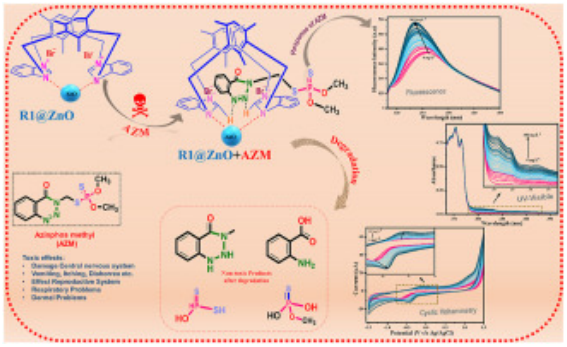
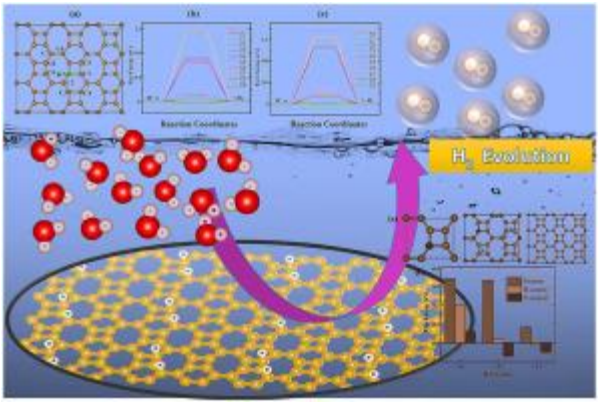
Sl. No.	IIT Ropar List of Recent Publications with Abstract Coverage: January, 2023
1.	A high-performance Calix@ZnO based bifunctional nanomaterial for selective detection and degradation of toxic azinphos methyl in environmental samples R Kaur, G Bhardwaj, S Saini, N Kaur, N Singh – Chemosphere, 2023 **Abstract:** One of the key tenets of sustainable agriculture and food safety is the removal of toxic pesticides from the environment. However, developing reliable, affordable, and efficient methods for detecting and degrading pesticides into non-toxic degradable products remains an immediate matter of concern. Herein, we attempt to develop a strategy for the detection as well as degradation of highly toxic phosphorodithioate pesticide, Azinphos methyl (AZM), using hybrid zinc oxide nanoparticles (ZnO NPs). Considering the non-selectivity of bare ZnO and receptor R1, we have fabricated the heterocalixarene-based Calix (R1) over zinc oxide (ZnO) surface in situ via the sol-gel process. The synthesized heterocaliaxrene-modified ZnO (R1@ZnO) NPs show an excellent affinity for the selective and sensitive detection of AZM with a tremendously low limit of detection (68 mg L^{-1}) and no interference from other pesticides. Degradation of AZM was fully supported by fluorescence spectroscopy, scanning electron microscopy (SEM), ^{1}H NMR titrations, FTIR spectroscopy, cyclic voltammetry, and mass spectroscopy, which unequivocally confirmed the formation of non-toxic products. According to our findings, R1@ZnO NPs are sustainable nanomaterials that can be employed for environmental remediation since they operate in an aqueous medium. **Graphical Abstract:** 
2.	A novel pedicle screw design with variable thread geometry: biomechanical cadaveric study with finite element analysis P Salunke, M Karthigeyan, P Uniyal, K Mishra, T Gupta, N Kumar - World Neurosurgery, 2022 **Abstract:** Background Pedicle screw fixation provides one of the most stable spinal constructs. Their designs together with osseous characteristics have been known to influence the screw-bone interplay during surgical maneuvers and thereafter the fusion process. Various technical modifications to enhance screw performance have been suggested. This study evaluated the pull-out strength and axial stiffness of a novel pedicle screw design with variable thread geometry and pitch. Methods The newly designed triple threaded pedicle screw is tapered, and has unique out-turned flanges

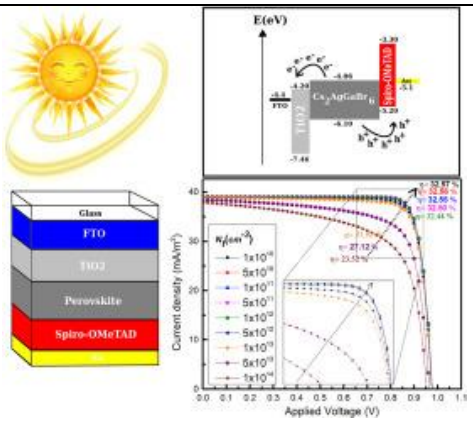
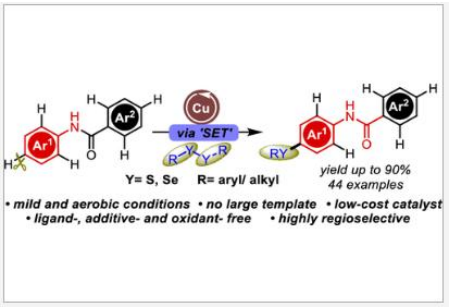
