hydration in remote regions. It contains many PGRs which play vital roles in many processes during seed development such as histodifferentiation, reserve accumulation, and germination. Many literatures are available highlighting the levels of PGRs in the tender and mature coconut water. However, a detailed account on the dynamics of PGRs during the coconut seed development and a comparative analysis of PGRs in the parental cultivars and their reciprocal hybrids is lacking. In the present study, fifteen hormones belonging to seven major classes of phytohormones, viz., IAA, IBA, SA, GA<sub>3</sub>, GA<sub>4</sub>, GA<sub>7</sub>, tZ, tZR,

BA, ABA, ACC, JA, cisJ, meJ, and 24-epiBL, were simultaneously assayed from the liquid endosperm of 120 days old young nuts collected from West coast tall cultivar, Gangabondam (dwarf cultivar) and their reciprocal hybrids (TxD and DxT) by LC-MS/MS method. According to the results, IAA was the predominant auxins while BA was the predominant cytokinins in the liquid endosperm of all cultivars and hybrids. SA was found in exceptionally higher levels in all the cultivars and hybrids. cisJ and 24-epiBL were found in significant levels in the tender water. These PGRs were found to be involved in the histodifferentiation process of seed development. All GAs and ABA were found in insignificant level in the liquid endosperm of all the cultivars and hybrids indicating their insignificance in early embryogeny process of nut development.



## Plastic trash to monomers and intermediates – PTMI



**Anne M. Gaffney**

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To address the issue of waste plastics in landfills, a hybrid approach is proposed. This would use low temperature plasma pretreatment followed by catalytic cracking to augment the conversion of waste polyolefins into monomers, intermediates, new polymers and value-added chemicals. Lightweight packaging (LWP) comprises about 50% of total plastics consumption and consists mainly of single and multilayer films and containers. LWP is heterogeneous, contaminated and is difficult to recycle. Mechanical recycling is currently the only commercial approach to recycling but is inadequate to address the growing volume of packaging plastics and degrades or downcycles both polyethylene (PE) and polypropylene (PP). In contrast, feedstock recycling converts polymers to monomer feedstock that can be used to make new products that have virgin-like performance in high volume single use packaging applications, thereby creating new value chains for what is currently a waste stream. Current high TRL feedstock recycling technologies like pyrolysis and gasification are highly energy intensive,

require multiple steps (plastics-syngas-methanol-olefins) and have low selectivity to polyolefin building blocks (ethylene, propylene). Alternatively, plastics upcycling aims at selectively deconstructing polymer in a one-step process directly into monomers and high value chemicals (HVC). Consequently, it is proposed to use a hybrid approach of preconditioning with a low temperature plasma followed by catalytic cracking for conversion of waste polyolefins into monomers, intermediates, new polymers and value-added chemicals. This offers improvement in carbon utilization, cumulative energy demand and selectivity to recycled high value products over current benchmark feedstock recycling processes like gasification and pyrolysis. It is suggested to use LTP treatment as a tunable polyolefin functionalization step to increase selectivity of subsequent catalytic deconstruction and reconstruction. The target waste stream is post-industrial and post-consumer packaging waste, mainly LDPE, LLDPE, and PP films. The primary target products from this novel process are C<sub>2</sub>-C<sub>4</sub> olefins (ethylene, propylene, butylene) which are the raw materials for

bulk of the volume of single use plastic production (PE and PP). Aromatic and other HVC precursors like benzene, toluene, xylene (BTX), ethyl benzene and polyols are also expected as by-products from the process. All the products and by-products

(C2- C4 olefins, BTX, polyols, HVC) can be upcycled to resins, bulk (polyethylene, polypropylene) and specialty polymers (polyurethanes, epoxy, polyester, Nylon-6) at different market entry points.





## Fruit peel bioactives, valorisation into nanoparticles and potential applications



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Nanotechnology is a rapidly growing field with profound applications in different domains, particularly in food science and technology. Nanoparticles (NPs) synthesis, an integral part of nanotechnology-based applications, is broadly classified into chemical, physical and biosynthesis methods. Chemically sensitive and energy-intensive procedures employed for NPs synthesis are some of the limits of traditional chemical approaches. Recent research has focused on developing easy, non-toxic, cost-effective, and environment-friendly NPs synthesis during the last decade. Biosynthesis approaches have been developed to achieve this goal as it is a viable alternative to existing chemical techniques for the synthesis of metallic nanomaterials. Fruit peels contain abundant

bioactive compounds including phenols, flavonoids, tannins, triterpenoids, steroids, glycosides, carotenoids, anthocyanins, ellagitannins, vitamin C, and essential oils with substantial health benefits, anti-bacterial and antioxidant properties, generally discarded as byproduct or waste by the fruit processing industry. NPs synthesised using bioactive compounds from fruit peel has futuristic applications for an unrealized market potential for nutraceutical and pharmaceutical delivery. Numerous studies have been conducted for the biosynthesis of metallic NPs such as silver (AgNPs), gold (AuNPs), zinc oxide, iron, copper, palladium and titanium using fruit peel extract, and their synthesis mechanism have been reported which will be discussed in the lecture.



## Relative age effects in track-and-field: Identification and performance rebalancing



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**Introduction:** Relative Age Effect (RAE) consists of a biased distribution of the dates of birth in a same-age group.

**Objectives:** This study aimed to investigate Relative Age Effect among French athletes in different track-and-field events, and propose a corrective adjustment method to highlight the true potential of an athlete with respect to his/her relative age.

**Methods:** 358,610 performances from 2009 to 2019 of female and male athletes between 12 and 21 years old were collected. Relative age distributions of performances were analyzed by level of competitiveness ("All," "Top50%," "Top10%" where "all" represents all athletes, top50% and top10% represent the best 50% and 10% of athletes per age category respectively) and age category, with chi-square and

odd-ratio statistics. A linear relationship between distribution of performances and age leads to a calibration coefficient allowing to rebalance the performance by considering the effect of Relative Age Effect. Validation is obtained by Wilcoxon statistical test on actual athlete data.

**Results:** Relative Age Effect is present in all types of events. It is larger when the level of competitiveness increases. In male 100 m sprint, 1 year difference between two athletes birth date represents an average gain of 931.01 ms (6.5%) in the U13 (Under 13 years old) and 229.65 ms (1.9%) in the U17 (Under 17 years old) categories. Our validated rebalancing methods allows to compensate for the biases induced by the relative age effect. By comparing the rebalanced performance and the realised performance of each athlete, we cannot

say that they are significantly different. On average, there is no significant difference between these two performances.

**Conclusion:** This study showed that there is a relative age effect among young French

athletes, with an even greater effect as the level of competition increases. Thanks to the rebalancing method that has been validated, performances can now be better appreciated according to category and event.



## **Silver nanoparticles induced hepatotoxicity with activation of TGF $\beta$ -1 and $\alpha$ -SMA triggered liver fibrosis in Sprague Dawley rats**

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Despite the extraordinary use of silver nanoparticles (AgNPs) in medicinal purposes and the food industry, there is rising worry about potential hazards to human health and the environment. The existing study aims to assess the hepatotoxic effects of different dosages of AgNPs by evaluating hematobiochemical parameters, oxidative stress, liver morphological alterations, immunohistochemical staining, and gene expression to clarify the mechanism of AgNPs' hepatic toxic potential. Forty male Sprague Dawley rats were randomly assigned into control and three AgNPs intraperitoneally treated groups 0.25, 0.5, and 1 mg/kg b.w. daily for 15 and 30 days. AgNP exposure reduced body weight, caused haematological abnormalities, and enhanced hepatic oxidative and nitrosative stress with depletion of the hepatic GSH level. Serum hepatic injury biomarkers with pathological hepatic lesions where cholangiopathy emerges as the main hepatic alteration in a dosage- and duration dependent manner were also elevated. Furthermore, immunohistochemical labelling of apoptotic markers demonstrated that Bcl-2 was significantly downregulated while caspase-3 was significantly upregulated. In

conclusion, the hepatotoxic impact of AgNPs may be regulated by two mechanisms, implying the apoptotic/antiapoptotic pathway via raising BAX and inhibiting Bcl-2 expression levels in a dose-dependent manner. The TGF- $\beta$ 1 and  $\alpha$ -SMA pathway which triggered fibrosis with incorporation of iNOS which consequently activates the

inflammatory process were also elevated. To our knowledge, there has been no prior report on the experimental administration of AgNPs in three different dosages for short and long durations in rats with the assessment of Bcl-2, BAX, iNOS, TGF- $\beta$ 1, and  $\alpha$ -SMA gene expressions.



## Analysis of the importance of the dispersion coefficient depending on the distance for the transport of solute in porous media



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Aquifers are subject to the intrusion of pollutants which may be of natural or anthropogenic origin. This can therefore affect human health through the consumption of borehole water, and also the development of vegetation. However, the natures of the adsorption and dispersion coefficients of the medium significantly influence the retention of pollutants in the underground environment. In this study, the advection dispersion equation whose dispersion and adsorption coefficient depend on distance was solved numerically to determine the spatio-temporal evolution of salinity in

aquifers. Analysis of the results shows that the concentration profiles remain very sensitive to the distance-dependent adsorption coefficient. The results obtained show that by considering 0.1g / L of salinity as a guide value in the aquifer and by considering an initial source of pollutant sinusoidally and exponentially varying as a function of time, the necessary time for a drinking water point is prolonged when the dispersion coefficient is dependent on the distance and the adsorption coefficient constant. These results show the importance of measuring these parameters before using them in models.



## **Spatial effect of digital economy on particulate matter 2.5 in the process of smart cities: Evidence from prefecture-level cities in china**



**Chen Lin and Tan Jingrong**

*Zhejiang University of Technology, China*

**D**uring the COVID-19 pandemic, the digital economy has developed rapidly. The airborne nature of COVID-19 viruses has attracted worldwide attention. Therefore, it is of great significance to analyze the impact of the digital economy on particulate matter 2.5 (PM2.5) emissions. The research sample of this paper include 283 prefecture-level cities in China from 2011 to 2019 in China. Spatial Durbin model was adopted to explore the spatial spillover effect of digital economy on PM2.5 emissions. In addition, considering the impact of smart

city pilot (SCP) policy, a spatial difference-in-differences (SDID) model was used to analyze policy effects. The estimation results indicated that (1) the development of the digital economy significantly reduces PM2.5 emissions. (2) The spatial spillover effect of the digital economy significantly reduces PM2.5 emissions in neighboring cities. (3) Smart city construction increases PM2.5 emissions in neighboring cities. (4) The reduction effect of the digital economy on PM2.5 is more pronounced in the sample of eastern cities and urban agglomerations.



**Numerical investigations of thermal radiation and activation energy imparts on chemically reactive Maxwell fluid flow over an exothermal stretching sheet in a porous medium** ”

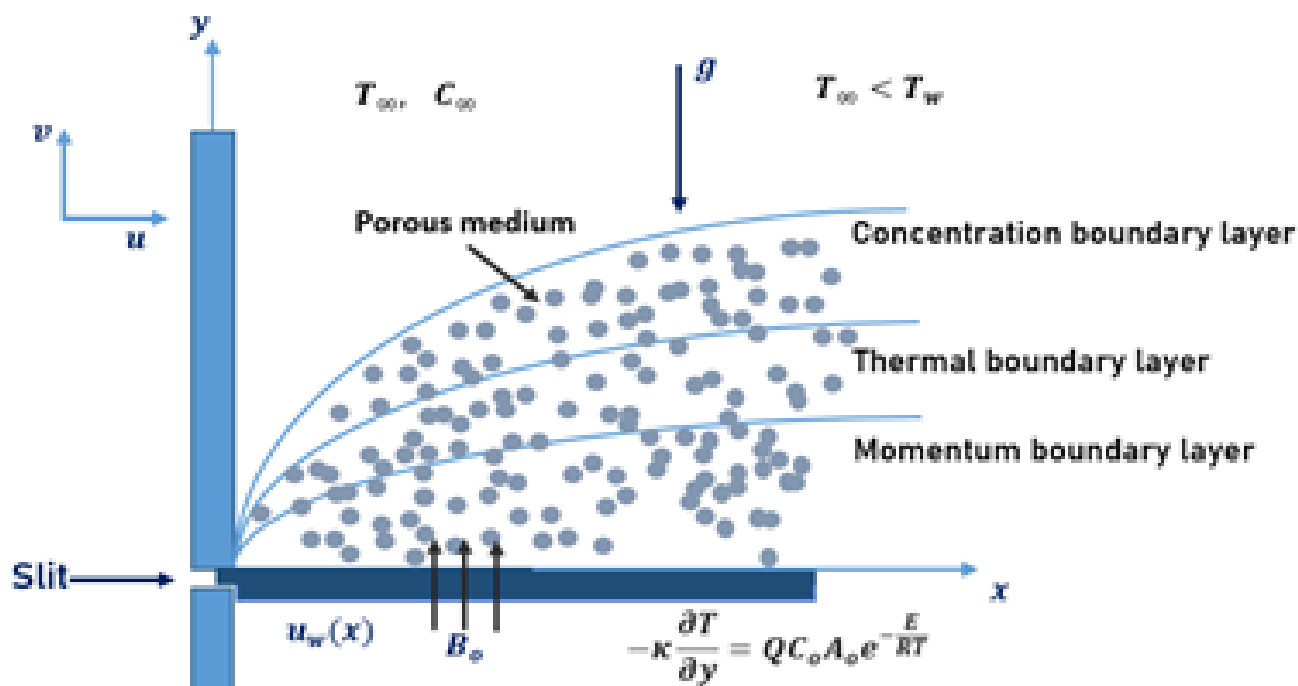
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The impacts of temperature dependent viscosity on radiative Maxwell fluid flow over an autocatalytic stretching sheet with chemical reaction is investigated in this work. Soret effect is invoked in the present study. The strongly nonlinear model equations are changed into system of ordinary differential structure with the help of proper non-dimensional quantities. The fourth order Runge-Kutta Fehlberg (RKF) numerical method is utilized to solve the transformed system of ODEs. The behaviors of flow, thermal and solutal fields under the influence of different model parameters are presented and discussed in detail via

graphs and tables. In this study, higher values of Frank-Kamenetskii parameter and permeability parameter is found to escalate temperature distribution. Also, concentration distributions drop rapidly by varying Schmidt number but enhances in the presence of Soret number. Comparison of the present results with previous study is examined and excellent concurrence is observed. The present study is relevant in chemical engineering applications where the formation of boundary layer is to be delayed or enhanced and in oil recovery processes.





