	IIT Ropar
Sl.	List of Recent Publications with Abstract
No.	Coverage: February, 2021
	A Novel Frequency Estimator for Protection Applications in Active Distribution Networks
	Y Bansal, R Sodhi - 21st National Power Systems Conference (NPSC), 2020
1.	<b>Abstract:</b> Frequency is a useful parameter for ensuring the proper functioning of the power system operation, control, and protection. In this paper, a fast and accurate frequency estimator is developed using a Zero-crossing and a Peak, occurring in the buffered data instead of two Zero crossings, which is commonly used to measure the frequency. Prior to this, the signal is preprocessed using the Sliding Goertzel Filter (SGF) that mitigates the impact of undesirable features such as harmonics, noise, etc. from the signal. The two frequency estimators, with and without SGF, then work in parallel to form the hybrid estimator and named as ZCPk—HFE. The estimated frequency is chosen based on the minimum error computed from the two parallel estimators. The performance of the estimator is, then, validated using the simulated signals polluted with harmonics, noise, transients etc. Moreover, the evaluation results with the IEEE-13 Active Distribution Network (ADN) incorporated with Photovoltaic DG using and dSPACE1104 and Real Time Digital Simulator (RTDS), show its capability to estimate real-time frequency
	with satisfactory output.
2.	A Novel Modular Approach for Kinematic Modelling and Analysis of Planar Hybrid Manipulators S Gupta, S Gupta, A Agrawal, E Singla - Journal of Mechanical Design, 2021  Abstract: For customized design of a hybrid-manipulator for a specific application, selection of an appropriate configuration is always a challenge. To assist in this foremost decision in data-driven synthesis, a novel approach is proposed for modular formation of quick configurations and developing respective kinematic model and differential relations for their performance analyses. This unified modular approach utilizes modular primitives to define a planar hybrid configuration. Three types of primitives are introduced as modular component, and pattern study is detailed. Modelling results from the proposed approach are compared to that with normally used partial differentiation with respect to the computational efforts, streamlined modular implementation and applicability in optimal design approaches. The strategy will help a designer as a tool for analysing several configurations. Two realistic case studies are demonstrated in the paper for application of the methodology in medical robotics field.
	A Serverless Cloud Computing Framework for Real-Time Appliance-Usage Recommendation S Dash, R Sodhi, B Sodhi - 21st National Power Systems Conference, 2020
3.	<b>Abstract:</b> Real-time appliance-usage recommendation (RTAUR) is an essential pre-requisite for various demand response (DR) programmes. This paper presents a simple yet effective integer programming (IP)-based model to solve the applianceusage scheduling problem in a dynamic pricing scenario. The proposed work further explores the viability of using a Serverless cloud-computing (SCC) framework for the actual implementation of RT-AUR algorithm. The efficacy of the overall proposal is demonstrated using a co-simulation architecture, combining a grid-simulation platform- MATLAB with a real-time cloudcomputing platform- Amazon Web Services (AWS). Various cosimulation results clearly reveal the effectiveness of the proposed SCC framework for RT-AUR.

A Simple Cyber Attack Detection Scheme for Smart Grid Cyber Security Enhancement S De, R Sodhi - 21st National Power Systems Conference (NPSC), 2020

Abstract: This paper proposes a simple framework for the detection of statistically crafted cyber-attacks, viz., random attacks, denial of service (DoS) attacks, False data injection(FDI) attacks, etc., in smart grids. A new cyber attack detector (CAD) is devised for this purpose which, in turn, is based on two statistical coefficients. The efficacy of the proposed framework is demonstrated on Real Time Digital Simulator (RTDS), along with its comparative assessments with another detector under various different attack scenarios.

Adapting Tellegen's Theorem for Synchrophasor-Assisted Fault Identification in Active Distribution Networks-An Illustration

Y Bansal, R Sodhi - 21st National Power Systems Conference, 2020

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Abstract: The integration of distributed generations at distribution level makes the traditional fault location schemes inappropriate, owing to bidirectional power flows and other challenges. It therefore becomes imperative to develop new and reliable fault identification methods in Active Distribution Network (ADN) in order to automatically isolate and restore the end-user services in a short space of time. To this end, this paper presents a synchrophasor-assisted Tellegen's theorem based fault identification method in ADNs. At first, the two adjoints of the original network are created and their phasor information is stored offline. Next, it is assumed that the distribution-level Phasor Measurement Units (PMUs) aka  $\mu$ PMUs are located at the extreme buses of the actual network that provides the real-time data, and finally, both the off-line and real-time information is utilized to detect the open or short circuit fault in the network. The proposed fault identification method is demonstrated in detail on a simple system, keeping in view the typical ADN characteristics.

Advancements in Microgrid Voltage Control Schemes
K Chauhan, R Sodhi - 21st National Power Systems Conference (NPSC), 2020

**Abstract:** Due to the intermittent behaviour of the renewable energy sources, containing the voltage rise issues and maintaining voltage regulation throughout the microgrids is of paramount importance. This paper presents a detailed literature survey on the available voltage control schemes. A unique approach for classifying and analyzing the voltage control techniques of active distribution system and/or microgrid, on the basis of their time scale, is proposed as short term voltage control and long term voltage control. Various architectures of their field implementation as decentralized, centralized and distributed are reviewed and discussed. Furthermore, the future trends in the voltage control are also reported.