	to hold the cancellous bone and a finer pitch at its distal and proximal end to engage the cortical bone. Five lumbar and 4 lower thoracic cadaveric vertebrae were divided into hemivertebrae. A standard cancellous pedicle screw and the newly designed pedicle screw were inserted into each hemivertebra. Axial stiffness and peak pull-out force between the screw types were compared; a finite element analysis was also performed to additionally compare the pull out under toggle forces. Results In cadaveric study, the axial stiffness of the new screw was significantly better than that of the standard screw. However, the peak load between the screws was not statistically different. Finite element analyses suggested lesser stress at bone-implant interface for the new screw along with better axial stiffness under both co-axial and toggle forces. Conclusions Our novel pedicle screw design with variable thread geometry demonstrates greater axial stiffness compared with the standard screws, and therefore is likely to withstand a greater surgical manipulation.
3.	Activation of metal-free porous basal plane of biphenylene through defects engineering for hydrogen evolution reaction MR Sahoo, A Ray, R Ahuja… - International Journal of Hydrogen Energy, 2023 **Abstract:** The biggest challenge in the commercial application of electrochemical reduction of water through the hydrogen evolution reaction (HER) is hampered due to the scarcity of inexpensive and efficient catalysts. Herein, we propose a metal-free biphenylene nanosheet, a recently proposed two-dimensional (2D) carbon allotrope, as an excellent HER electrocatalyst. The dynamical and thermal stability of biphenylene nanosheet is validated through phonon dispersion and *abinitio* molecular dynamics (AIMD) calculations, respectively. At a low H coverage (1/54), the biphenylene nanosheet shows excellent catalytic activity with the Gibbs free energy (ΔG_{H*}) of 0.082 eV. The Bdoping and C-vacancy in biphenylene further improve ΔG_{H*} to −0.016 eV and 0.005 eV, respectively. The interactions between the H atom and the nanosheet are explained through the relative position of the *p*-band center. Our study opens new possibilities to use non-metallic porous materials as highly efficient electrocatalysts for HER. **Graphical Abstract:** 
4.	Addressing data intrinsic characteristics for augmentation for breast cancer classification A Garg - Proceedings of the 6th Joint International Conference on Data Science & Management of Data, 2023 **Abstract:** Breast cancer is the most frequently diagnosed cancer among females worldwide. The task of correctly diagnosing cancer using histopathology in its very earlier stages is a challenging

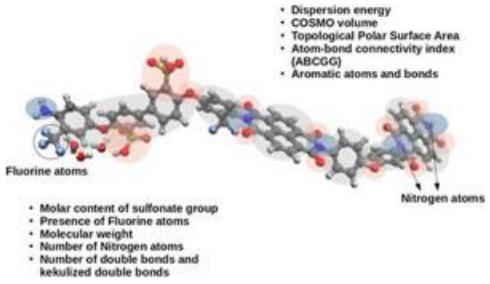
	and critical task. Most of the present machine learning techniques require a lot of data to analyze and predict a benign tumour in its early stages, and such data is not available readily. In this paper, we propose the idea of data augmentation of breast cancer tissue images by addressing data intrinsic characteristics. The aim is to detect the micro presence of the tumour cells and highlight it over multiple synthetic images for classifiers to predict benign tumours in very early stages with high accuracy. The initial experimental analysis highlights the proposed technique's impact and significance in boosting the performance of standard classifier(s).