**Flow configuration**



## Ultraviolet actinometry: Determination of the incident photon flux and quantum yields for photochemical systems using low-pressure and ultraviolet light-emitting diode light sources



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The study of the interaction of light with photochemical and photobiological systems requires an accurate assessment of the incident photon flux. The determination of photon fluxes for various light sources (monochromatic and polychromatic) has an inherent advantage since the use of standard quantum yields for the actinometer assures that the photon flux has been calculated against accepted standards. Alternatively, if the photon flux is known, chemical actinometry can be used to determine quantum yields. This study illustrates how incident photon fluxes and quantum yields can be estimated for photochemical and photobiological systems. First, an example is developed to calibrate a spectroradiometer using a low-

pressure (LP) UV lamp using either the ferrioxalate or iodide/iodate actinometers. The Calibration Factors (CFs) (defined as the ratio between the actinometer and the spectroradiometer) agreed very well, demonstrating the consistency of quantum yields between well-researched actinometers. Second, since UV-LEDs have a bandwidth almost twice that of LP lamps, should UV-LEDs be treated as monochromatic or polychromatic light sources? Results showed no significant differences between the monochromatic analysis and the polychromatic analysis. Third, the uridine quantum yield is  $0.025 \pm 0.001$  over the 254-279 nm wavelength range, independent of these wavelengths.



## Motion as a concept, an insufficient element in the kantian philosophy



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This article examines the Kantian ideas on motion in his work *Metaphysical Foundations of Natural Science*. In that essay, Kant holds that motion as a concept—from its connotation as elemental and fundamental predicament of the material reality—mobilises in matter all the characteristics of its essence as a property. Nevertheless conceiving motion as a concept does not enable us to confirm the existence of motion itself in the natural world because ‘the possibility of specific natural things can’t be discovered from their mere concepts.’ (Kant in *Principios metafísicos de la ciencia de la naturaleza*. Tecnos, Madrid, 7. 1991). Therefore, the concept of movement does not evidence the existence of the movement or its

characteristics and properties. Such claim would imply that motion as a concept is not evidence of the existence of motion as such and, therefore, the properties of matter cannot be mobilised based on that concept because they are characteristics of the essence of motion. Then, how does Kant intend to denote motion? Why pretend to explain matter form the concept of motion if a pure concept is, by definition, independent of the data obtained from the sensibility? (Colomer in *El pensamiento alemán. De Kant a Heidegger*. Herder, Tomo I. Barcelona, 114. 1986). Therefore, we will demonstrate that such weakness is the breaking point of the Kantian concept of motion in his “dynamic-metaphysical” model.



## **Recycling pollutants and used oils as substrates for producing useful lipids by using microbial biotechnological process**



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Oleaginous microorganisms have the ability to use oils and fats as carbon source, making them a promising cell factory for the design of alternative bioprocesses based on renewable substrates. The non-pathogenic oleaginous yeast *Yarrowia lipolytica* has become more useful in the field of biotechnology and its environmental applications, since it contains an excellent enzyme system that enables it to degrade and assimilate a wide range of substrates. Therefore, single-cell oil production that can potentially be used as a supplier of functional oils and/or biodiesel, could be coupled with the use of hydrophobic waste, as a low-cost culture medium. Our latest studies showed the high potential of the yeast *Y. lipolytica* to degrade used oils and olive mill wastes (effluents). The latter are effluents resulting

from olive oil extraction industry, they are known as highly polluting and harmful to the environment.

Thus, the profiles of accumulated fatty acids were not strictly dependent on carbon substrates but also on the microbial strain, which it showed a clear biomodification effect on the substrate's lipids used to a higher degree. Most of the fatty acids of the microbial accumulated lipids were unsaturated and corresponded mainly to oleic, and linoleic acids, making the used strain of *Yarrowia lipolytica* valuable from a nutritional point of view. Consequently, the strain in question can be considered as a good tool for integration into bioremediation solutions that realize the requirements of the circular economy and of environmental sustainability.



## Expression of de novo ceramide synthesis enzymes in local fat depots in smoking patients with coronary artery disease



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**Aim:** To study the relationship between the expression of de novo ceramide synthesis enzymes in adipose tissue (AT) and smoking in coronary heart disease (CAD).

**Methods:** The study included 30 patients with CAD, undergoing coronary artery bypass grafting. Biopsies of subcutaneous, epicardial, perivascular AT (SAT, EAT, PVAT, respectively) were obtained during surgery. Expression of de novo ceramide synthesis enzyme genes (serine palmitoyltransferases C1 and C2 subunits SPTLC1, SPTLC2; ceramide synthase 1-6 CERS1-6; dihydroceramide desaturase DEGS1) was assessed by quantitative real-time polymerase chain reaction (qPCR) using TaqMan™ in a ViiA 7 Real-Time PCR system (Applied Biosystems, USA). Smoking is classified as current (at least one cigarette per day within the past year) or former smokers. Statistical analysis of the results was performed using GraphPad

Prism 8 (GraphPad Software).

**Results:** Among the examined patients with coronary artery disease, 17 were smokers, 13 were not. Analysis of the studied parameters depending on the fact of smoking in patients with CAD showed that smokers were characterized by increased expression of SPTLC1, SPTLC2, CERS1, 2, 4, 6 and DEGS1 in adipocytes of subcutaneous, epicardial and perivascular localization ( $p < 0.005$ ).

**Conclusions:** Thus, in patients with CAD, smoking revealed an increase in the expression of most enzymes of the main pathway for the synthesis of ceramides in all types of AT. The data obtained indicate a close relationship between the expression of enzymes of the main ceramide synthesis pathway in AT and smoking in patients with CAD. One of the reasons for this may be the development of hypoxia, which activates de novo ceramide biosynthesis.



## **Positive magnetoconductivity and inelastic scattering time at low temperatures with magnetic field in InSb semiconductor**



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In this work, we investigate the temperature dependence of the perpendicular electrical conductivity in presence of magnetic field of InSb sample measurements obtained by S. Abboudy [1]. First we determine the value of the critical magnetic field  $B_C$  for which the Metal Insulator Transition (MIT) occurs.

On the metallic side of the MIT, we are interested in the study of positive magneto conductivity as a function of magnetic field by modeling it with complex theoretical models. The validity of these models is tested by calculating and comparing the inelastic scattering time  $\tau_\epsilon$  for each model used.



## **Blockchain Technology prospects in transforming Ghana's economy: A phenomenon-based approach**



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A phenomenon-based approach is used to learn more about how blockchain technology could improve Ghana's economic sectors in terms of cost savings, efficiency, and reliability with reduced risks. With our proposed blockchain-enabled frameworks, we describe how blockchains' Internet-of-Things (IoTs) and Distributed Ledger Technologies (DLTs) might reduce transaction, contract, and monitoring-related costs in the Agriculture & Agro-processing sector's supply chains. We also demonstrate how Smart Contracts (SMCs) and Distributed Ledger Technologies

(DLTs) can improve time and cost-based efficiencies in local procurements, logistic contract execution, and supply chains across the Mining & Minerals processing sector. With the help of IoTs, DLTs, and SMCs, information asymmetries in the finance sector can be reduced to improve the financing for Small and Medium-sized Enterprises (SMEs). The Technological-Organizational-Environmental (TOE) elements remain crucial in the adoption of blockchain technology. As a result, it's critical to provide adequate frameworks for blockchain adoption.



**Applying a social-ecological model to understand factors impacting demand for childhood vaccinations in Nigeria, Uganda, and Guinea**



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Low vaccination demand threatens global child mortality reduction. Demand frameworks prioritize primary caregiver decision-making. We used an adapted socio-ecological model to analyze 158 interviews with primary caregivers, fathers of young children, and community influencers in Nigeria, Uganda, and Guinea to better understand vaccine demand.

This study collected qualitative and quantitative data from Nigerian, Ugandan, and Guinea-Conakry mothers and fathers of infants. The qualitative phase participants were over 18 and had a child aged 2–4 (in Nigeria) or 1–3 (in Ghana) (in Guinea and

Uganda). Convenience sampling was used to recruit the participants, and a moderator led a 90-minute discussion on household roles, child protection, and vaccination. Participants gave written consent. An honorarium for their time was provided. Each country's ethics boards approved the research.

The findings showed that the decision to vaccinate a child is informed by a primary caregiver's web of family and community relationships and a range of environmental and contextual factors. In addition, even though directly taking care of the child is seen as the mother's role, fathers are



involved in decisions about child health. Fathers often grant permission for mothers to vaccinate children, or even for them to leave the house. This suggests that fathers have decision making powers over vaccination decisions and could act as an enabler or blocker. Also, belief in God's and traditional protection may in some cases lead to rejection and replacement of vaccination.

Low vaccination demand in many countries may lead to under-immunization and higher childhood mortality. This research provides guidance on how to design demand creation interventions for fathers. Linking vaccination with the financial and social success of the family and ensuring that encouragement to vaccinate is delivered by trusted community figures are likely to have a positive impact on completion of immunization schedules.



## Surface markers of stem cells from epicardial and perivascular adipose tissue in patients with coronary artery disease



**Olga Gruzdeva, Evgenya Uchasova, Yulia Dyleva, Ekaterina Belik, Vera Matveeva, Maxim Zinets and Olga Barbarash**

*Federal State Budgetary Scientific Institution Research Institute for Complex Issues of Cardiovascular Diseases, Russia*

**Aim:** To describe the immunophenotype of ADSCs isolated from epicardial and perivascular fat depots in patients with coronary artery disease.

**Methods:** The study included 5 patients with CAD. The average age is  $65.5 \pm 5.5$  years. Patients had indications for open intervention on the heart-direct myocardial revascularization by CABG. ADSCs from biopsy samples of epicardial and perivascular AT that were obtained from patients during surgery (CABG or correction of heart defects) and isolated according to the method of Zeng G(2013). When cells grew to 80–90% confluence, they were digested with 0.25% trypsin and proliferation for subsequent experimental analyses. Flow cytometry analysis was performed on passage 2 cells.

**Results:** On the 29<sup>th</sup> day of cultivation (pas. 2), it was shown that CD105 and CD90 were present in the EAT of a patient

with CAD on 79.71%, while one antigenic marker CD105 was present in 17.54% of the cells. Membrane proteins CD73 and CD90 were present in 79.47%, only one CD73 in 18.26% of cells, while CD34 was present in only 3.76%. Thus, the phenotype of the resulting culture of cells isolated from EAT CD73+, CD90+, CD105+, CD34-. In addition to the main population, 2 minor: 1-CD90-, CD105+, CD34-, CD73+ CD45- presumably endothelial population, 2-CD90+, CD105-, CD34-, CD73-, CD45- presumably hematopoietic population. In PVAT, a high (over 90%) expression of membrane proteins characteristic of stem cells. CD34 was expressed by 3.46%. In PVAT, we observe 3 populations, as in EAT.

**Conclusion:** At the early stages of cultivation, SVF PVAT and EAT contain cells that carry markers inherent in both AT stem cells and markers of hematopoietic and endothelial populations.



## Mixed stochastic heat equation with fractional laplacian and gradient perturbation



**Eya Zougar** and **Mounir Zili**

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We introduce a new stochastic heat equation with a mixed operator, which is a combination of the standard Laplacian, a fractional Laplacian and the gradient operator, driven by an additive Gaussian noise which is white in time and in space. We establish the existence of the solution and we study its

behavior with respect to the time variable. In particular, we establish sharp two-sided interesting estimates of its variance increments, which allow us to get some regularity characteristics of the solution sample paths, among many other possible applications.



## Surface modification of the membrane used in commercial air gap membrane distillation system



**Ganesh Bapu Shirsath**

*Adsul's Technical Campus, India*

Water can be cleansed with a hydrophobic layer in membrane distillation system especially in AGMD design. The current work presents trial information for such a framework. The significance of individual jobs of feed water temperature and stream rate, cold water temperature and stream rate and the degree of air gap on water distillation rate is examined. Potential enhancements in the experimental setup is analyzed by utilizing surface modification of the hydrophobic film. In this regard, a layer of

lead from a pencil is covered over the film. Rate of evaporation through the pencil-covered layer were estimated in a solar simulator powered test system with 1 sun, 2 sun and 3 sun settings. A significant improvement in the rate of evaporation was seen when a pencil covered film was utilized. Following this perception, an increased two-sided AGMD framework is proposed, that conveys a covered layer presented to sun based radiation on one side and an uncoated film on the other.



## Challenges in developing strategies for the valorization of lignin—A major pollutant of the paper mill industry



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**A**part from protecting the environment from undesired waste impacts, wastewater treatment is a crucial platform for recovery. The exploitation of suitable technology to transform the wastes from pulp and paper industries (PPI) to value-added products is vital from an environmental and socio-economic point of view that will impact everyday life. As the volume and complexity of wastewater increase in a rapidly urbanizing world, the challenge of maintaining efficient wastewater treatment in a cost-effective and environmentally friendly manner must be met. In addition to producing treated water, the wastewater treatment plant (WWTP) has a large amount of paper mill sludge (PMS) daily. Sludge management and disposal are significant problems associated with wastewater treatment

plants. Applying the biorefinery concept is necessary for PPI from an environmental point of view and because of the piles of valuables contained therein in the form of waste. This will provide a renewable source for producing valuables and bio-energy and aid in making the overall process more economical and environmentally sustainable. Therefore, it is compulsory to continue inquiry on different applications of wastes, with proper justification of the environmental and economic factors. This review discusses current trends and challenges in wastewater management and the bio-valorization of paper mills. Lignin has been highlighted as a critical component for generating valuables, and its recovery prospects from solid and liquid PPI waste have been suggested.