An analytical approach for frequency modulated thermal wave imaging for testing and evaluation of glass fiber reinforced polymers

A Rani, R Mulaveesala, V Kher - IoP SciNotes, 2021

**Abstract:** Frequency modulated thermal wave imaging (FMTWI) has been considered as one of the promising nondestructive testing and evaluation approach due to its merits such as economical, safe, fast, sensitive and high depth resolvability. The present work provides a novel analytical solution for FMTWI using one-dimensional heat conduction equation with adiabatic (Neumann) boundary conditions. The temperature gradient over the glass fiber reinforced polymer specimen has been analyzed and validated with a commercially available three

dimensional mathematical finite element model to retrieve the quantitative information regarding the subsurface defects. The efficiency of the proposed method is highlighted using matched filter based approach for a frequency modulated imposed heat flux. The depth resolvability of the proposed method has been studied from the obtained correlation lag and the time domain phase obtained for FMTWI technique.

Cavitation Erosion Resistant Nickel-based Cermet Coatings for Monel K-500 NK Singh, ASM Ang, DK Mahajan, H Singh - Tribology International, 2021

**Abstract:** WC-NiCr and WC-Hastelloy C coatings were deposited on Monel K-500 substrate by HVOF-spray with an aim to enhance cavitation erosion resistance of the alloy. The cavitation tests were performed for 10 hours following ASTM G32-10 standard. Both WC-NiCr as well as WC-Hastelloy C coatings successfully reduced the erosion volume loss of the alloy by 59 % and 9 % respectively. The relatively superior performance of WC-NiCr coating could be attributed to better combination of its microhardness and fracture toughness. Formation of craters, cavities, and debonding of splats were found to be the signatures of cavitation erosion in the coatings. Whereas, microplastic tearing and microcracks were observed as the primary erosion mechanism in Monel K-500.

Communication-free Approach for Frequency Support in the MTDC grids-A Comparative Study AS Kumar, BP Padhy - 21st National Power Systems Conference, 2020

Abstract: Frequency Support (FS) through the Multi-Terminal HVDC (MTDC) grids is become obligatory by most of the Transmission System Operators (TSOs). Providing this support without any communication between converter stations is challenging. In the literature, researchers try to obtain the FS from the dc grid in a communication-free manner to improve the stability and reliability of the AC surrounded MTDC (AC-MTDC) grids. Moreover, in most of the literature, based upon the test system considered, the researchers have adopted a suitable control scheme. However, a study of various communication-free based FS control schemes and comparison among them are unavailable in the literature, which is the subject matter of this paper. Further, to conclude the various frequency supporting control methodologies, simulation of two case studies have been carried out with three schemes in PSCAD/EMTDC software. The conclusion is drawn based upon the simulation results and comparative study.

Comparison of enhanced second harmonic generation in pyramid-like in-plane MoS2 flakes to vertically aligned MoS2 flakes

AV Agrawal, R Lemasters, C Li, A Mojibpour...M Kumar - Journal of Applied Physics, 2021

**Abstract:** Here, we report the comparative study of enhanced second harmonic generation using defect engineering in pyramid-like MoS2 (P-MoS2) flakes to vertically aligned MoS2 (VA-MoS2) flakes. P-MoS2 and VA-MoS2 is synthesized via the modified chemical vapor deposition technique. The second harmonic generation measurements on P-MoS2 and VA-MoS2 are performed by sweeping the excitation wavelength from 1200 nm to 1310 nm in identical conditions. The P-MoS2 flakes show a high SHG signal. The high SHG signal in pyramid-like MoS2 is attributed to the broken inversion symmetry and high thickness of grown MoS2 flakes. VA-MoS2 flakes under the identical conditions show a 34% enhanced SHG signal in comparison to P-MoS2. The midgap states generated due to defects in the form of S vacancies in VA-MoS2 are responsible for this enhancement. These midgap states confine the photons and result in enhanced SHG properties. Our study will pave a new path to understand the role of 2D material

morphology in fabricating versatile optical and photonics devices.

Constrained Autoencoder based Pulse Compressed Thermal Wave Imaging for Sub-surface Defect Detection

K Kaur, R Mulaveesala, P Mishra - IEEE Sensors Journal, 2021

**Abstract:** Non-destructive testing & evaluation techniques play an essential role in ensuring safety of materials in operation at various industry sectors. Pulse compressed favourable thermal wave imaging is one of the widely used non-destructive testing techniques due to its excellent noise rejection capabilities. However, the high dimensional thermal imaging data needs to be encoded into lossless compressed form to highlight the hidden defects inside the materials. This paper proposes a novel constrained and regularized autoencoder based thermography approach for sub-surface defect detection in a mild steel specimen. Certain properties such as noncorrelation of encoded data, weight orthogonality, and weights with unit norm length have been highlighted which are non-existent in linear autoencoders but are responsible for better defect detection inside the materials inspected by frequency modulated thermal wave imaging. Novel constraints are formulated for autoencoder cost function to incorporate these significant properties. The proposed approach is able to provide better defect detection, in terms of signal to noise ratio of defects, than linear autoencoder as well as traditional principal component thermography approach. Also, non-correlation of encoded data is found to be the most significant factor in achieving better defect detection followed by properties ensuring weight orthogonality and weights with unit norm length.