5.	Algorithmic recourse based on user's feature-order preference M Singh, SS Kancheti, S Gupta, G Ghalme, S Jain… - Proceedings of the 6th Joint International Conference on Data Science & Management of Data, 2023 **Abstract:** The state-of-the-art recourse generation methods solely rely on the user's profile (feature vector). However, two users having the same profile may still have different preferences. Consequently, the recourse generated from a single profile may not have the same appeal to both the users. For example, one rejected loan applicant may prefer changes in Savings Amount, whereas, another - being a financial expert - may prefer changes in Investment Amount. Taking into account these preferences in feature-change can be very helpful in generating more user-satisfying recourses. To this end, we propose a simple user-preference representation and design a method to generate a recourse that adheres to the user preference. We empirically demonstrate the effectiveness and ease of the proposed method at generating recourses satisfying user preferences.
6.	Analytical framework of S-parameter based efficiency for secondary-parallel compensation WPT system to authenticate data using VNA A Bharadwaj, A Sharma, CC Reddy - IEEE Transactions on Instrumentation and Measurement, 2023 **Abstract:** Resonant Wireless Power Transfer (R-WPT) is the most efficient system in near-field applications. Predominantly, four distinct resonant topologies exist for R-WPT to enhance the power transfer efficiency (PTE) under different load conditions. Here, the PTE is considered crucial for gauging the R-WPT system performance. In a typical experimental scenario, measurement of the PTE is performed by exciting the Tx coil with a sinusoidal signal using a high-frequency inverter source. Thereby, the input and output power measurements are conducted using an oscilloscope. Here, the measurement using an oscilloscope is highly susceptible to external noise. As an alternative, the vector network analyzer (VNA) is the most accurate instrument to measure S-parameters with high precision, even at very high frequencies. The S-parameter-based analytical expressions for evaluating PTE are available only for series-series compensation topology. Therefore, the VNA usage is severely limited for experimental validation of the other compensation topologies. This paper proposes an analytical evaluation of S-parameter-based PTE for secondary parallel compensation topology as a contribution. Moreover, the mathematical proof is deduced to determine the active operating load condition for the secondary parallel capacitor. Error analysis of experimental data is performed where the SNR of the measurement system is greater than 35 dB and the percentage error rate ϵ is less than 1.3%, which implies high precision and accuracy of the S-parameter-based VNA measurement system.
7.	Applications and developments of thermal spray coatings for the iron and steel industry S Singh, CC Berndt, RK Singh Raman, H Singh… - Materials, 2023 **Abstract:** The steel making processes involves extreme and harsh operating conditions; hence, the production hardware is exposed to degradation mechanisms under high temperature oxidation, erosion, wear, impact, and corrosive environments. These adverse factors affect the product quality and efficiency of the steel making industry, which contributes to production downtime and maintenance costs. Thermal spray technologies that circumvent surface

	degradation mechanisms are also attractive for their environmental safety, effectiveness and ease of use. The need of thermal spray coatings and advancement in terms of materials and spray processes are reviewed in this article. Application and development of thermal spray coatings for steel making hardware from the molten metal processing stages such as electric arc and basic oxygen furnaces, through to continuous casting, annealing, and the galvanizing line; to the final shaping process such as cold and hot rolling of the steel strips are highlighted. Specifically, thermal spray feedstock materials and processes that have potential to replace hazardous hard chrome plating are discussed. It is projected that novel coating solutions will be incorporated as awareness and acceptance of thermal spray technology grows in the steel making sectors, which will improve the productivity of the industry.