## **ANN-based modeling of combined O<sub>3</sub>/ H<sub>2</sub>O<sub>2</sub> oxidation, and activated carbon adsorption treatment system: forest polluting site leachate**



**Ghorban Ali Dezvareh<sup>1</sup> and Erfan Nabavi<sup>2</sup>**

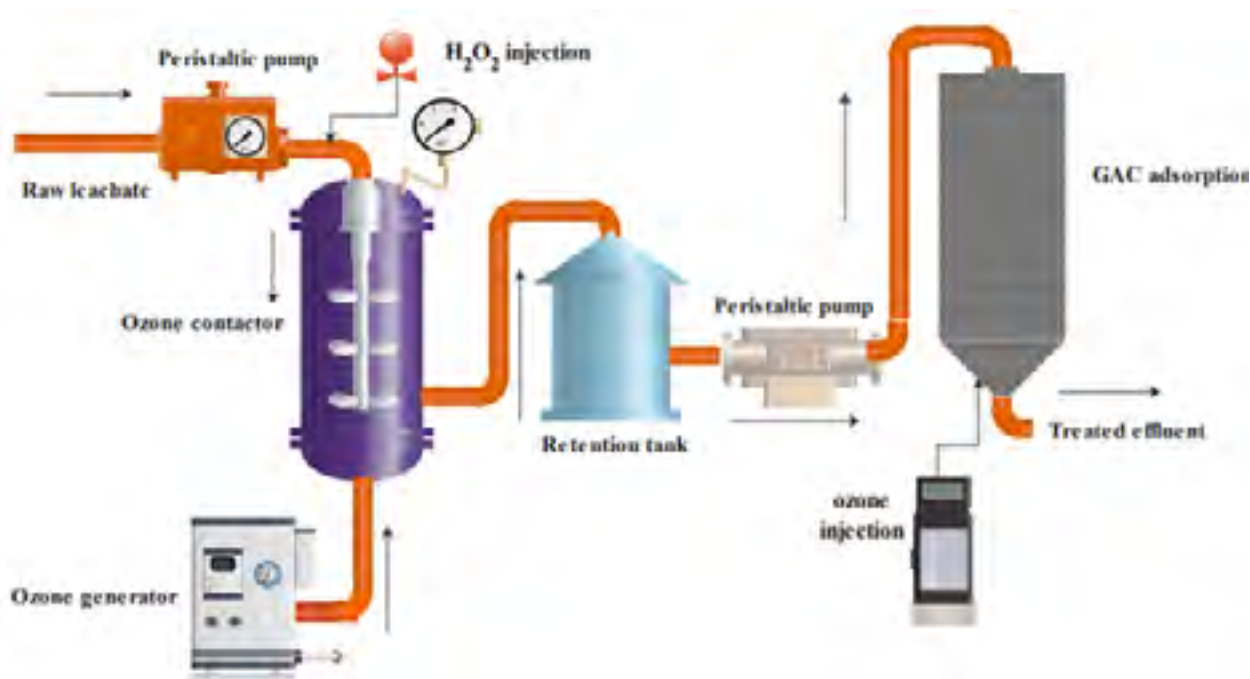
<sup>1</sup>Tarbiat Modares University , Iran

<sup>2</sup>Khaje Nasir Toosi University of Technology , Iran

**T**reatment of organic leachate is one the most controversial topics around the world which led this study to assess the efficiency of the combined oxidation and adsorption treatment (COAT) process in the treatment of forest polluting site (FPS) leachate by considering local experiments. The removal of effluent parameters (TDS, COD, BOD) was enhanced by oxidizing the GAC surface as a catalyst with NaOH before the process and by ozone within the procedure as well. comparison between COAT process and ozone-GAC was investigated based on variation in ozone dose, H<sub>2</sub>O<sub>2</sub> and pH. Assessing the interacting effect of operating variables (i.e., ozone concentration, GAC density, reaction time and pH) provides valuable information for optimization. Response Surface Methodology (RSM) and for better

prediction, another modeling tool, Artificial Neural Networks (ANN), were employed. Moreover, the results of both software were compared and ANN showed a higher R<sup>2</sup> of 0.908, 0.923 and, 0.919 for TDS, COD and BOD respectively in contrast with RSM (R<sup>2</sup>: TDS= 0.8538, COD=0.9105, BOD=0.8108). The optimized model's circumstances are the reaction time of 30.77 min, ozone dosage of 141.29 mg/l, pH of 7.2, and the GAC density of 1.29 gr/cm<sup>3</sup> with the predicted removal percentage of 51.63%, 62.84% and 56.13% for TDS, COD and, BOD respectively. Meanwhile, in the experimental situation amongst the various methods, the COAT process by the removal percentage of TDS=59.47%, COD=68.37%, and BOD=67% showed proper efficiency.

*Fig. 1. The schematic of the COAT process*





## The concentration and health risk assessment of potentially toxic elements (PTE's) in vegetables from southern districts of Punjab, Pakistan



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**Context/Purpose:** The present study was aimed to evaluate the concentration and health risk assessment of potentially toxic elements in vegetable samples (spinach, mustard greens and cauliflower) which were collected from different sites of drought and salinity hit areas of southern districts of Punjab Pakistan.

**Methods:** Cadmium, copper, cobalt, chromium, iron, manganese, nickel, lead and zinc concentrations were detected by the help of atomic absorption spectrophotometer. Chronic daily intake (CDI), Hazard quotient (HQ) and cancer risk (CR) of PTEs were calculated by using the appropriate formulas.

**Results:** The order of mean concentrations observed in spinach, mustard greens and cauliflower from district Dera Ghazi Khan were as follows Fe > Mn > Zn > Cu > Cr > Co > Pb > Cd > Ni, Fe > Mn > Zn > Cu > Cr > Cd > Ni > Co = Pb and Fe > Zn > Mn > Cu > Cr > Co > Cd > Ni > Pb respectively. While the order of mean

concentrations observed in mustard greens and cauliflower from district Rajan Pur were as follows Fe > Mn > Zn > Cu > Cr > Co > Pb > Cd > Ni, Fe > Zn > Mn > Cu > Cr > Cd > Pb > Ni > Co and Fe > Zn > Mn > Cu > Cr > Pb > Cd > Ni > Co respectively. The order of mean concentrations observed in mustard greens and cauliflower from district Rahim Yar Khan were as follows Fe > Mn > Zn > Cu > Cr > Co > Pb > Ni > Cd, Fe > Mn > Zn > Cu > Cr > Co > Cd > Ni > Pb and Fe > Zn > Mn > Cu > Cr > Co > Pb > Cd > Ni respectively. Co and Pb were not detected in most of the vegetable samples. Cu was observed under the range recommended by WHO/FAO (73ppm) in all vegetable samples. Highest concentration was found of iron in spinach from Iqbal Abad was 1872.6 ppm that exceeds the maximum permissible limit (425ppm) suggested by WHO/FAO. CDI values of Zn were equal to the permissible value (0.3mg/kg/day). CDI values of Cd, Co and Ni were found in the range of permissible limits (0.001, 0.03 and 0.02mg/kg/day) by WHO/FAO. Meanwhile CDI values of Cr, Cu, Fe, Mn



and Pb were higher than the suggested limits (0.003, 0.037, 0.7, 0.083 and 0.0015mg/kg/day respectively) by WHO/FAO. HQ values of Zn were almost equal to limits and values of Co and Ni were under the range of limits meanwhile values of Cd, Cr, Cu, Fe, Mn, and Pb were exceed the limit (should be less than 1) by WHO/FAO. CR values of Cr were almost near about the range and Zn, Cd, Co, Ni and Pb were in the range meanwhile values of Cu, Fe, Mn and Zn were exceeding the range (10<sup>-4</sup>-10<sup>-6</sup>) suggested by WHO/FAO.

**Interpretation:** Environmental pollution and industry processing are the main attributes to the elevated level of potentially toxic elements.

**Conclusion:** Checking the exposure and plausible involvement for reducing further exposure to the potentially toxic elements in human and the environment can become a significant step concerning prevention.



## Glycemic response of volunteers to the consumption of supplements and food formulas for oral and/or enteral nutrition



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<sup>2</sup>Danone Brazil LTDA, Medical Affairs Department, Brazil

**Purpose:** The objective of this study was to determine the glycemic index (GI) and glycemic load (GL) of three products from the Brazilian market used as a supplement and food formula for oral and/or enteral nutrition.

**Methods:** The volunteers (n=16) attended Food Research Center weekly for six weeks after a 10–12-h overnight fasting. Blood was sampled in the fasting state (t=0) and at 15 min, 30 min, 45 min, 60 min, 90 min, and 120 min after starting to eat each evaluated meal: glucose solution (reference food, three times) and three products: Cubitan® vanilla (specific for wounds healing), Diasip® chocolate, and Diasip® vanilla (diabetic supplements). GI was determined by calculating the area under the glycemic response curve using the trapezoidal rule and ignoring the areas below the fasting line and considering the

GI of glucose to be 100. To determine GL, it was considered the amount of carbohydrates available in a standard serving of the product and GI.

**Results:** The three products studied showed low GI and low GL (Cubitan® GI=35, GL=6; Diasip® chocolate GI=49, GL=7; Diasip® vanilla GI=47, GL=7), with significant differences from those and the reference food, but no significant difference between them. Similar results were also observed for the blood glucose peak, which occurred 30 min after the consumption of all products.

**Conclusions:** GI and GL of the products were considerably lower than those of the reference food. The products evaluated presented a low glycemic response, shown by a glycemic response curve with a slightly accentuated shape and no high peaks.



## Improvement in cowpea variety Videza for traits of extra earliness and higher seed yield



**Godwin Amenorpe<sup>1,2</sup>, Innocent Kwaku Dorvlo<sup>2</sup>, Harry Mensah Amoatey<sup>2</sup>, Samuel Amiteye<sup>2</sup>, Jacob Teye Kutufam<sup>1</sup>, Emmanuel Afutu<sup>3</sup>, Elvis Asare-Bediako<sup>3</sup> and Alfred Anthony Darkwa<sup>3</sup>**

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The cowpea variety Videza, which was used as the control, matures early (70 days after planting), although it produces low yields. Gamma irradiation mutagenesis was used to induce Videza into extra-early maturing and higher yielding mutant genotypes. A single seed descend population was developed for radio-sensitivity test, and a Lethal Dose 50 (LD50) of 240.5 Gy was determined, and applied from a cobalt-60 (60Co) source, to acutely mass irradiate 1800 Videza seeds, at the Ghana Atomic Energy Commission. The irradiated seeds (M1) were planted to produce M2 seeds bearing plants and subsequently advanced to M3 plants for selection of nine induced plants based on extra earliness and significantly higher seed yields than the parental control. It took 48 days after planting (DAP) for the genotype coded P1N02#1 to reach 50 % maturity followed by 52 DAP for genotypes

with codes P4N03#3; P3N01#5; P5N05#6, P4N14#7, P5N07#8, P5N05#10 and 54 DAP for genotype P4N14#11. P1N06#9 had the highest yield (97.38 g/plant), followed by P5N05#10 (95.97 g/plant), P1N08#13 (81.24 g/plant), P2N09#12 (73.94 g/plant), P6N10#19 (70.83 g/plant), P1N06#20 (65.36 kg/plant), P5N07#14 (61.23 g/plant), P4N14# (58.05 g/plant) and P1N08#17 (56.23 g/plant). M3 seeds were advanced to M4 plants for a Preliminary Yield Trial which revealed that induced plants P5N05#10 (1235 kg/ha), P2N09#12 (1206 kg/ha), P5N07#14 (1185 kg/ha), P1N06#20 (1171 kg/ha), P1N06#9 (1051 kg/ha), P1N08#13 (1041 kg/ha), and P6N10#19 (999 kg/ha) outperformed the control (517 kg/ha) and two other commercial varieties. Overall, the two highest performing candidates for further evaluation for varietal release were P5N05#10 and P2N09#12.



## Facile green synthesis of zinc oxide nanoparticles: Phytotoxicity, design experiments and optimization of photocatalytic activity using Box-Behnken design



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*Laboratory of water Membrane and Environmental Biotechnology CERTE, Tunisia*

In this research, zinc oxide nanoparticles (ZnO-NPs) were successfully prepared using the extract of verbena as a capping agent and were used in photodegradation of crystal violet dye. The obtained powder was characterized using XRD, FTIR, SEM and DLS. The X-ray diffraction results confirmed that the synthesized ZnO nanoparticles had a hexagonal wurtzite structure. The average crystalline size of around 25nm was observed by the Debye-Scherrer formula. SEM analysis showed the shape of the NPs to be spherical whereas the Dynamic Light Scattering showed a range of sizes 20nm. The Box-Behnken design (BBD) in response surface methodology (RSM) was used to optimize several process variables, including concentration dye [CV] (A: 10–30 ppm), catalyst dose (B: 1–3mg/

L), and contact time (C: 20–70min). The used model was clearly very appropriate, as indicated by the adjusted coefficient of determination (R<sup>2</sup>) value 0.99 and the RSM chosen was efficient in optimizing Crystal Violet degradation conditions. The current study takes a fresh look at the effects of nanosized biosynthesized ZnO NPs on agricultural production (development and photosynthesis) and plant defensive performance (defense systems) in White beans (*Phaseolus vulgaris* L.). Changes in metabolic responses in plant sections, exposure duration and NPs concentrations all influenced the impacts of NPs exposed. These results suggest that a heterogeneous photocatalytic process utilizing ZnO NPs is efficient in environmental remediation.



## Synthesis, characterization and evaluation of anti- arthritic potential of curcumin loaded chitosan nanoparticles



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*University College of Conventional Medicine, Islamia university of Bahawalpur, Pakistan*

**Background:** Curcumin is a versatile phytomolecule derived from *Curcuma longa*'s dried rhizome, which have a lot of biological activities and have hydrophobic property.

**Objectives:** The current study was conducted to fabricate, characterize and optimize Curcumin loaded chitosan and STPP Nanoparticles and improved bioavailability.

**Methods:** Curcumin loaded Chitosan and STPP Nanoparticles were fabricated employing Ionic gelation method. Four formulations were developed based on the selected variable like STPP concentration, chitosan concentration, Rotations per minute, temperature and pH of chitosan solution. Nanoparticles were characterized for morphology, drug-polymer compatibility, percentage yield, mean particle size, encapsulation efficiency, release behavior, anti-inflammatory and antiarthritic activity.