Controlling the flow and heat transfer characteristics of power-law fluids in T-junctions using a rotating cylinder

A Maurya, N Tiwari, RP Chhabra - International Journal of Thermal Sciences, 2021

**Abstract:** In this work, the combined influence of the power-law rheology and isothermal rotating cylinder has been investigated numerically on the flow and heat transfer characteristics in a T-channel. The cylinder placed at the T-junction imitates the functioning of a rotating valve which controls the flow rate and the enthalpy distribution of the exiting streams in two branches. The range of parameters considered in this work is as: Reynolds number,  $1 < \text{Re} \le 50$ , power-law index,  $0.2 \le n \le 1$ , Prandtl number,  $10 \le Pr \le 100$  and non-dimensional circumferential velocity of the cylinder,  $-5 \le \alpha \le 5$ . Results suggest that the rotating cylinder can be used as a technique to create and/or reduce the formation of momentum and thermal boundary layers in the flow domain. The rotational velocity ( $\alpha$ ) and power-law flow index (n) are seen to have a strong effect on the critical Reynolds number for both the main and side branches. The hydrodynamic forces acting over the cylinder surface exerted by the fluid in the flow and perpendicular to the flow direction show a strong relationship with the cylinder rotation. For a particular combination of the studied parameters, these forces are also seen to be negative. Further, it is interesting to note that as the power-law index increases, the flow split ratio decreases while it shows an opposite trend with the Reynolds number. It can also be varied by switching the rotation direction. The dimensionless exiting temperature and enthalpy distribution are seen to have a strong relationship with the direction of rotation, fluid power-law index, Reynolds and Prandtl numbers. The mean values of the Nusselt number are seen to increase and/or decrease with the rotational velocity. For the anticlockwise rotation, the maximum suppression in the heat transfer is seen to be 79% while 62% for the clockwise rotation for the Newtonian fluid behaviour at low Prandtl number and high Reynolds numbers.

Convolution Filter based Efficient Multispectral Image Demosaicking for Compact MSFAs

V Rathi, P Goyal - Proceedings of the 16th International Joint Conference on Computer Vision,
Imaging and Computer Graphics Theory and Applications, 2021

Abstract: Using the multispectral filter arrays (MSFA) and demosaicking, the low-cost multispectral imaging systems can be developed that are useful in many applications. However, multispectral image demosaicking is a challenging task because of the very sparse sampling of each spectral band present in the MSFA. The selection of MSFA is very crucial for the applicability and for the better performance of demosaicking methods. Here, we consider widely accepted and preferred MSFAs that are compact and designed using binary tree based approach and for these compact MSFAs, we propose a new efficient demosaicking method that relies on performing filtering operations and can be used for different bands size multispectral images. We also present new filters for demosaicking based on the probability of appearance of spectral bands in binary-tree based MSFAs. Detailed experiments are performed on multispectral images of two different benchmark datasets. Experimental results reveal that the proposed method has wider applicability and is efficient; it consistently outperforms the existing state-of-the-art generic multispectral image demosaicking methods in terms of different image quality metrics considered.

Cyber Security Enhancement of Smart Grids Via Machine Learning-A Review PU Rao, B Sodhi, R Sodhi - 21st National Power Systems Conference, 2020

Abstract: The evolution of power system as a smart grid (SG) not only has enhanced the monitoring and control capabilities of the power grid, but also raised its security concerns and vulnerabilities. With a boom in Internet of Things (IoT), a lot a sensors are being deployed across the grid. This has resulted in huge amount of data available for processing and analysis. Machine learning (ML) and deep learning (DL) algorithms are being widely used to extract useful information from this data. In this context, this paper presents a comprehensive literature survey of different ML and DL techniques that have been used in the smart grid cyber security area. The survey summarizes different type of cyber threats which today's SGs are prone to, followed by various ML and DL-assisted defense strategies. The effectiveness of the ML based methods in enhancing the cyber security of SGs is also demonstrated with the help of a case study.

Dynamic correlations and volatility spillovers between stock price and exchange rate in BRIICS economies: evidence from the COVID-19 outbreak period K Rai, B Garg - Applied Economics Letters, 2021

**Abstract:** This paper examines the impact of COVID-19 pandemic on dynamic correlations and volatility spillovers between stock prices and exchange rates in BRIICS economies. Using volatility modelling, we demonstrate significant negative dynamic correlations and volatility spillovers between stock and exchange returns in most of the BRIICS economies. Further, the relationship strengthened during the initial days of lockdowns. Our results pass the sensitivity analysis, and hence robust. Overall, our findings indicate that there have been significant risk transfers between the two markets, during the COVID-19 outbreak, which led to decline in domestic stock returns and subsequent capital outflows thereby increasing the exchange rates.

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Electric Field and DC Breakdown Voltage of Multi-layer Dielectrics in Parallel-Plane Geometry P Muppala, CC Reddy - IEEE Transactions on Dielectrics and Electrical Insulation, 2021

**Abstract:** In this paper, the electric field, space charge and temperature distributions across a double layered dielectric are investigated under DC voltage. The dissimilarity of material properties of different layers, the effect of electric field and temperature dependent conductivity are found to play critical role in the electro-thermal problem of multi-dielectrics. At the interface, Maxwell-Wagner polarization is incorporated for electric field and interfacial charge, while temperature is considered as a continuous function of space inside the material. The current continuity equation, thermal continuity equation and Poisson's equation are simultaneously solved using numerical methods in parallel-plane electrode geometry. The electric field distribution, temperature distribution, space charge distribution and thermal breakdown limits are obtained at various boundary temperatures for different thickness proportions of layers.

<u>Electrochemical Rearrangement Protocols towards the Construction of Diverse Molecular</u> Frameworks

D Saha, IM Taily, R Kumar, P Banerjee - Chemical Communications, 2021

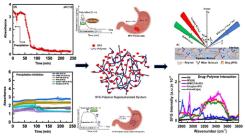
Abstract: Rearrangement reactions constitute a critical facet of synthetic organic chemistry and demonstrate an attractive way to take advantage of existing structures to access various important molecular frameworks. Electroorganic chemistry has emerged as an environmentally benign approach to carry out organic transformations by directly employing the electric current and avoids the use of stoichiometric chemical oxidants. The last years are witnessing a resurgence of electroorganic chemistry that has promoted a renaissance of interest in the development of novel redox electroorganic transformations. This review manifests the evolution of electrosynthesis in the area of rearrangement chemistry and covers the achievements in the field of migration, ring expansion, and rearrangements along with the mechanisms involved.

Elucidating the Molecular Mechanism of Drug-Polymer Interplay in a Polymeric Supersaturated System of Rifaximin

R Singh, V Thorat, H Kaur, I Sodhi, SK Samal, KC Jena... - Molecular Pharmaceutics, 2021

Abstract: Supersaturated drug delivery system (SDDS) enables the solubility and sustained membrane transport of poorly water-soluble drugs. SDDS provides higher drug concentration in the dispersed phase and equilibrium in the continuous phase, which corresponds to amorphous solubility of the drug. Rifaximin (RFX) is a nonabsorbable BCS class IV drug approved for the treatment of irritable bowel syndrome and effective against Helicobacter pylori. RFX shows slow crystallization and precipitation in an acidic pH of 1.2-2, leading to obliteration of its activity in the gastrointestinal tract. The objective of the present study is to inhibit the precipitation of RFX, involving screening of polymers at different concentrations, using an inhouse developed microarray plate method and solubility studies which set forth hydroxypropyl methylcellulose (HPMC) E15, Soluplus, and polyvinyl alcohol to be effective precipitation inhibitors (PIs). Drug-polymer precipitates (PPTS) are examined for surface morphology by scanning electron microscopy, solid-phase transformation by hot stage microscopy, the nature of PPTS by polarized light microscopy, and drug-polymer interactions by Fourier transform infrared and nuclear magnetic resonance spectroscopy. Besides, the unfathomed molecular mechanism of drug-polymer interplay is discerned at the air-water interface using sumfrequency generation spectroscopy to correlate the interfacial hydrogen bonding properties in

bulk water. Surprisingly, all studies disseminate HPMC E15 and Soluplus as effective PIs of RFX.



Evaluation of three approaches to probable maximum precipitation estimation: a study on two Indian river basins

SR Chavan, VV Srinivas - Theoretical and Applied Climatology, 2021

Abstract: Estimates of probable maximum precipitation (PMP) and corresponding probable maximum flood (PMF) are necessary for planning, design, and risk assessment of flood control structures whose failure could have catastrophic consequences. For PMP estimation, multifractal approach (MA) is deemed to be better than conventional approaches, which are based either on statistical concepts or physical aspects. The MA yields physically meaningful PMP estimates by attempting to capture scale-invariant multiplicative cascade mechanism inherent in rainfall. This paper attempts to gain insights into the performance of MA by comparing PMP estimates obtained using the approach with those resulting from the use of two widely used empirical approaches (storm maximization approach (SMA) and Hershfield method (HM)) on two floodprone river basins (Mahanadi and Godavari) in India. The results indicate that rainfall data of the two river basins exhibit multifractal properties, and the use of MA has an advantage over HM and SMA in estimating PMP corresponding to longer durations (>3 days). PMP estimates obtained using HM are generally lower (higher) than those obtained using SMA for 1-day (higher) duration. PMP maps are prepared for the two Indian river basins corresponding to 1-day to 5-day durations. Further, PMP estimates obtained based on the PMP maps are provided for 18 catchments in the Mahanadi basin and 53 catchments in the Godavari river basin.

Ferrohydrodynamics governed evaporation phenomenology of sessile droplets A Kaushal, V Mehandia, P Dhar - Physics of Fluids, 2021

Abstract: In this article, we report the morphing of the evaporation kinetics of paramagnetic saline sessile droplets in the presence of a magnetic field stimulus. We explore the evaporation kinetics both experimentally and theoretically and study the kinetics on hydrophilic and superhydrophobic substrates for various magnetic field strengths. We show that the evaporation rates of the paramagnetic droplets are augmented significantly and are observed to be a direct function of the magnetic field strength. Additionally, we note the modulation of the contact line transients due to the presence of the field. The influential role of solvated ions in modulating the flow behavior, and subsequently the evaporation, of droplets is present in the literature. Taking cue, we show using particle image velocimetry and infrared thermography that the magnetic field augments the thermo-solutal advection within the droplets. A mathematical analysis, based on the different internal advection mechanisms, has been proposed. We reveal that the magneto-thermal and magneto-solutal modes of internal ferrohydrodynamics are the dominant mechanisms behind the augmented evaporation dynamics. The experimentally obtained internal

velocities are in excellent compliance with the model predictions. Furthermore, the enhanced evaporation rates are predicted accurately using a proposed model to scale the interfacial shear modified Stefan flow. The inferences drawn from these findings may hold several important implications in magnetic field-modulated microfluidic thermal and species transport systems.

Fluorescence modulation of naphthalene containing salicyl hydrazide based receptor through aggregation induced emission enhancement (AIEE) approach: Dual detection of lanthanum and cyanide ions in semi-aqueous medium

P Joshi, SR Ali, VK Bhardwaj - Luminescence: the journal of biological and chemical luminescence, 2021

Abstract: The sensing activity of naphthalene containing salicyl hydrazide-based fluorescence receptor has been improved through aggregation-induced enhanced emission mechanism approach in semi-aqueous medium. The receptor has been found to be selective toward La3+ with approximately 70-fold fluorescence enhancement due to a combined effect of keto-enol tautomerism inhibition and chelation enhanced fluorescence with a detection limit of 3.91 × 10–6 M. In addition, the receptor is also able to sense CN– with a detection limit of 3.55 × 10–6 M via deprotonation effect, justifying its multiple analyte sensing behaviour. Hence, the current analytical methodology improves the sensing activity of the probe and also provides a greener alternative for La3+ and CN– detection.