**Results:** FTIR spectroscopic analysis established the stable character of Curcumin in nanoparticles and produced

sharp characteristic peaks representing at 3519cm<sup>-1</sup> of O-H group, C-OH bending at 1366cm<sup>-1</sup> and bending vibration of -CH bond of alkene group at peaks 728cm<sup>-1</sup> and 950cm<sup>-1</sup>. Maximum percentage yield was found to be 60%. Encapsulation efficiency of Nanoparticles ranged from 30.2 μm to 76.7μm and 78.8 to 96.2% respectively. Curcumin release from optimized formulation was maintained in vitro up to 24 hours following first order release kinetics and non-fickian transport mechanism. 600 microgram per ml of Curcumin shows 52% anti-inflammatory activity by membrane stabilization method which is less than standard drug result whereas 71% antiarthritic activity by protein denaturation method which is equivalent to standard drug (Dicloran).

**Conclusion:** The study concluded that Curcumin loaded Chitosan and STPP Nanoparticles can be formulated successfully by Ionic gelation method, which increased Curcumin absorption leading to reduced dosing rate and improved patient compliance.

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**Selection of  
conventional  
preservation  
technologies  
using analytical  
hierarchy process**  
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**Hailemariam Gebru<sup>1</sup>, Baba Abdissa<sup>1</sup>, Betelhem Addis<sup>2</sup>, Sisay Alebachew<sup>2</sup> and Abaysew Ayele<sup>3</sup>**

<sup>1</sup>*Materials Science and Engineering Directorate, Bio and Emerging Technology Institute, Ethiopia*

<sup>2</sup>*Technology and Innovation Institute, Ethiopia*

<sup>3</sup>*Armauer Hansen Research Institute (AHRI), Ethiopia*

Vegetable crop quality loss commences right along the route of harvesting, transportation, storage, and delivery to consumers. Despite the huge postharvest loss of horticultural crops recorded, no reports have been disclosed on alternative preservation technologies in Ethiopia. Herein, an analytical hierarchy process was employed to select the best food preservation technology. Pairwise comparison of the criteria with respect to the goal was performed based on the suggestion's food technology experts. Considering the economic feasibility and

personal skill, fermentation (29.0%) took the greatest weight followed by the hot water treatment technique (27.3%). Likewise, those techniques for tomato preservation in different ways like solar dryer, cold house storage, and modified atmosphere packaging account for 20.7%, 15.6%, and 7.3% respectively. This finding would serve as input data for small to large holding farmers, retailers, investors as well as stakeholders in the food processing sector and support the sustainable development intent.



## Enhanced structural and microwave applications of M -Type (Ca-Ba) hexaferrites



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<sup>2</sup>Centre of excellence in solid state physics, University of The Punjab, Pakistan

Effect of rare earth and Divalent (InMn) substitution on the structural electrical and dielectric properties of  $\text{Sr}_{0.5-x}\text{Ba}_{0.5}\text{In}_x\text{Mn}_y\text{Fe}_{12-y}\text{O}_{19}$  ( $x = 0.00-0.10$ ;  $y = 0.00-1.00$ ) Hexaferrites prepared by sol-gel auto combustion is reported. The synthesized samples were characterized by Fourier transform infrared spectroscopy, X-ray diffraction, scanning electron microscopy electrical and dielectric properties (resistivity and conductivity). The X-ray diffraction analysis confirmed single phase M-type hexa-ferrite structure.

The lattice parameters were found to increase as In Mn contents increases, which is attributed to the ionic sizes of the implicated cations. The InMn seems to be completely soluble in the lattice. The results of scanning electron microscopy shows that the grain size decreases with increase of In Mn substitution. The increased anisotropy and fine particle size are useful for many applications, such as improving signal noise ratio of recording devices.



## **Preparation of nonionic softener based on wool wax and its utilization in functionalization of textile fabrics**



**Hosam El-Sayed, Salwa Mowafi and Marwa Abou Taleb**

*Proteinic and Man-made Fibres Department, Textile Technology Research Institute, National Research Centre, Egypt*

**T**extile industries utilize huge amounts of auxiliaries to impart certain desired properties to the final textile goods. Herein we prepared a nonionic softener based on wool wax which is a by-product from the wool scouring process. Fatty acid(s), isolated from wool wax, was reacted with a bifunctional amino aliphatic compound to synthesize the proposed auxiliary. The prepared softener was utilized as a finishing agent that imparts luxurious desirable touch for selected textile fabrics with the minimum accumulated electrostatic charge. Wool wax was extracted and purified from wool fleece

to obtained lanolin. The extracted lanolin was saponified followed by neutralization to obtain free fatty acid. The free fatty acid was reacted with a dihydroxy amino saturated aliphatic hydrocarbon to produce a condensate whose softening action of textile fabrics. The chemical structure of the prepared nonionic softener was elucidated using FTIR and <sup>13</sup>C NMRC. The physical, chemical, and mechanical properties of the treated fabrics were evaluated using the appropriate methods of analysis. The scanning electron microscopy was used to monitor the change in the fibre morphology after application of the prepared softener.



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**An innovative  
ballasted track  
utilizing stabilized  
clayey subgrade**

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**H. Ghorbani Dolama<sup>1</sup>, J.Zakeri<sup>2</sup>, M.Esmaeili<sup>2</sup> and P. Hayati<sup>1</sup>**

<sup>1</sup>SRBIAU, Iran

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The traditional ballasted tracks have been used widely in railway transportation infrastructure. Construction of ballasted tracks on the clayey soft subgrade causes high settlement and low bearing capacity. Significant maintenance cost and time-consuming operation have been encountered due to presence of clay. Using road construction experience with Royal Road Product (RRP235 Special), as an innovative method for the first time, the layers underneath the sleeper have been replaced with the clayey subgrade stabilized with RRP 235 special. A series of static and dynamic lab experiments such as Maximum Compaction test, California Bearing Ratio, Unconfined

Compressive Strength, Brazilian Indirect Tensile test, Direct Shear Strength, and Uniaxial Cyclic tests were carried out. Samples with different dosages of additive were made, and an optimal percentage was found. Using the obtained dosage a part of track with length of 50 meters was made and tested with RRP. Plate loading test (PLT) and single tie push test (STPT) was carried out on track. The advantages revealed that RRP 235 special has positive effect on soil strength; therefor sleeper can put directly on the stabilized substructure as shown in figure 1. Subsequently, new proposed track needs lower construction and maintenance costs and has low environment impacts.



## Forecasting tropical cyclone-induced rainfall intensity in Australia: A comparison between bayesian approach and traditional regression method



**Kamal K Saha**

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Extreme weather such as tropical cyclone (TC) often causes major threats to life and property. Providing accurate, reliable and timely forecasts of extreme weather is a subject of great importance for meteorological agencies. It has also an immense use to the coastal peoples around the world. In this paper a Bayesian approach is applied to develop the accurate TC rainfall forecast using the Best Track database of the Australian Bureau of Meteorology (BoM). Correlation analysis was conducted to examine the individual relationship of each independent variables with the dependent variable. A multiple regression model is developed in the form of  $y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \dots + \beta_p X_p + e$ , where  $y$  is the response variable,  $X_p$  is the  $p$ th explanatory variable,  $\beta_p$  is the coefficient of the  $p$ th explanatory variable  $\beta_0$  is the constant coefficient and  $e$  is the

error term. Then the developed Bayesian model has then been compared with the traditional regression model using forecast accuracy measures. From the analytical point of view both the models are capable to produce forecasts with satisfaction. But considering precision of the findings from both models it can conclude that the Bayesian approach would be more reliable for TC rainfall forecast as compared to the traditional regression method. The mean squared error (MSE) reduced by the Bayesian model is approximately 1.75% as compared to the traditional regression model.

The result of this analysis is presented in Table 1. Only two of them  $G_{cp}$  and  $G_{lon}$  among all the independent variables showed significant relationship with dependent variable RI.



## Synthesis and metrological characterization of carboxy containing starch nanoparticles as an adsorbent for Cd (II) ions from waste water effluent



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Tailor-made and fully characterized starch nanoparticles (SNPs) having a particle size ranging from 80-100 nm was used as a starting substrate for cadmium ions removal from wastewater effluent after carboxylation with citric acid via esterification reaction using the dry preparation technique. The latter process is simple, safe, and environmentally friendly method. The obtained adsorbent is designated as cross-linked esterified starch nanoparticles (CESNPs). To validate the esterification reaction and existence of carboxylic groups in the adsorbent, CESNPs were characterized metrologically via analytical tool for carboxyl content estimation and instrumental tools using FT-IR spectra and SEM morphological analysis. The batch technique was used to determine the CESNPs adsorption capacity, while atomic adsorption spectrometry was used to determine the residual cadmium ions concentration in the filtrate before and after adsorption. Different factors affecting

adsorption were examined with respect to pH, contact time, adsorbent dose, and degree of carboxylation. The overall adsorption potential of CESNPs was found to be 136 mg/g when a 0.1 g adsorbent dose having 190.8 meq/ 100 g sample carboxyl content at pH 5 for 60 min contact time was used. Besides, increasing the degree of carboxylation of the CESNPs expressed as carboxyl content would lead to the higher adsorption capacity of cadmium ions. FTIR spectroscopy analysis elucidates the esterification reaction with the appearance of a new intense peak C=O ester at 1700 cm<sup>-1</sup>; while scanning electron microscopy observations reveal some atomic/molecules disorder after esterification. The work was further extended to study the ability of CESNPs to remove basic dye from its solutions at different degrees of carboxylation in addition to the comparison with other adsorbents cited in the literature.



**Quality and  
tool stability  
improvement in  
turning operation  
using plastic  
compliant damper**



**Kitmo**

*Department of Renewable Energy, National Advanced School of Engineering of University of Maroua, Cameroon*

The major hindrance for any production industry in obtaining higher yield is the lack of achieving full material removal rate in the machine tools. If achieved, the surface quality of the machined works will be compromised. An attempt was made in this work to reduce the compromise of surface finish by integrating a plastic compliant damper that is capable of reducing the effects of unwanted vibrations generated during the machining process. The damper is designed

to degenerate the effects of vibration and thereby improve product finish. It is made of Acrylonitrile butadiene styrene by fused deposition modelling (an additive manufacturing technique). Measuring the vibration and cutting force is indirectly related to finish in product and tool wear rate. The stability of tool is improved greatly by the new compliant damper possessing displacement resistance. The peak surface roughness is reduced by 48% by using the proposed compliant damper.



## Spontaneous speech feature analysis for Alzheimer's disease screening using a random forest classifier



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Detecting Alzheimer's disease (AD) and disease progression based on the patient's speech data can aid non-invasive, cost-effective, real-time early diagnostic and repetitive monitoring in minimum time and effort using machine learning (ML) classification approaches. The paper aims to predict early AD diagnosis and evaluate stages of AD through exploratory analysis of 22 acoustic features, non-stationarity, and non-linearity testing, and applying data augmentation techniques on AD and cognitively normal (CN) spontaneous speech. Evaluation of the proposed AD prediction and AD stages classification models using Random Forest classifier yielded accuracy rates of 82.2% and 71.5%. This study involved exploratory data analysis to understand why machine learning models make the decisions they do, and why it matters. It was found that the speech signals have a non-linear and a non-stationary expression. Signal segmentation was applied as pre-processing step for non-

stationary signal analysis. Non-linearity property was handled by applying a large portion of acoustic features with a non-linear expression. This will enrich the Alzheimer's research community with further understanding on methods to improve models for AD classification and addressing non-stationarity and non-linearity principles on audio features to determine the best suited acoustic features for AD identification. The model can be used to screen and successfully distinguish between sick and healthy individuals and can further be applied to distinguish the stage of the disease and can therefore be applied to a telemedicine platform to provide patients with limited mobility and/or geographic limits access to specialists, making medical consultations and diagnostics more affordable and convenient. Although further procedures and tests are still mandatory, patient engagement and early intervention would be aided by a telemedicine platform.

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**Thermal  
consequences of  
dynamic phantom  
AdS black hole by  
utilizing barrow  
and logarithmic  
corrections**  
”

**Lubna Nosheen, Alia Hanif and M. Umair Shahzad**

*University of Okara, Pakistan*

We will interpret the thermal consequences of the dynamic phantom Anti-de sitter (AdS) black hole by utilizing Barrow and Logarithmic corrections. Both techniques are compatible and lead us to better results. In this work, we first examine the pressure, how it behaves using barrow corrected entropy, and Bekenstein entropy with the impacts of the cosmological parameter as well as electric charge and magnetic charge the pressure gets increases using barrow in comparison with Bekenstein entropy. When we compare it to the results of logarithmic corrections, we can conclude that pressure is more accurate using barrow entropy instead of logarithmic corrected entropy. Our major analysis is the comparison of the barrow and logarithmic corrected entropies on dynamic phantom AdS black hole and in our analysis, we find better results by using barrow's corrected entropy as compared to logarithmic corrected entropy. Furthermore, we compare different

significant thermodynamical amounts like entropy, specific heat, Helmholtz free energy, and Gibb's free energy. In the same line, we talk about the stability of dynamic phantom AdS black holes at constant pressure and volume. We have also discussed here  $\gamma$  the ratio of specific heat at constant pressure and volume. Gamma  $\gamma$  shows the maximum value at 1 with the barrow entropy and shows fluctuation with logarithmic corrected entropy. Moreover, we discuss the behavior of Gibbs free energy and Helmholtz free energy for specific values of parameters, initially both (Gibbs free energy and Helmholtz free energy) show instability. We also observe that Gibbs free energy and Helmholtz free energy do not only depend upon lambda but also on electric charge and magnetic charge. One can analyze those dynamic phantom AdS black holes becoming more stable by increasing the worth of the cosmological constant.



## Creation and realization of quasicrystal with ultracold atoms in optical lattices



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This paper introduces the creation and realization of quasicrystal with ultracold atoms in optical lattices. A single-site resolution fluorescence imaging technique is paramount for the strongly interacting bosons in an optical lattice because we can entirely reconstruct the atom distribution on the microtraps and detect individual atoms with high fidelity. Superlattice provides unprecedented

control over individual atoms in optical traps and manipulates the atomic system. Optical lattices contain thousands of strongly-interacting bosons, analogous to strongly-correlated material or electrons in the crystal. So quantum gas microscopy allows us to create of optical nano-crystal or quasicrystal with remarkable control of excitations and observes them through a high-resolution system.