Frontispiece: Utilization of CO2 Feedstock for Organic Synthesis by Visible-Light Photoredox Catalysis

S Pradhan, S Roy, B Sahoo, I Chatterjee - Chemistry—A European Journal, 2021

**Abstract:** Visible-light photoredox-catalyzed transformation of carbon dioxide has emerged as a privileged technique for forging C–C and C–X bonds. Both nucleophilic and electrophilic activation of CO2 by visible-light photocatalysis enable efficient access of essential functionalities. The easy access of pervasive CO2 can readily be incorporated into various synthetic organic motifs, delivering value-added products. The advancements of visible-light-mediated photoredox-catalyzed processes for CO2 fixation onto organic matters are elaborately discussed, especially focusing on reports from 2018 to 2020. For more details see the Minireview by I. Chatterjee, B. Sahoo, et al. on page 2254.



Hydrogen assisted crack initiation in metals under monotonic loading: A new experimental approach

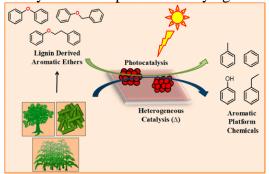
A Arora, R Kumar, H Singh, Dhiraj K. Mahajan - Theoretical and Applied Fracture Mechanics, 2021

**Abstract:** Hydrogen is foreseen as a promising energy carrier that can control global warming by reducing CO2 emissions. However, hydrogen is associated with an embrittlement phenomenon that imparts substantial damage to the infrastructure by reducing the ductility, fracture strength, strength bearing capacity, etc., of metallic components. Therefore, understanding hydrogeninduced crack initiation mechanisms in metals are of prime importance. Greater insights into this critical phenomenon are expected if the hydrogen-induced crack initiation can be correlated with the local microstructure and corresponding stress-strain state towards their propensity for hydrogen accumulation. With this motivation, in this work, crack initiation is studied for the uncharged and hydrogen charged nickel specimens during in-situ tensile loading under the scanning electron microscope. By assuming the material to be elastic at low strains, a novel approach is implemented for generating the microstructural stress maps through strain and stiffness tensor extracted at each point in the region of interest on the specimen surface using high-resolution digital image correlation (HR-DIC) and Euler angles (given by electron backscattered diffraction data), respectively. Based on this analysis at low strain, the crack initiation sites for uncharged and hydrogen charged nickel specimens are correlated with microstructural maps of maximum Schmid factor, elastic modulus in the loading direction, hydrostatic stress, von Mises stress, and triaxiality factor. The analysis highlighted two independent factors responsible for hydrogen enhanced decohesion (HEDE) based intergranular failure observed only at the random grain boundaries, (i) strain localization due to hydrogen enhanced localized plasticity (HELP) mechanism of hydrogen embrittlement, and (ii) hydrostatic stress-based hydrogen diffusion to the crack initiation sites. These critical insights thus can help to design hydrogen embrittlement resistant metals. In addition, the novel experimental approach can be used to calibrate advance micromechanical models while providing quantitative estimate of the hydrogen distribution in realistic metallic microstructure responsible for hydrogen-assisted crack initiation with deformation.

<u>Hydrogenolysis of Lignin-Derived Aromatic Ethers over Heterogeneous Catalysts</u>
A Shivhare, D Jampaiah, SK Bhargava, AF Lee, R Srivastava... - ACS Sustainable Chemistry & Engineering, 2021

**Abstract:** Global temperature has risen >1 °C since the preindustrial era, resulting in well-documented adverse climate impacts including extreme weather (floods, droughts, storms, and heat waves), a rise in sea level accompanying melting polar and glacial ice, and disrupted crop growth. These changes are closely correlated with anthropogenic greenhouse gas emissions, predominantly arising from the combustion of nonrenewable fossil fuels. Lignin derived from lignocellulose is the second most abundant biopolymer on Earth, and a rich source of renewable aromatic hydrocarbons to replace those currently obtained from fossil resources. Lignin depolymerization by cleavage of C–O and C–C linkages in the biopolymer can be achieved by direct pyrolysis or catalytic transformations, involving oxidation, hydrolysis, or hydrogenolysis reactions. Hydrogenolysis, in which H2 gas (or in-situ generated reactive H species) is supplied to lignin under relatively mild conditions, has attracted significant attention. This Perspective summarizes recent progress in the development of heterogeneous catalysts for the cleavage of C–

O linkages in lignin-derived aromatic ethers by hydrogenolysis: it encompasses strategies using H2, hydrogen transfer, and photocatalysis for aromatic monomers production, and the determination of structure—activity relationships and underlying reaction mechanisms.



<u>Impact of magnetic field on the thermal properties of chemically synthesized Sm-Co</u> nanoparticles based silicone oil nanofluid

A Oraon, BP Das, M Michael, T Adhikary, P Dhar... - Journal of Thermal Analysis and Calorimetry, 2021

**Abstract:** This work aims to study the enhanced thermal conductivity of silicone oil on increasing mass % of hard magnetic Sm-Co based nanoparticles (NPs) in the presence of external magnetic fields. Sm-Co NPs were synthesized using the low temperature 'Pechini-type sol-gel' process. The presence of mixed phases is evident through XRD, FESEM, and TEM. The average hydrodynamic size of Sm-Co NPs was measured 51 nm by DLS. The study of magnetization vs. magnetic field reveals the weak ferromagnetic ordering along with the paramagnetic behaviour of the Sm-Co NPs. Thermal conductivity enhancement of Sm-Co nanofluids showed an increasing trend with the rising particle concentration and magnetic flux density. A high thermal conductivity enhancement of  $\sim 373\%$  is reported at 15 mass % concentration of Sm-Co nanofluids and at a magnetic flux density of 0.5 T. The mechanism behind this thermal conductivity enhancement in the presence of an externally applied magnetic field has been discussed on the basis of near field magneto-static interactions of the magnetic nanoparticles. Microstructural, magnetic, and heat transport studies of Sm-Co based MNFs are very useful for device applications.

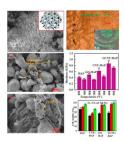
Improved nanomechanical and in-vitro biocompatibility of graphene oxide-carbon nanotube hydroxyapatite hybrid composites by synergistic effect

J Jyoti, A Kiran, M Sandhu, A Kumar, BP Singh, N Kumar - Journal of the Mechanical Behavior of Biomedical Materials, 2021

**Abstract:** Hydroxyapatite (HAP) is an attractive bio-material for new bone growth process, hard tissue repair, bioactivity, osteoblast adhesion and proliferation due to its physicochemical resembles natural apatite. The intrinsic brittleness and poor mechanical properties of HAP restrict it for potential clinical applications. This problem is undertaken by exploiting the unique properties of carbon nanofillers (carbon nanotube (CNTs), graphene oxide (GO), graphene oxide-carbon nanotube (GCNTs) hybrid) which are used as reinforcement for preparing the carbon nanofillers based HAP composites. The nanomechanical and in-vitro biocompatibility of carbon nanofiller reinforced HAP composites have been studied. Carbon nanofiller reinforced HAP composites led to an improvement in nanomechanical and biocompatibility properties. The

nanoindentation hardness and elastic modulus of GCNTs-HAP composites are significantly higher than other carbon nanofiller reinforced composites and pristine HAP powder. The in-vitro cytotoxicity of the prepared carbon nanofillers reinforced HAP composites is examined using MTT-assay on the MDCK cell line. The prepared GCNTs-HAP composites containing 2% of GCNTs nanofiller show higher cell viability, improved compatibility, and superior one cell proliferation induction than the other carbon nanofillers and HAP. These findings will provide the new prospects for utilizing the GO and its hybrid in HAP composites in bone repair, regeneration, augmentation and implantation.

## **Graphical Abstract:**



Mathematical modeling and analysis for controlling the spread of infectious diseases S Tyagi, SC Martha, S Abbas, A Debbouche - Chaos, Solitons & Fractals, 2021

**Abstract:** In this work, we present and discuss the approaches, that are used for modeling and surveillance of dynamics of infectious diseases by considering the early stage asymptomatic and later stage symptomatic infections. We highlight the conceptual ideas and mathematical tools needed for such infectious disease modeling. We compute the basic reproduction number of the proposed model and investigate the qualitative behaviours of the infectious disease model such as, local and global stability of equilibria for the non-delayed as well as delayed system. At the end, we perform numerical simulations to validate the effectiveness of the derived results.

Multiphysics simulation of plasma channel formation during micro-electrical discharge machining

S Raza, CK Nirala - AIP Advances, 2021

Abstract: A 2D axisymmetric plasma model for micro-electrical discharge machining (µEDM) is developed, and the discharge phenomenon is discussed in this paper. Variations in different plasma properties, such as density, temperature, and collisions of the electrons bombarding the anode and cathode electrodes, were simulated to comprehensively explain the discharge process. The said properties of the plasma channel will be extremely helpful in determining the heat flux available at the tool and workpiece of µEDM. The governing equations of electrostatics, drift-diffusion, and heavy species transport were coupled together and solved simultaneously for computing the properties of the plasma channel in water vapor. The simulation describes the movement of electrons and ions in the inter-electrode gap during the discharge initiation under the applied electric field. The anode spot responsible for the material removal was formed much earlier compared to the cathode spot formed at the tool. Both the temperature and the density of the electrons were observed to be higher near the workpiece, compared to the tool electrode. The temperature of the electrons and the current density of the plasma obtained during the simulation will be useful to determine the heat flux responsible for the material removal. The non-

equilibrium nature of the plasma sheath is responsible for the steep changes in the collisional power loss and higher capacitive power deposition near the workpiece electrode.

Network resilience of FitzHugh-Nagumo neurons in the presence of nonequilibrium dynamics S Bhandary, T Kaur, T Banerjee, PS Dutta - Physical Review E, 2021

Abstract: Many complex networks are known to exhibit sudden transitions between alternative steady states with contrasting properties. Such a sudden transition demonstrates a network's resilience, which is the ability of a system to persist in the face of perturbations. Most of the research on network resilience has focused on the transition from one equilibrium state to an alternative equilibrium state. Although the presence of nonequilibrium dynamics in some nodes may advance or delay sudden transitions in networks and give early warning signals of an impending collapse, it has not been studied much in the context of network resilience. Here we bridge this gap by studying a neuronal network model with diverse topologies, in which nonequilibrium dynamics may appear in the network even before the transition to a resting state from an active state in response to environmental stress deteriorating their external conditions. We find that the percentage of uncoupled nodes exhibiting nonequilibrium dynamics plays a vital role in determining the network's transition type. We show that a higher proportion of nodes with nonequilibrium dynamics can delay the tipping and increase networks' resilience against environmental stress, irrespective of their topology. Further, predictability of an upcoming transition weakens, as the network topology moves from regular to disordered.