## **Realistic economic design of $\bar{X}$ control charts with independent multiple assignable causes under weibull shock model**



**M. Bameni Moghadam and S. R. Shojaei**

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It has been more than six decades since Duncan (1956) proposed the economic design of control chart in the presence of multiple independent assignable causes. In all the economic designs derived from his model under the exponential shock model, it is assumed that after an assignable cause occurs, until the correct alarm is issued, another assignable cause will not occur, which is clearly unrealistic. Thus, for the first time in this paper, after proving the dependence of the probability of occurrence of this assumption in Chen and Yang economic model on design parameters, a realistic economic design for  $\bar{X}$  control chart in the presence of

$m$  assignable causes under Weibull shock model is presented. The optimal values of the design parameters show that not only in the model of Chen and Yang, the average cost per unit time of the quality cycle is severely underestimated, but by increasing the Weibull distribution shape parameter, the probability of this assumption is greatly reduced. Therefore, it is suggested to use this realistic economic model to eliminate the shortcomings of economic design of various control charts performed in the presence of multiple assignable causes on Duncan (1956) and Chen and Yang economic models.





## **Soil-to-plant transfer factor for stable elements in lemon balm (*Melissa officinalis* L.) and estimates of the daily intakes**



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<sup>2</sup>*Universidade de Taubaté, Brasil*

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This study evaluated the transfer factor (TF) of stable elements from soil to *Melissa officinalis* and the estimated daily intakes for potentially toxic elements. Lemon balm (*Melissa officinalis* L.) originates from Europe and is now grown all over the world. INAA, GFAAS, and ICP-OES techniques were applied to determine the elemental concentration. Br, Ca, Cd, K, Ni, and Rb accumulated the most with the TF ( $> 1.0$ ), followed by Ba, Co, Cr, Cu, Mg, Mn, Na, Pb, Sb, and Zn (0.1–1.0), while As, Fe, Hf, La, Sc, Sm, Th, Ti, and V had

the lowest accumulation ( $< 0.1$ ). The daily intake ( $\mu\text{g day}^{-1}$ ) of As (1.35–10.35), Br (22.5–297), Cd (0.09–0.54), Cr (220–1,270), Cu (31.5–76.5), Ni (0.09–0.54), Pb (4.5–31.5), and Zn (139.5–400.5) even overestimated was still lower than values established by WHO/FAO. This work does not only improve understanding of soil-to-plant transfer mechanism of stable elements but also increase available TF data on *Melissa officinalis* used as medicinal plants and contributing to design a best quality control of plant materials.



**Nutritional,  
organoleptic, and  
physical properties  
of biscuits made with  
cassava flour: Effects  
of eggs substitution  
with kidney bean milk  
(Phaseolus vulgaris L.)**



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Common bean forms a significant part of the diet in Africa and hence plays a critical role in human nutrition. In order to promote it, this study was designed to investigate the effects of fully substituting eggs with bean milk on the physical, nutritional and organoleptic properties of biscuits made with cassava flour. Replacement of egg by bean milk increased the biscuits' fat, carbohydrates, crude protein, and energy content. On the other hand, there were no significant differences in mineral contents between the cassava biscuits with eggs which served as the control and cassava biscuits with bean milk following substitution by bean

milk. There was no significant difference ( $p < 0.05$ ) in the Saponin and Phytate contents regarding anti-nutrients contents between bean milk and cassava bean milk biscuits. In contrast, Tannin contents were significantly higher in biscuits than in bean milk. Biscuit made with eggs, was rated as "very good," while the test biscuits were rated as "good." Substitution of egg by bean milk in cassava biscuits increased the biscuits' protein, the fat, and carbohydrates contents with an appreciable taste. These biscuits made with bean milk can be used as a food supplement to help fight protein malnutrition in vulnerable groups.



## **Experimental investigation on pyrolysis of agricultural biomass residues: Khat stem for bio-oil application**



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**K**hat stem is commonly available agricultural residue in Ethiopia and pose serious environmental hazards through the eutrophication of water streams and greenhouse gas emissions. To alleviate these impacts, thermochemical conversion of this residue through fast pyrolysis can be employed. The sample are characterized for their composition, experimental investigation has been carried out using thermogravimetric analysis at different heating rates (10, 20, 30, 40, and 50 °C/min) in the temperature range 30 °C – 800 °C under an inert atmosphere to scrutinize the decomposition characteristics. Estimation of pyrolysis kinetic parameters for this material, which is not widely available in the literature, has been done using different model-free approaches: Kissinger, Flynn–Wall–Ozawa, and Kissinger–Akahira–

Sunose. Validation of experimental data has been done and evolved pyrolysis product yields are predicted using the CRECK-S-B model. The effect of biomass characterization parameters and heating rate are also examined. The CRECK-S-B model revealed good agreement with the experimental data the sample, while being capable of capturing the hemicellulose shoulder and the residual decomposition of char at higher temperatures. The yields and composition of gas, bio-oil and char fractions are estimated, for which the biomass characterization and heating rates have influenced the distribution of the products. This study reveals the potential of this residue to promote local sustainable economies and also gives a possible solution to the environmental issue caused by their disposal.



## **Bimetallic (Cu/ Bi) oxide based dumbbell-shaped nanorod: Effective photocatalyst for the degradation of caffeic acid**



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Environmental challenges associated with organic/biological contamination and their treatment is one of the most urgent requirements, globally. Therefore, there is the requirement of developing a newer materials for the removal and treatment of wastewater. The present study reports on the synthesis of Cu-bismuth oxide (CuBi<sub>2</sub>O<sub>4</sub>)-based nanorods by using a simple co-precipitation method for the photocatalytic degradation of caffeic acid (CA). The incorporation of Cu metal ions during the synthesis of CuBi<sub>2</sub>O<sub>4</sub> nanorods might be advantageous to avoid the aggregation and control the leach out of metal ions. The calculated bandgap values of ~ 1.04, 1.02, and 0.94 eV were observed for CuBi<sub>2</sub>O<sub>4</sub> with different amounts of Cu

1.0, 0.50, and 0.25 g, respectively. Varying the quantity of Cu metal ions easily tuned the bandgap value within the CuBi<sub>2</sub>O<sub>4</sub>-based nanorods. However, a further decrease in the bandgap value increased the recombination rate, and the less photocatalyst performance was observed. The CA degradation could be explained based on the species distribution. The CA pKa was mainly located between pKa<sub>1</sub> and pKa<sub>2</sub> of 4.43 and 8.6, respectively. The Cu within the CuBi<sub>2</sub>O<sub>4</sub>-based nanorods changed the electronic properties and the antibacterial ability. Therefore, the synthesized CuBi<sub>2</sub>O<sub>4</sub>-based nanorod cluster might be a promising material for the photocatalytic degradation of CA.



**On neighborhood and closed neighborhood M-polynomial and computer based computational techniques of some closed neighborhood degree sum-based tis and their predictive**



**Mohammad Essa Nazari**

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In this work I consider some neighborhood degree sum-based topological indices (TIs) and their closed forms with two computational methods; a theoretical method using a proposed Closed Neighborhood M-polynomial (CNM-polynomial) and a computer-based method by utilizing a written MATLAB algorithm. Both the methods are useful for computational purpose of TIs under consideration. We verified closed neighborhood degree-sum based TIs on considered 22 lower Polycyclic Aromatic Hydrocarbons (PAHs) as experiment compounds and we have done a detailed

statistical analysis for prediction ability of considered TIs, we used linear regression model for analysis. Our analysis shows excellent result of prediction ability of considered TIs. Here we compare the predictive ability of closed neighborhood and neighborhood (open neighborhood) degree sum-based TIs. Our comparison shows a considerable result of predictive power of closed neighborhood degree sum-based TIs. This may help researchers in QSPR/QSAR methods to predict physicochemical properties of molecules.



## Synthesis and characterization of novel semi-IPN hydrogels of poly (Acrylic Acid) (PAAc)- poly (Allylamine) (PAIAm) and PAAc-poly(Allylamine Hydrochloride) (PAH)



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This study was an attempt to synthesize novel semi-IPN Hydrogels of Poly(acrylic acid) (PAAc)-Poly(allylamine) (PAIAm) and PAAc-poly(allylamine hydrochloride) (PAH) with different molar ratio of components. The influence of pH, time, temperature and salinity of water, as well as cross-linker amount, were also investigated. The synthesized PAAc/PAIAm and PAAc/PAH hydrogels were characterized using Fourier Transform Infrared Spectroscopy. The swelling behavior of the semi-IPN hydrogels revealed that the maximum swelling ratio was obtained for the sample SAPH1 with a PAAc/PAH ratio of 1/0.25 and for the sample SAP3 with a PAAc/PAIAm ratio of 1/1. Moreover, for the PAAc/PAH system, the maximum swelling degree was observed in alkaline pH, while for PAAc/

PAIAm system, the maximum swelling was shown in pH=7. The swelling study of the hydrogels in the aqueous solution of NaCl showed that increasing the salt concentration caused the limitation of water absorption. It was also shown that the increase in temperature of the swelling process led to an enhancement of the swelling ratio in distilled water. According to the results, the optimum amount of cross-linker was found for achieving the maximum swelling degree. UV-Vis spectroscopy was employed to determine the dynamic change of the 4-nitrophenol concentration. The results revealed the complete absorption of the 4-nitrophenol pollutant. This suggests that the prepared semi-IPN hydrogel is an appropriate system for treating the wastewater.



## Predicting of acid red 14 removals from synthetic wastewater in the advanced oxidation process using artificial neural networks and fuzzy regression



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The titanium dioxide (TiO<sub>2</sub>) photocatalyst reactor is a widely used approach for eliminating non-biodegradable compounds in water and wastewater. Predicting the performance of the reactor in removing acid red 14 (AR14) was investigated using radial basis function (RBF), Adaptive Neuro-Fuzzy Inference System (ANFIS), and fuzzy regression analysis. The input variables in the models were radiation, irradiation time, the initial concentration of nanoparticle TiO<sub>2</sub> to cement ratio (nTiO<sub>2</sub>/c), pH, initial concentration of AR14, flow rate, and initial concentration of oxidizing peroxydisulfate. In addition, for reducing the overfitting of the training process, we used K-fold cross-validation. The results of using the three methods indicated that the ANFIS performance was more suitable in comparison with the fuzzy regression models, such that the coefficient of determination (R<sup>2</sup>), index of agreement (IA), Nash–Sutcliffe efficiency (E) for model efficiency, Mean Squared Error (MSE), and

Mean Bias Error (MBE) for training between the observed data and predicted data reached 0.965, 0.991, 0.73, 0.0132 and 0.019, respectively. Normalized input data improved slightly the training processes and performance of RBF compared with non-normalized input data. The ANFIS neural network for training process and model performance slightly achieved better results than the RBF neural network. The performance of the fuzzy regression approach was less suitable in comparison with RBF and ANFIS modeling. The sensitivity analysis of the RBF neural network depicted that the initial concentration of peroxydisulfate (S2O8) was the most effective factor (25.6%) in predicting the removal of AR14 from synthetic wastewater. After that, the effective factors were irradiation time (12.44%), initial concentration of AR14 (10.37%), pH (10.37%), flow rate (8.55%), and the weight ratio of the initial concentration of nanoparticle TiO<sub>2</sub> to cement ratio (nTiO<sub>2</sub>/c) (1.75%), respectively



## **Fabrication and characterization of carnauba wax-based films incorporated with sodium alginate/ whey protein**



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Edible films and coatings developed through biopolymers have good tensile strength and gaseous barriers but lack moisture barrier properties. To improve the moisture barrier properties of sodium alginate and whey protein-based films, carnauba wax at different concentrations (0.5, 1.0, and 1.5%) was incorporated. Results showed significant variations as the concentration of the carnauba wax increased. The addition of wax at a higher concentration (1.5%) significantly improved the moisture barrier properties ( $3.12 \pm 0.31$  g mm/kPa h m<sup>2</sup>). However, tensile strength reduced ( $3.92 \pm 0.04$  to  $3.34 \pm 0.04$  MPa) with the increase in

wax concentration. The incorporation of lipid constituents in the emulsion-based films also affects the physicochemical properties including thickness, droplet size, transparency, and microstructure of the films as well. At lower concentrations (0.5%) films showed uniform microstructure and better transparency ( $81.82 \pm 1.63\%$ ) but lack in moisture barrier properties. Emulsified edible films with improved moisture barrier and tensile properties are preferable in the food packaging industry. Emulsion-based films and coatings have potential applications in foods, especially in fresh and processed foods, dairy, bakery products, meat, and sausages.





## **Carboxymethyl cellulose/gelatin hydrogel films loaded with Zinc Oxide nanoparticles for sustainable food packaging applications**



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The current research work presented the synthesis of carboxymethylcellulose-gelatin (CMC/GEL) blend and CMC/GEL/ZnO-Nps hydrogel films which were characterized by FT-IR, XRD and applied to antibacterial and antioxidant activities for food preservation as well as biomedical applications. ZnO-Nps were incorporated into Carboxymethylcellulose (CMC) and Gelatin (GEL) film-forming solution by solution casting followed by sonication. Homogenous mixing of ZnO-Nps with

CMC/GEL blend has improved thermal stability, mechanical properties, moisture contents, and water vapor permeability of neat CMC/GEL films. Further, a significant improvement was observed in antibacterial activity, and antioxidant properties of CMC/GEL/ZnO films against two food pathogens, *Staphylococcus aureus* and *Escherichia coli*. Overall, CMC/GEL/ZnO films are eco-friendly and can be used for sustainable food packaging applications.