nSite-Selective, Chemical Modification of Protein at Aromatic Side Chain and Their Emergent Applications

A Chowdhury, S Chatterjee, A Pongen, D Sarania, NM Tripathi, A Bandyopadhyay - Protein and Peptide Letters, 2021

Abstract: Site-selective chemical modification of protein side chain has probed enormous opportunities in the fundamental understanding of cellular biology and therapeutic applications. Primarily, in the field of biopharmaceutical where formulation of bioconjugates is found to be potential medicine than an individual constituent. In this regard, Lysine and Cysteine are the most widely used endogenous amino acid for these purposes. Recently, the aromatic side chain residues (Trp, Tyr, and His) that are low abundant in protein have gained more attention in therapeutic applications due to their advantages of chemical reactivity and specificity. This review discusses the site-selective bioconjugation methods for aromatic side chains (Trp, Tyr and His) and highlights the developed strategies in the last three years, along with their applications. Also, the review highlights the prevalent methods published earlier. We have examined that metal-catalyzed and photocatalytic reactions are gaining more attention for bioconjugation, though their practical operation is under development. The review has been summarized with the future perspective of protein and peptide conjugations contemplating therapeutic applications and challenges.

Quantitative Assessment and Analysis of Non-Masing Behavior of Materials under Fatigue SS Yadav, SC Roy, J Veerababu, S Goyal - Journal of Materials Engineering and Performance, 2021

**Abstract:** Quantitative assessment of non-Masing behavior is studied, and a new method is proposed for the estimation of cyclic plastic strain energy density and fatigue life. Low cycle fatigue tests were performed on 304L stainless steel employing strain amplitudes ranging from

 $\pm 0.25\%$  to  $\pm 1.0\%$  at a strain rate of 3  $\times$  10-3 s-1. The material exhibited Masing behavior at lower strain amplitudes and non-Masing behavior at higher strain amplitudes. Secondary hardening was observed at relatively higher strain amplitudes. Both the secondary hardening and non-Masing response were found to be associated with the deformation induced martensitic transformation. The master curve approach, which is generally used for the analysis of non-Masing response, could not be used as experimental data could not be represented in the form of a master curve. The proposed method of quantification of non-Masing response could estimate the cyclic plastic strain energy density of 304L stainless steel well within a scatter band of 1.2. The fatigue life of 304L stainless steel could also be predicted within a scatter band of 2. The proposed approach could also estimate the cyclic plastic strain energy density and fatigue life of materials of different grades within scatter factors of 1.2 and 2, respectively.

Significance of surface modification on nucleate pool boiling heat transfer characteristics of refrigerant R-141b

S Deb, M Das, DC Das, S Pal, AK Das, R Das - International Journal of Heat and Mass Transfer, 2021

Abstract: Experimental investigations were conducted to study the significance of surface modification on the heat transport phenomena under nucleate pool boiling configuration of saturated R-141b at ambient condition over SiO2 thin film (TF) nanocoated surfaces. The experiments were conducted within the heat flux variation of 50 to 185 kW/m2 at an interval of 15 kW/m2. The diameter of the heating surface was 9 mm, and the thickness was 3 mm. Five Cu heating surfaces of circular shape having zero (Emery polished surface (S1)), 125 (S2), 250 (S3), 375 (S4), and 500 (S5) nm coating thicknesses were fabricated employing the Sol-Gel approach accompanied by spin coater and characterized by surface profilometer and field emission scanning electron microscopy (FE-SEM). The current experimental results were verified with the existing correlations proposed in the literature. It was found that the heat transfer coefficient increased with an increase in the heat flux, and it is also witnessed here that modification in the surface significantly contribute towards the improvement in the heat transfer coefficient. The maximum and the minimum heat transfer were revealed at 375 (S4) and 500 (S5) nm coating thickness, respectively. Modification of the surface leads to an increase in the heat transfer coefficient due to the existence of a large number of dynamic nucleation sites. Finally, a mathematical model to predict the optimum nucleate pool boiling heat transfer coefficients for different coating thicknesses was proposed which reflects the effects of surface thickness, coating thickness, and the imposed heat flux. The model predicts good agreement with the experiment of R-141b and other existing findings within an accuracy of %.

<u>Spaceborne C-band SAR remote sensing-based flood mapping and runoff estimation for 2019</u> flood scenario in Rupnagar, Punjab, India

A Tripathi, L Attri, RK Tiwari - Environmental Monitoring and Assessment, 2021

Abstract: Floods are one of the most disastrous and dangerous catastrophes faced by humanity for ages. Though mostly deemed a natural phenomenon, floods can be anthropogenic and can be equally devastating in modern times. Remote sensing with its non-evasive data availability and high temporal resolution stands unparalleled for flood mapping and modelling. Since floods in India occur mainly in monsoon months, optical remote sensing has limited applications in proper flood mapping owing to lesser number of cloud-free days. Remotely sensed microwave/synthetic aperture radar (SAR) data has penetration ability and has high temporal data availability, making

it both weather independent and highly versatile for the study of floods. This study uses space-borne SAR data in C-band with VV (vertically emitted and vertically received) and VH (vertically emitted and horizontally received) polarization channels from Sentinel-1A satellite for SAR interferometry-based flood mapping and runoff modeling for Rupnagar (Punjab) floods of 2019. The flood maps were prepared using coherence-based thresholding, and digital elevation map (DEM) was prepared by correlating the unwrapped phase to elevation. The DEM was further used for Soil Conservation Service-curve number (SCS-CN)-based runoff modelling. The maximum runoff on 18 August 2019 was 350 mm while the average daily rainfall was 120 mm. The estimated runoff significantly correlated with the rainfall with an R2 statistics value of 0.93 for 18 August 2019. On 18 August 2019, Rupnagar saw the most devastating floods and waterlogging that submerged acres of land and displaced thousands of people.

The nexus between the exchange rates and interest rates: evidence from BRIICS economies during the COVID-19 pandemic

B Garg, KP Prabheesh - Studies in Economics and Finance, 2021

#### **Abstract:**

Purpose

This paper aims to investigate whether the interest rate differentials Granger cause expected change in the exchange rate during the COVID-19 period. The study examines if the investors in the international assets and exchange rate markets take advantages of the relevant information obtained during the COVID-19 pandemic.

## Design/methodology/approach

This paper used daily data ranging from January 31, 2020 to June 30, 2020 and considered BRIICS economies. The study implemented the Toda—Yamamoto's Granger causality approach to identify the causality between interest rate differentials and exchange rates. For robustness checks, the study used ARLD short-run dynamics to infer causal relations.

### **Findings**

Overall, the results indicate that the interest rate differentials improve the predictability of subsequent exchange rate changes in all six BRIICS economies during the COVID-19 period wherein investors are forward-looking. The empirical results pass the robustness checks.

#### Originality/value

There is a lack of studies exploring the relationship between interest rate differentials and exchange rates in the presence of an unanticipated event such as the current pandemic. To the best of the authors' knowledge, this is the first study to explore the causal linkages between interest rate differentials and expected change in exchange rates, focusing on the COVID-19 outbreak period.

Thermal Mixing of Shear-Thinning and Newtonian Fluids in a T-Channel Using Impinging Streams

A Maurya, N Tiwari, RP Chhabra - Proceedings of 16th Asian Congress of Fluid Mechanics: 35. Part of the Lecture Notes in Mechanical Engineering book series, 2021

**Abstract:** In this work, thermal mixing of shear-thinning (i.e. CMC solutions) and Newtonian fluids has been numerically investigated in a rectangular T-channel for a specified heat flux

boundary condition at the mixing zone walls. The influence of the Reynolds number  $(10 \le \text{Re} \le 50)$ , power-law index  $(0.6161 \le n \le 1)$ , Nusselt number (a dimensionless form of convective heat transfer coefficient for external air flow,  $103 \le \text{Nuo} \le 104$ ), and ambient temperature  $(-2.7 \le \theta a \le 1.3)$  is studied on the mixing behaviour. The flow is assumed to be steady, laminar, and incompressible. The new results are presented in terms of isotherm contours, mixing index, and required channel length to achieve complete mixing. The mixing index decreases along channel length for both shear-thinning and Newtonian fluids. Better mixing is seen at high power-law index, ambient temperature, and Nusselt number and low Reynolds numbers. The length required to achieve the 95% of the ambient temperature or the exact ambient temperature is shorter for mildly shear-thinning fluids (high power-law index) and Nusselt number, and low Reynolds numbers. Also, for the case of heating (high ambient temperature), the complete mixing demands a shorter channel length than that in the case of cooling.

<u>Understanding the priorities of designers for an ecodesign support during environmentally</u> sustainable product development

PK Singh, P Sarkar - World Journal of Science, Technology and Sustainable Development, 2021

#### **Abstract:**

Purpose

The main purpose of this research is to understand the priorities of designers for an ecodesign support, while developing environmentally sustainable products. Also, this study identifies the requirements of the designers for managing the environmental quality of products.

# Design/methodology/approach

This research is conducted in two phases of survey. In the first phase, various requirements of designers are collected, refined and segregated under certain well defined characteristics of the ecodesign support. In second phase, the designers are asked to rank each characteristic of the ecodesign support in a questionnaire. The responses obtained from the designers are analyzed separately for engineering designers and design researchers by using Henry Garrett ranking technique to identify the priorities of designers for an ecodesign support.

#### Findings

Results show that there is a contrast between the perspective of engineering designers and design researchers, and their priorities for an ecodesign support are opposite to each other. Thus it can be understood that the features which are added by design researchers in ecodesign support may not be adequate for engineering designers to manage the environmental quality of products.

#### Originality/value

The designers play a key role in the development of environmentally benign products through the use of different ecodesign supports (i.e. tools or methods). Therefore, it is important to understand the desired characteristics of the ecodesign support from designer's perspective. Also, the priorities of designers from academia (design researchers) and industry (engineering designers) must be understood because they are the two stakeholders indulged in the development and usage of various ecodesign supports for environmentally conscious product development (ECPD).

<u>Visible light promoted tandem dehydrogenation-deaminative cyclocondensation under aerobic condition for the synthesis of 2-aryl benzimidazoles/quinoxalines from ortho-phenylenediamines and arylmethyl/ethyl amines</u>

FA Sofi, R Sharma, R Rawat, AK Chakraborti... - New Journal of Chemistry, 2021

Abstract: Visible light promoted domino synthesis of 2-aryl benzimidazoles is reported through the reaction of ortho-phenylenediamines and arylmethyl amines under aerobic condition. The methodology has wide substrate scope and tolerates wide range of functional groups affording the products in high yields. Use of arylethyl amines replacing arylmethyl amines gives 2-aryl quinoxalines.

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