## Eco-friendly thin PDLC films technology



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Smart glass technology is widely used in today's world. The smart glass containing epoxy monomer and liquid crystal dispersed in it is called polymer dispersed liquid crystal (PDLC). Eco-friendly thin PDLC films composite with variable concentration induces into the films. The variable concentration of variables epoxy resin gives the pristine morphology of the sample A1-A4. The electrooptical properties are measured by a liquid crystal detector and abbe-refractophotometer for refractive index measurement. PDLC thin films technology is widely used in today's world. It offers several advantages over the conventional LCD materials, such as simple manufacturing process, no polarizers, no viewing angle problem, unnecessary for the strict control of the space between substrates and easy to fabricate large-

area display. The thin PDLC films were fabricated by the polymerization induced phase separation (PIPS) method with curing monomers/LC/hardener/catalyst mixtures. It was demonstrated that the curing monomers with catalyst of various sizes affect the structure of the polymer network remarkably. Especially, the crosslinking density of the polymer network containing this 35-55 nm size tended to increase with increasing the content of the curing monomers with -NH<sub>2</sub> group in the curable monomers in epoxy monomers/LC/hardener/catalyst mixtures. This film can display On and Off State, transparent to opaque medium due to the polymer composite and feed ratio of the LC which enable to use of a wider choice of PDLC thin films technology and other optical devices.



## **Anchored ferrocene based heterogeneous electrocatalyst for the synthesis of benzimidazoles**



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A facile and sustainable electrochemical synthetic strategy for phenyl benzimidazole has been developed using a ferrocene-based electrocatalyst anchored on Toray carbon paper (TCP) coated with conducting polymeric films. The developed electrode was used for the electrochemical dehydrogenative cyclization reaction of o-phenylene diamine and benzaldehyde using lithium perchlorate/acetonitrile as electrolyte. The surface characteristic properties of the developed electrode were characterized

by FESEM, Optical profilometer and X-ray photoelectron spectroscopy. Electron transfer mechanism of the anchored ferrocene-based electrocatalyst was thoroughly studied. To determine the efficacy of the catalyst, the electron transfer coefficient (0.5) and apparent rate constant  $41.4 \text{ s}^{-1}$  were determined. The oxidation for the synthesis of benzimidazole occurs at 0.48 V. We have identified & quantified the product by Gas chromatography and Nuclear Magnetic Resonance spectroscopy.



## **Design and implementation of a sub-optimal explicit mpc using a novel complexity reduction approach based on fuzzy reshaped active regions**



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The Explicit Model Predictive Control (EMPC) has emerged as a powerful technique to solve the optimization problem for embedded applications. Despite practical obstacles in implementation of EMPC, the main drawback of MPC, due to its need for repetitively solving optimization problem is removed. This paper addresses the complexity issue of EMPC implementing in terms of online evaluation and memory requirement. In this paper, a novel reshaping method is applied for active region selection in order to have regular boundaries in polyhedron definitions. In this approach, several improvements have been achieved. First, it employs low memory for practical implementation compared to the traditional

EMPC. Next, because of less number of new polyhedrons, searching time among explicit look-up table is decreased, so the overall implementation speed is increased. For this purpose, a reshaping method for traditional polyhedrons is introduced and then, a novel fuzzy-based Piece-Wise Affine (PWA) explicit formulation is developed for control action calculation. Stability of the proposed scheme is investigated using Lyapunov stability criterion. The proposed algorithm is tested on a nonlinear chemical reactor of propylene glycol as an industrial pilot plant. The simulation tests show that the proposed approach can significantly outperform the traditional explicit MPC methods in real-time implementation.



## How do temperature, humidity, and air saturation state effect the COVID-19 transmission risk?



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**E**nvironmental parameters have a significant impact on the spread of respiratory viral diseases (Temperature(T), Relative Humidity (RH), and air saturation state). T and RH are strong correlated with viral inactivation in the air, whereas supersaturated air can promote droplets deposition in the respiratory tract. This study introduces a new concept, the dynamic virus deposition ratio ( $\alpha$ ), that reflects the dynamic changes in viral inactivation and droplets deposition under varying ambient environments. A non-steady-state modified Wells-Riley model is established to predict the infection

risk of shared air space, and highlight the high risk environmental conditions. Findings reveal that a rise in T would significantly reduce the transmission of COVID-19 in cold season, while the effect is not significant in hot season. The infection risk under low-T and high-RH conditions, such as the frozen seafood market, is substantially underestimated, should be taken seriously. The study encourages selected containment measures against High-risk environmental conditions, and cross-discipline management in the public health crisis based on meteorology, government, and medical research.



## **Modelling total soil runoff of Syngkai river basin Domiasiat Meghalaya India using radionuclides**



**Niranjan Kumar**

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For the correct estimation of minerals washing off rate and quantity of annual dumping to the river or low gradients territory is not yet done in Domiasiat Meghalaya; Urnaium mineralized bed. So a research were conducted to quantify the value of runoff and washoff using beta spectroscopy techniques and sedimentation rate in the radius of 5 Km at the elevation 795 were estimated  $9 \times 10^6$  tons annually

and where natural annual precipitation was 1000cm. The Gross beta activity counted by Liquid scintillation counter was 18.7347 bq/l. And it was found that the estimation of soil loads using ( $^{14}\text{C}_6$   $t_{1/2} = 5775$  years) hydrogeochemical properties of radionuclides were quite easier and not much complex process involved like in flood or unit hydrograph runoff estimation methods.



## Surface markers of stem cells in local fat depots in patients with coronary artery disease



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**Aim:** To describe the immunophenotype of ADSCs isolated from epicardial and perivascular fat depots in patients with coronary artery disease.

**Methods:** The study included 5 patients with CAD. The average age is  $65.5 \pm 5.5$  years. Patients had indications for open intervention on the heart-direct myocardial revascularization by CABG. ADSCs from biopsy samples of epicardial and perivascular AT that were obtained from patients during surgery (CABG or correction of heart defects) and isolated according to the method of Zeng G (2013). When cells grew to 80–90% confluence, they were digested with 0.25% trypsin and proliferation for subsequent experimental analyses. Flow cytometry analysis was performed on passage 2 cells.

**Results:** On the 29<sup>th</sup> day of cultivation (pas. 2), it was shown that CD105 and CD90 were present in the EAT of a patient

with CAD on 79.71%, while one antigenic marker CD105 was present in 17.54% of the cells. Membrane proteins CD73 and CD90 were present in 79.47%, only one CD73 in 18.26% of cells, while CD34 was present in only 3.76%. Thus, the phenotype of the resulting culture of cells isolated from EAT CD73+, CD90+, CD105+, CD34-. In addition to the main population, 2 minor: 1-CD90-, CD105+, CD34-, CD73+ CD45- presumably endothelial population, 2 - CD90+, CD105-, CD34-, CD73-, CD45- presumably hematopoietic population. In PVAT, a high (over 90%) expression of membrane proteins characteristic of stem cells. CD34 was expressed by 3.46%. In PVAT, we observe 3 populations, as in EAT.

**Conclusion:** At the early stages of cultivation, SVF PVAT and EAT contain cells that carry markers inherent in both AT stem cells and markers of hematopoietic and endothelial populations.



## Use of indocyanine green fluorescence imaging in the extrahepatic biliary tract surgery



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**C**holelithiasis presents in approximately 20 % of the total population, ranging between 10% and 30 %. It presents one of the most common causes for non malignant surgical treatment. The cornerstone therapy is laparoscopic cholecystectomy, urgent or elective. Laparoscopic cholecystectomy is nowadays the gold standard surgical treatment method, however bile duct injury occurred to as high as 0.4-3% of all laparoscopic cholecystectomies. The percentage has decreased significantly to 0.26-0.7% because of increased surgical experience and advances in laparoscopic imaging the past decade which have brought to light new achievements and new methods for better intraoperative visualization such as HD and 3D imaging system. However, bile duct injury remains a significant

issue and indocyanine green fluorescence imaging, mainly cholangiography but also angiography, can further enhance the safety of laparoscopic cholecystectomy as it allows the earlier recognition of the cystic and common bile duct, even in several times before dissecting the Callot triangle. Fluorescence cholangiography could be an ideal method in order to improve bile tree anatomy identification and enhance prevention of iatrogenic injuries during laparoscopic cholecystectomies and also it could be helpful in young surgeons training because it provides enhanced intraoperative safety, but however this method does not replace CVS. Finally, our ongoing current study results comparing intravenous to direct administration of ICG in the gallbladder will be presented.





## **Construction and investigation of new drug delivery systems; From Nanobandages to Nanorobots**



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Nanotechnology is a science that has improved the quality of products in various fields. Many advances in medicine and drug delivery with the help of nanostructured materials have been achieved in recent decades. Creating a smart substrate that can load high medicinal substances makes it possible for low concentrations of medicinal substances to be transferred so that side effects, dosage, and problems related to them are significantly reduced.

During the last decade, the work done by our research team includes the construction and investigation of one-dimensional, two-dimensional, and three-dimensional nanostructures that can be used as drug delivery systems and cellular scaffolds. The main focus has been on the use of natural-based materials, chemicals with green

synthesis methods, and materials with minimal toxicity. In order to achieve this goal, nano drug delivery systems with desired morphologies and characteristics were first made, and then their performance as active agent transfer systems (medicine, growth factor, etc.) was investigated by chemical, physical, and biological methods. In the next phase, the goal was accessing intelligent drug delivery systems with the ability to control the release rate was achieved. Therefore, the behavior of these systems was investigated with external stimuli. In the final phase, the intelligent transmission of the drug delivery system was introduced by the design and construction of intelligent micromotors. Therefore, in the present speech, a summary of the most important results obtained in the said direction will be presented.



## **Apatite of metamorphic rocks of the northern part of the subpolar Urals**



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Studies devoted to variations in the composition of metamorphic apatites and their typomorphic properties are not so numerous. Scientific works on apatite applicable to metamorphic rocks include studies of the fugacity of metamorphic fluid components in apatite-bearing samples (Korzinsky, 1981; Smith and Yardley, 1999), apatite-biotite OH-F exchange thermometry (Sallet and Sabatier, 1996;) and thermodynamics of the distribution of F and CL between minerals and fluids (Zhu and Sverjensky, 1991, 1992; Brennan, 1993).

Apatite occurs in rocks of different facies of metamorphism from low-temperature alteration to ultra-high pressures (Liou et al., 1998), which is probably dictated not by its resistance to other phosphates, but rather by the presence of the main components (P, Ca, F), therefore, the use of the mineral for the purpose of subdivision and correlation of metamorphic formations

has great prospects. The study of apatites from metamorphic formations in the Southern Urals showed that, depending on the degree of metamorphism, the REE composition in the mineral changes, so in apatites from rocks that have undergone an amphibolite facies of metamorphism, yttrium REE and Y predominate, and in apatites from rocks that have undergone a granulite facies of metamorphism, cerium REE (La) (Krasnobaev and Kholodnov, 1981).

We have studied accessory apatite from rocks that have undergone various degrees of metamorphism in the Subpolar Urals: the degree of prograde metamorphism of the rocks of the Nyarta complex and the Shchokur'inskaya suite corresponds to the level of the amphibolite facies of moderate pressures: T=650–750°C, P=6–9 kbar; pressure: 350–450°C, P=4–6 kbar.

The data obtained showed that the

morphological features of apatite, the presence, mineral composition and amount of solid and gas-liquid inclusions, the chemical composition of the mineral itself (strontium content, qualitative composition and REE content), and spectroscopic properties are associated

with rock metamorphism. Thus, according to the typomorphic features of apatites, one can judge not only the similarity or difference in the degree of metamorphism of the compared rock associations, but also solve the important problem of separating mono- and polymetamorphic formations.



## **Solid-state synthesis and single crystal growth of novel fluorescent compound worth for detection of Cr<sup>+6</sup> Ions**



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A novel organic compound ANNBA has synthesized adopting the solid-state green synthesis and utilizing knowledge of phase diagram studies. The phase diagram studies has inferred that the complexation occurs at 1:1 molar ratio of the parent compounds. The synthesized ANNBA has studied by DSC, FTIR, NMR, PXRD and single crystal XRD for its novelty and identity. The experimental heat of fusion value, obtained from DSC, has helped in studying its various thermodynamics parameters. The emission from the synthesized compound, on exciting of the synthesized compound, has revealed the remarkable fluorescence emission which is far better than known fluorescent organic compound pyrene. The significant fluorescent emission efficiency of this novel compound is employed for its outstanding affinity for selective detection of hexavalent chromium (Cr+6) ions in water samples. It has wide dynamic range in between 2-50 mM concentration with

limit of linearity (LOL) within 2-10 mM of Cr+6. The single crystals of ANNBA were grown from mixture of solvents (acetone and water) using slow evaporation technique. The peculiar observation has been noted from the analysis of single crystal XRD that the solvent (acetone), used for crystal growth, has itself reacted and cyclized with the anthranilamide molecule which is connected with 3-nitrobenzoic acid molecule via intermolecular hydrogen bonding. The single crystal XRD studies reveals that synthesized ANNBA compound has crystallized in monoclinic-P21/n space group having two molecules in crystal asymmetric and eight molecules present in its unit cell. The approach of phase diagram study, to have novel materials with 100% yield, and solvent free solid-state synthesis method are inspiring to develop and design such other novel fluorescent organic crystalline materials to be used as sensors.



## Recycling and applications of expired medicinal materials for corrosion protection of metals and alloys



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Significant inhibition efficiency of several drugs have been proved many years ago, but unfortunately, drugs are expensive and their practical applications as corrosion inhibitors for metal and alloys has been delayed. Several reports have mentioned the application of novel environmentally friendly molecules as corrosion inhibitors. One of these prominent areas in this field is pharmaceutical products. In the present review, the studies on the inhibition properties in metal corrosion processes

of expired drugs have been emphasized, starting with the paper of R. S. Abdel Hameed, published in 2009. This review presents most of the contributions made to the literature on the use of expired drugs as corrosion inhibitors of various metals. All the reported survey of literatures proved that the use of expired drugs as corrosion inhibitors traced back to 2009's by the scientist Reda Abdel Hameed that introduced the new idea for application of the expired drugs as Environmentally Sustainable Corrosion Inhibitors.



**Engineering at  
the nanoscale:  
A strategy for  
developing high  
performance  
functional materials  
from biopolymers**



**Sabu Thomas**

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**G**reen chemistry started for the search of benign methods for the development of nanoparticles from nature and their use in the field of antibacterial, antioxidant, and antitumor applications. Bio wastes are eco-friendly starting materials to produce typical nanoparticles with well-defined chemical composition, size, and morphology. Cellulose, starch, chitin and chitosan are the most abundant biopolymers around the world. Cellulose nanoparticles (fibers, crystals and whiskers) can be extracted from agrowaste resources. Chitin is the second most abundant biopolymer after cellulose, it is a characteristic component of the cell walls of fungi, the exoskeletons of arthropods and nanoparticles of chitin (fibers, whiskers) can be extracted from shrimp and crab shells. Starch nano particles can be extracted from tapioca and potato wastes. These nanoparticles can be converted into smart and functional biomaterials by functionalization through chemical modifications due to presence of large amount of hydroxyl group on the surface. The preparation of these nanoparticles includes both series of

chemical as well as mechanical treatments; crushing, grinding, alkali, bleaching and acid treatments. Since large quantities of bio wastes are produced annually, further utilization of cellulose, starch and chitins as functionalized materials is very much desired. The cellulose, starch and chitin nano particles are currently obtained as aqueous suspensions which are used as reinforcing additives for high performance environment-friendly biodegradable polymer materials. These nanocomposites are being used as biomedical composites for drug/gene delivery, nano scaffolds in tissue engineering and cosmetic orthodontics. The reinforcing effect of these nanoparticles results from the formation of a percolating network based on hydrogen bonding forces. The incorporation of these nano particles in several bio-based polymers have been discussed. The role of nano particle dispersion, distribution, interfacial adhesion and orientation on the properties of the ecofriendly bio nanocomposites have been carefully evaluated.



## Numerical investigation of injection angle and injection rate of drug-loaded nanoparticles on their capture efficiency at tumor site considering RBCS-particles



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Cancer is considered as one of the most leading causes of human mortality. There are different ways for treatment of cancer each has their own pros and cons. Magnetic drug targeting (MDT), among others, is one of the most promising methods for cancer treatment with minimum side effects. In this method, the carrier particles are injected into the blood vessel and are captured at tumor site by applying an external magnetic field. In this study, trajectories and capturing of drug-loaded nanoparticles in a 3D vessel under the effect of an external magnetic field have been investigated. Magnetic field was produced by a current carrying wire and a permanent Halbach array. Two different models, i.e., modified Carreau and Casson, were considered for the non-Newtonian behavior of blood. The effect of different parameters, including drag

force, magnetic force, particles' diameter, vessel's diameter, injection angle, blood velocity, wall shear stress (WSS) and interaction forces have been investigated. The injection angle ranged from 30° to 90°. Results revealed that drug-loaded nanoparticles were effectively captured at tumor site by MDT method. Besides, it was revealed that considering the non-Newtonian behavior of blood would result in lower capture efficiency for all cases. It was found that by increasing the injection rate of the nanoparticles, the CE was increased. Besides, it was noticed that the difference between the values of CE for injection angle of 30° and 90° is 10%. Finally, it was found that considering particles-RBCs interaction negatively affect, except for few cases, the CE of nanoparticles; although considering the interaction forces would significantly increase the calculational time.



## **Optimizing Wildlife Patrols based on prior spatial Information, attribute data and vulnerability to illegal activities**



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The problem of adversarial multi-path guard dependent patrol has gained interest in recent years, mainly due to its immediate relevance to various security applications. In this problem, patrol guards are required to repeatedly visit a protected area in a way that maximizes their chances of detecting poachers and indulge in illegal activity. When facing a strong adversary that knows the patrol strategy of the guards, if the guards use a deterministic patrol algorithm, then in many cases it is easy for poachers to penetrate undetected (in fact, in some of those cases the adversary can guarantee penetration). Besides a landscape has differential vulnerability in space and time to poaching and subsequent illegal activity. Covariates associated with this vulnerability were modelled to generate a spatial cost surface to depict pixel vulnerability to poaching. Herein, we develop a program for generating a non-deterministic, dynamic, and optimal patrol framework in time and space for Protected Area guards. We used a polynomial-time algorithm for determining an

optimal patrol under the Markovian strategy assumption, such that the probability of detecting poachers at the Protected Area's most vulnerable locations is maximized. Once a spatial pixel is patrolled, its vulnerability is programmed to decline immediately following a patrol and builds up again with time. Detection of poaching activity (traps, snares, logging, campfire, etc.) by patrols enhances the pixel vulnerability score to poachers. We use Game, Graph theory to model, and design a patrol path using Hawk and Dove game construct. We construct minimum spanning tree or a Hamiltonian path, depending on the start and end, decided by guards, is then obtained by employing Kruskal's algorithm or Travelling Salesman problem. We build upon this framework and describe an optimal patrol strategy for several patrol guards based on their movement abilities (directed or undirected) and sensing abilities (perfect or imperfect), and in different environment models - either patrol around a perimeter (closed polygon) or an open fence (open polyline).





## Cross-linked naphthalene diimide-based polymer as cathode material for high-performance organic batteries

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In the field of rechargeable batteries, redox organic compounds have attracted huge attention owing to their eco-friendliness, resource abundance, good flexibility, and low cost. However, the high solubility of the organic compounds in electrolytes results in poor cell performance. In this paper, we report that a cross-linked naphthalene diimide-based polymer, which is a three-dimensional network structure, exhibits outstanding cell performance in organic batteries. The polymer is synthesized by the imidization condensation of naphthalene-1,4,5,8-tetracarboxylic dianhydride (NDA) and 4-vinylaniline to form N,N'-di(4'-vinylphenyl)naphthalene-1,4,5,8-dicarboxydiimide (DVP-NDI) and by subsequent radical polymerization to

a cross-linked DVP-NDI (CL-DVP-NDI) polymer. The cross-linking of the polymer is characterized by using infrared and solid-state <sup>13</sup>C nuclear magnetic resonance spectroscopy. Thermogravimetric analysis shows that the polymer with a three-dimensional network structure exhibits better thermal stability than an organic molecule. The solubility test indicated that the CL-DVP-NDI polymer can suppress the dissolution of the polymer in organic electrolytes. The discharge capacity of the CL-DVP-NDI electrode is 121.3 mAh g<sup>-1</sup> at a C-rate of 0.2 C. The cycle-life performance of the Li||CL-DVP-NDI cell is 84% remaining after 200 cycles at a charging-discharging rate of 1 C.



## Unaccounted environmental factor – Anticoagulants of the 2<sup>nd</sup> generation



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**A**groecosystems have no physical boundaries, therefore, the processes occurring in them affect the biological diversity of adjacent territories, which are considered natural. Current changes increase the proportion of intensive processing fields, which are introduced agrochemical preparations. Of particular importance are modern rodenticides - superwarfarins. The literature indicates their danger not only for animals, but also for humans (poisoning in the Russian Federation, Europe, Asia, North America).

There are many reports of the death of animals of non-target species after the use of rodenticides (for example, bustard in the Crimea in 2020-21), but only in two regions of Russia the facts were officially registered (Krasnodar Territory, Volgograd region). Veterinary examinations of a part of the collected carcasses excluded infectious diseases as a cause of death. The range of species of dead animals includes brown hares, badgers, grain-eaters, omnivores and birds of prey, i.e. consults not only

of the first, but also the second order consumers. It proves the transmission of toxicants through food chains.

The animals of different species are not equally sensitive to superwarfarins. The death of dogs from relatively low doses was established, which excluded the use of pets as indicators of danger to humans.

The most common toxicants are based on bromadiolone and brodifacum. They are considered to be drugs of intestinal action, combining a multicomponent mechanism with an acute effect, related to extremely dangerous substances when injected into the stomach, with a possible skin-resorptive effect.

The results of pathologic-anatomic autopsies show that absorbing to the respiratory system is greatly underestimated and that effects on the state of the brain cannot be excluded. The collection of carcasses of dead birds that died after the use of superwarfarins made it possible to conduct systemic complex pathomorphological and toxicological studies. The presence of

bromadiolone in tissues has been proven. Vascular and respiratory system lesions predominate, the poison reached the gastrointestinal tract only in less than half of the birds.

The numerous autopsies of dead animals approved the lack of knowledge of the routes of entry of the toxicant and its lethal doses.

Modern agriculture is based on the constant introduction of agricultural chemistry. The increase in the proportion of plowed fields into which they are introduced allows us to assert that this effect is a permanent environmental factor affecting all types of animals and humans.



## **Qubit and bit- based quantum hybrid secret key generation**



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For the generation of a secret key, hardly a quantum algorithms integrating states and bits have yet developed. Integrating random states and bits is difficult for a combiner component. The underlying problems of the study are the design of a quantum circuit, an algorithm, state polarization setup, and the concatenation of bits and states. By combining either rectilinear, orthogonal (superposition), or both states with bits, we have investigated three different possibilities for the quantum hybrid protocol. We investigated errors in each case and compared them

with regard to decoherence and other quantum mechanics properties by taking into consideration the effectiveness of states during transmission time across an untrusted channel. Furthermore, we observed that key size, state errors, design complexity, and security are all addressed in a reasonable manner for identifying solutions while comparing our results to earlier proposed quantum protocols. Because of this, the suggested key protocol's effectiveness is greater than that of earlier proposed protocols.



## Fractionalized mathematical models for drug diffusion



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An attempt has been made in this work to construct a mathematical model to understand the concepts of the processes occurring between the human body and the chemical substance drug. The diffusion process was utilized to create three models applying Fick's principle and the law of mass action. The Caputo Fractional Derivative and Sumudu Transform methods were used in this study to determine the answer of the specified

model more accurately. Mathematical modeling of drug diffusion is a useful predictive method for understanding the bio-transport process. Mathematical modeling is theoretical, but the results are established to lead to realistic results when confirmed empirically. In the absence of experimentation, the local operations in each compartment perform many mathematical models and numerical simulations with high efficiency.



**How the physico-chemical properties of the soil affect the distribution and vegetative characteristics of the medicinal plant *Dorema ammoniacum* (D. Don) in south-central Alborz, Iran**



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**D**orema ammoniacum (D. Don) is one of the medicinal plants that is found in natural sites of Semnan province in the south-central Alborz Mountains, Iran. This plant is famous all over the world for its valuable milky juice known as gum Ammoniacum (an oleo-gum-resin latex) and its essential oil, which has been considered in the fields of health, trade and industry. This research was conducted to evaluate the soil physicochemical factors affecting functional characteristics (frequency, coverage and density) of *Do.ammoniacum* in this region. Based on field surveys, four main habitats were identified in the rangeland ecosystems: Garmsar (A), Semnan (B), Damghan (C), and Shahroud (D). In each habitat, 4 to 6 transects of 150 meters were established for sampling of vegetation and soil parameters. Totally 53 soil samples were taken (from 0-50-cm depth) and organic carbon, CaCO<sub>3</sub>, CaSO<sub>4</sub>, pH, EC, calcium, magnesium, sodium, potassium, phosphorus, nitrogen, and soil texture were measured. Habitats were compared with

Duncan test and correlation relationships between functional characteristics with soil factors were determined by RDA that was performed with Canoco4.5. Habitat A has the highest average densities, frequencies, and cover (0.098 m<sup>2</sup>, 48.7%, and 29.7%, respectively) and the most amount of CaSO<sub>4</sub> (23.67%), Ca (31.53Meq/l) and the lowest amount of CaCO<sub>3</sub> (3%), SAR (0.65) and pH (7.06). RDA results showed that the gypsum content in soil had the greatest positive effect on the functional characteristics of *Do.ammoniacum* habitats; by contrast, increasing factors such as calcium carbonate reduced them. Salinity and alkalinity were not limits to soils in the studied habitats (average pH and EC of 7.56 and 2.60). Presence of gypsum, lime, calcium, magnesium and sodium significantly affected the distribution and density of species such as gypsum and calcium increased density. Conversely, magnesium and sodium of soil have a negative correlation with density of *Do.ammoniacum*.



## Bioinformatic Tools for CRISPR/ Cas9 Applications in plants



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The development of numerous bioinformatic tools to allow Cas9-mediated genome editing greatly enabled the research in genome editing field. These online tools allow the creation of certain gRNAs, forecast the off-target sites of specific gRNAs, and perform other beneficial tasks (e.g., assessing restriction enzyme cut sites). Only CRISPR-PLANT and CRISPR-P are intended especially for Cas9-mediated plant genome editing among these technologies. CRISPR-PLANT provides restriction enzyme analysis of target sites and has a genome-wide survey of highly specific gRNAs in eight plant species (Xie et al., 2014). Nearly all plant species whose genome sequence is accessible can create gRNA with the help of CRISPR-P, which also offers off-target site analysis and restriction enzyme sequence analysis (Lei et al., 2014).

The widespread application of CRISPR/Cas9 technologies in plants and their

quick evolution need the inclusion of more features in these online tools. A plug-and-play online tool would assist plant biologists who are unfamiliar with genomic sequence analysis in creating a CRISPR/Cas9 experiment. Such bioinformatics platforms should also contain gRNA design for various Cas9 proteins with diverse PAM specificities, forecast the on-target editing effectiveness and off-target risk of gRNAs, and help choose the best Cas9 target sites from among a large number of options. Aside from that, because many significant crops are polyploid or outcrossing species, the sequence variation between various alleles should be taken into account while designing gRNA. A platform that incorporates Cas9/gRNA design tools with genome annotation data would help genome-engineering experiments in fundamental research and crop breeding since CRISPR/Cas9 genome editing is becoming a common method.



## H<sub>2</sub>S: A new look at its role in human activity



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The concept on the decisive role of solid catalysts in the reaction of low-temperature decomposition of H<sub>2</sub>S is considered in the framework of non-equilibrium thermodynamics of an irreversible process in an open system [1]. The reaction proceeds at room temperature without the use of external energy sources due to the internal (kinetic and potential) energy of hydrogen sulfide molecules. In the gas phase, this reaction is thermodynamically impossible. The reaction products are, along with hydrogen, either solid sulfur (sulfide catalysts) or diatomic gaseous sulfur in the ground triplet state (metal catalysts) [2]. The

concept makes it possible to solve not only the problem of efficient utilization of H<sub>2</sub>S, but also opens new pages in the chemistry of this substance as both a source of atomic hydrogen and an energy supplier for activation of the chemically inert molecules. Moreover, the gaseous triplet sulfur discovered by us can be used in various fields of chemistry, pharmacology, medicine, etc. Therefore, "useless" H<sub>2</sub>S acquires the status of a "useful" chemical that will be probably in demand to solve problems which could not be realized within the framework of the previous paradigm of the high-energy disposal of H<sub>2</sub>S [3].





## Pharmaceutical Cocrystallization as an emerging trend to modify the physico-chemical properties



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Crystal engineering[1] serves as an opportunity window to develop new solid forms based on non-covalent intermolecular forces interactions among crystal formers. Pharmaceutical cocrystallization is being widely investigated as a strategy to improve the physicochemical and stability properties of solid dosage forms of APIs. Formulation of two or more APIs having complementary functional groups into a single dosage can save manufacturing, packaging and storage resources as well as being provide convenient to patients. Isoniazid is a key antitubercular agent which exhibits poor chemical stability in the solid state. Solid-state NMR and single crystal XRD serves as key characterization tools to establish the crystalline form structure

and to distinguish among cocrystal or salt formation. Cocrystallization of isoniazid with hydroxyl derivatives of cinnamic acid[2], possessing antitubercular and antioxidant activity, may produce solid forms with improved pharmaceutical properties[3] due to the complementary nature of the functional groups[4] of isoniazid and the chosen cofomers and resulted in a high success rate for cocrystal formation. All synthesized cocrystals were characterized by solid-state NMR, DSC, PXRD and single crystal XRD. NMR chemical shifts were observed to distinguish between key synthons involving the carboxylic acid of cinnamic acid[5].



## Numerical solution of contaminant transport model



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Contamination of fluids in rivers, channels, lakes, tanks... may be caused due to chemicals from factories, animal wastes, human activities, environmental pollutions [floods, gases, toxic substances...]. Its transport (flow) is expressed in the form of PDE models of 1D, 2D or 3D; such as advection /convection-diffusion equations [ADEs / CDEs or singular perturbation equations, SPPDEs]. The diffusion equations (PDEs) are important models in applications. They occur in physical, chemical reactions, financial, biological, fluid mechanics, economic and other prediction processes. These PDE are used to describe the dynamics, migrations, transportations, distributions and concentrations of the pollutants in a typical medium. Particularly heat diffusions, wave motions, fluid flows/ dispersions... are real examples where PDE-models are involved. Most of PDEs are naturally nonlinear or complex and intricate to solve. So it may be impossible or difficult to find their analytic solutions (by separation, Fourier transform, Laplace transform, Taylor/

power series...). Few analytical solutions may be used to solve science & engineering PDE problems. Practically it is not simple to solve convection-diffusion problems of complex nature (BCs or ICs) by direct methods. Finite element methods (FEMs), FDMs, FVMs and BEM are numerical approaches for PDEs. These methods can be applied to analyze, compute or predict the model parameters. The main motive of this study is to model CDEs and develop CFDMs based on Taylor's series & new approaches of domain grids geometry for solving (convection / advection equations) representing flow of contaminants in porous media. The convergences of the FDMs are also discussed, with test problems in Python. We focus on (1) theoretical discussion on modeling of convection-diffusion equation, (2) numerical modeling of finite difference schemes (3) analysis of the FDMs (4) we also discuss SPPDEs in chemistry, their fitted mesh (FMFDMs) and fitted operator (FOFDMs).



## Functionalization of carbon nanodots and their application in biomedicine



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Carbon nanodots (CNDs) are an developing branch of nanomaterials and nanoscience, this have generating much more interest in the field and class of biomedicine science by way of unique particular properties, such as high stability, great photoluminescence, easy green synthesis, and simple surface modification. Numerous applications, such as bioimaging, biosensing, and treatment, have made use of CNDs. In this review, we describe the most recent developments in CND research and talk about major changes in our understanding of CNDs and their prospects as biomedical tools. The functional

modification of CNDs through the changing of dopants and surface molecules, which has led to an improved knowledge of their antioxidant behaviour and mechanisms of action, is discussed in this review. Interest in in vivo procedures has grown as a result of the growing body of in vitro research on CNDs. We start by talking about the development of studies looking at CNDs as potential therapeutic agents for various disease states. Each topic is discussed while considering potential future research that could expand our understanding of CNDs.



## Study on the preparation of epoxy resin materials from nano-lignin polyols



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Formaldehyde attacks the ortho phenolic hydroxyl groups on the p-hydroxyphenyl and guaiac-based structures in the lignin, shedding the hydrogen atom on the ortho-position carbon and grafting hydroxymethyl group to obtain the hydroxymethylated modified lignin (HMKL). The infrared spectroscopy, hydrogen NMR spectroscopy, thermogravimetric (TG), and derivative thermogravimetric (DTG) analysis show that the hydroxymethylation modification of alkali lignin is successful. Then, lignin nanoparticles (LNPs) are prepared by the acid precipitation self-assembly method in ethylene glycol solution of hydroxymethylated modified lignin. The particle size and shape of lignin nanoparticles are determined by scanning electron microscopy and dynamic light scattering (DLS) analysis. In the liquefaction agent prepared from polyethylene glycol

400 and glycerol, the graft polyol is liquefied under methanesulfonic acid. The Fourier transform infrared spectroscopy, hydrogen NMR, and thermogravimetric analysis indicate the successful formation of nano-lignin polyols. In addition, epoxy resin is synthesized by two-step epoxidation of nano-lignin polyols including ring-opening and closed-loop epoxidation in an alkaline environment. The prepared epoxy resin from nano-lignin polyol exhibits excellent performance and wide application prospects. The optimum process conditions are the mass fraction of LNP-P is 19.98 %, the amount of catalyst (NaOH) is 20.10 %, the reaction time is 6.99 h, the solid content of the epoxy resin is 57.05 %, the viscosity is 615.58 mPa.s, the tensile strength is 44.80 MPa, the elastic modulus is 2.77 GPa.



## The lining responses for shallow mountain tunnels subjected to frost heaving



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Mountain tunnels in cold regions are vulnerable to adverse effects of freezing action. Thus, it is necessary to identify the lining responses of shallow mountain tunnels subjected to freezing action. To quantify the influence of freezing action and key design parameters (such as cross-sectional shape; lining thickness; and waterproof measures) on the lining response, a thermal-hydro-mechanical coupled finite element (FE) model is established and verified. Then, specific consideration is given to the lining internal force and resulting axial stresses. And the influences of the cross-sectional shape, concrete parameters, and

waterproof measures on the lining responses are investigated. Generally, the rectangular tunnel has the worst security; the circular tunnel is the safest. On the other hand, when the thermal conductivity is less than 2.2 [W/(m•K)], a greater thermal conductivity will cause a greater risk of damage to the lining. Moreover, the drainage plate can reduce the value of minimum axial stresses, whether frozen or not, even eliminating the tension-damaged area. Overall, this study helps to estimate the lining responses and prevent frost damages for shallow mountain tunnels during freezing period.



## Evaluation of oilseed proteins as precursors of antimicrobial peptides using bioinformatics method



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In this study, the potential of oilseed proteins from soybean, peanut, sesame, sunflower seed and flaxseed as antimicrobial peptide (AMP) precursors was assessed using the bioinformatics method. Thirty-four novel potential AMPs were obtained by in silico hydrolysis of 12 oilseed protein sequences, and twelve of them were positive in all four algorithm tests in CAMP. Subtilisin was most effective for flaxseed AMPs release, obtaining 3 AMPs. More than 70% of AMPs

were predicted to be cationic peptides, and some AMPs were hydrophobic and formed alpha helix structure. These potential AMPs were classified as non-toxic peptides, and 15 peptides were non-allergenic. All the AMPs were unstable to digestive enzymes according to in silico simulated digestion. The results of this study provide a theoretical basis for further development of AMPs using oilseed proteins.



**The Ergosterol single  
crystal from Cordyceps  
Militaris differential  
anticancer mechanism  
with regulation estradiol  
17  $\beta$ - dehydrogenase  
and 3  $\beta$  - hydroxy  
steroid dehydrogenase**



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Cancer is one of the main diseases threatening human health. Although Traditional Chinese Medicine (TCM) shows prominent applications for difficult and miscellaneous diseases, it still lacks in-depth research on its anticancer mechanism. Therefore, this research aims to base on metabolic enzyme mutation to find key ingredients and clarify the mechanism of its key targets and pathways. Based on the cells experiments of A549 and HepG2 in vitro, 31 active compounds were extracted from TCM through the solvent and chromatographic system. Analyzed by the key compound-target-pathway network (contained 28 compounds, 52 targets, and 25 pathways). We combined with the mice experiments of Lewis and H22 in vivo and transcriptome Single

Molecular Real-time (SMRT) sequencing to screen out some key enzymes. TCM exerts anticancer effects through multi-interactions of components, targets, and pathways. Furthermore, combined with the mice experiments of Lewis and H22 in vivo, we found that 5 compounds had the effect of inhibiting the growth of Lewis cancer, and 3 can inhibit the growth of H22 cancer, precisely, Cordyceps militaris HN strain (C. militaris HN) fruiting body specifically inhibited the growth of cancer cells through regulating the oxidation of estradiol to estrone in A549 and reducing the 3 $\beta$ -hydroxysteroid dehydrogenase (3 $\beta$ -HSD) in HepG2. Transcriptome SMRT sequencing results confirmed that the estradiol-17 $\beta$  dehydrogenase (17 $\beta$ -HSD) was mutated in A549 cells (ref. XP\_011523034.1),

respectively, with 79% identity, 49 gaps. And in HepG2, glyceraldehyde-3-phosphate dehydrogenase (GAPDH) was mutated (ref. NP\_001243728.1), with 97% identity, 1 gap; 3 $\beta$ -HSD was mutated cells(ref. NP\_079469.2), with 86% identity, 52 gaps. The TCM anticancer mechanisms mainly involved multiple

interactions with targets and pathways. And the ergosterol single crystal from *C. militaris* HN specifically inhibited cancer by regulating the 17 $\beta$ -HSD and GAPDH in A549 and reducing the 3 $\beta$ -HSD in HepG2. That may provide an important metabolic to treat lung cancer and new targets to treat lung and liver cancer.





## Enzymes of the sphingomyelinase pathway synthesis of ceramides in adipose tissue of the heart in patients with cardiovascular diseases



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**Objective:** To study the expression of enzymes of ceramide metabolism in the heart and blood vessels of patients with coronary artery disease and valvular heart disease.

**Materials and Methods:** The study included 30 patients with coronary artery disease (CAD) and 30 patients with heart defects (aortic valve stenosis/insufficiency). During surgery, biopsies of subcutaneous adipose tissue (SAT), epicardial (EAT) and perivascular (PVAT) were obtained. In AT samples the enzymes of ceramide synthesis genes expression (acid sphingomyelinase: SMPD1, neutral sphingomyelinase: SMPD3) and ceramide utilization (sphingomyelin synthase 1: SGMS1, sphingomyelin synthase 2: SGMS2) by quantitative PCR. Statistical analysis of the results was performed using GraphPad Prism 8 (GraphPad Software).

**Results:** We found that SMPD1 was more expressed in cardiac AT than SMPD3. In the group of CAD, the SMPD1 expression was the highest in SAT ( $p=0.011$ ) and EAT ( $p=0.002$ ) compared to PVAT, in the group of heart defects - in SAT compared to PVAT ( $p=0.026$ ). the maximum gene expression of SGMS1 In EAT was found in CAD group which was combined with a high mRNA level of SGMS2 in the SAT and PVAT. The SGMS1 expression in EAT in the CAD group was higher ( $p=0.0011$ ) and SGMS2 in SAT ( $p=0.013$ ) and PVAT ( $p=0.0013$ ) compared with patients with heart defects.

**Conclusion:** Regional fat depots of the heart differed in the level of expression of enzymes of ceramide biosynthesis the sphingomyelinase pathway and synthesis of sphingomyelin from ceramides. The results obtained indicate the probable activation of this ceramide synthesis

pathway in adipocytes of predominantly epicardial localization in coronary pathology, which may contribute to the accumulation of certain ceramides associated with the pathophysiological aspects of atherosclerosis in the AT of this localization.

**Source of financing:** Russian Science Foundation grant No. 22-15-20007 "Ceramide profile of local heart fat depots: clinical and pathogenetic significance and therapeutic potential".



## Preparation of hollow Zn<sub>2</sub>SnO<sub>4</sub> / ZnSn(OH)<sub>6</sub> cubes and their gas-sensitive and visible light photocatalytic properties



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**M**etal oxide semiconductors with porous or hollow heterostructures can significantly improve the gas-sensing properties of materials by promoting the increase in free electron density and the diffusion of test gases. Compared with solid nanostructures, hollow micro/nanostructures have low density, It has large specific surface area, good surface permeability, high light-harvesting efficiency, and excellent photocatalytic activity. Firstly, using zinc acetate, sodium stannate and ammonium fluoride as raw materials, using NH<sub>4</sub>F etching, a hollow structure of ZnSn(OH)<sub>6</sub> cubes with a size of 250 nm was prepared by the hydrothermal method, and then calcined in air to obtain hollow Zn<sub>2</sub>SnO<sub>4</sub>/SnO<sub>2</sub> nanocubes with inter-n-n heterojunctions. The research shows that the ZnSn(OH)<sub>6</sub> prepared by hydrothermal treatment for 2

h has a complete hollow structure, and the degradation efficiency of methylene blue under visible light is the best. O<sub>2</sub><sup>-</sup> plays a major role in the degradation process, and the stability is good, indicating that the hollow ZnSn(OH)<sub>6</sub> cubic photocatalytic material is a promising visible light catalytic degradation material. Further, the Zn<sub>2</sub>SnO<sub>4</sub>/SnO<sub>2</sub> sensor has a good response (Ra/Rg) to ethanol and formaldehyde compared with other volatile organic compound (VOC) gases. Specifically, in 100 ppm ethanol and formaldehyde at 200°C, the Ra/Rg are 11.12 and 9.16, respectively. Furthermore, the repeatability, stability and ambient humidity, and enhancement mechanism of this sensor are systematically discussed, which suggests that Zn<sub>2</sub>SnO<sub>4</sub>/SnO<sub>2</sub> nanocubes with hollow structures are a promising material for VOC gas detection.



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