8.	Bank competition and SMEs access to finance in India: evidence from world bank enterprise survey B Rakshit, S Bardhan - Asian Review of Accounting, 2023 **Abstract:** Purpose The primary purpose of this study is to investigate the effects of bank competition on SMEs' access to finance in selected Indian states. Using 9,281 firm-level observations from World Bank Enterprises Survey (WBES), this study tests the market power hypothesis versus the information hypothesis to determine whether bank competition promotes access to finance for financially constrained firms. Design/methodology/approach The authors measure state-level bank competition using two structural indicators: the Herfindahl Hirschman Index (HHI) and three bank concentration ratios (CR3). The authors apply simple probit regression, probit model with sample selection (PSS) and two-stage least squares (2SLS) to examine the effects of bank competition on firms' financing constraints. Findings The results obtained through PSS and 2SLS indicate that bank competition alleviates firm's financing constraints and positively impacts its need for a bank loan and the decision to apply for bank credit. However, the prevalence of bank competition in promoting access to finance is more pronounced for small and medium-sized firms than for large firms. Higher bank competition also alleviates the credit constraints faced by female entrepreneurs. Practical implications Reserve Bank of India (RBI) and other government stakeholders should ensure bank competition without hampering the agenda of bank consolidation to facilitate access to credit for SMEs. Regulators should also identify and monitor the financial institutions that make an insignificant contribution to promoting competitiveness in the financial system. Originality/value Previous studies primarily investigate the effect of bank competition on a firm's access to finance from advanced and cross-country perspectives. This study contributes to the literature on bank competition by examining its role in promoting access to finance from an emerging economy standpoint. Measurement of bank competition indicators at the state level is an additional contribution.
9.	Cassava starch-derived aerogels as biodegradable packaging materials P Joshi, K Gupta, P Uniyal…N Kumar… - Materials Chemistry and Physics, 2023 **Abstract:** Biodegradable and natural materials can provide transformational solutions to environmental issues, particularly those associated with ubiquitous fossil-resources-derived

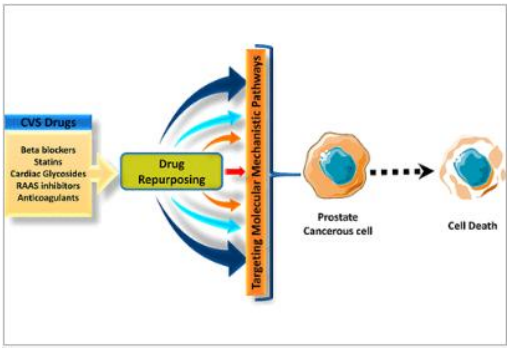
	conventional polymers like polyolefin thermoplastics and polystyrene foam as packaging materials. Herein, a facile approach is presented for preparing biodegradable and biocompatible lightweight structural scaffolds as an alternative to conventional plastic-based packaging materials. A variable dosage of polyvinyl alcohol (PVA) is used along with cassava starch to govern the structural integrity, mechanical properties, and porosity of resultant aerogels. The incorporation of PVA as a strengthening precursor improved the compressive modulus of starch aerogel from 2.0 to 18.2 MPa. Hydrogen-based interactions between the starch and PVA components, as revealed by infrared spectroscopic and differential scanning calorimetric measurements, extended the structural integrity. The high and regulated porosity of these aerogels furnished significantly low density (0.13–0.21 mg mm^{-3}). A 98.5% of the starch-PVA aerogel is converted to CO_2 by the microbial consortia within 23 days, signifying excellent biodegradability of these aerogels. Moreover, cassava starch-PVA aerogel is demonstrated as alternative packing material to conventional non-biodegradable black plastic bags for growing, transporting, and transplanting young plants. The improved thermal stability (<270 °C), low density, good compressive modulus (2.0–18.2 MPa), and excellent biodegradability reveal the potential of starch-based aerogels as excellent alternatives to conventional polyolefin thermoplastics and polymer-foam-based packaging materials.
10.	Community-based intervention targeting depressive symptomatology in indian women: an exploration of its efficacy in a non-specialized healthcare setting N Mishra, P Singh - Community Mental Health Journal, 2023 **Abstract:** Depressive symptomatology casts a more adverse impact on the well-being of women in countries with unfavourable societal norms. The prevalence of depressive symptomatology in Indian women and the treatment gap in case of mental health issues are alarming and thus may require interventions at a community level. The present study tested the efficacy of a psychosocial community-based intervention in managing depressive symptomatology and associated factors like rumination, reappraisal, psychological resilience, and self-efficacy using a pre-test post-test control group design. A total of 114 (M_{age}=23.03, SD = 5.29) and 37 (M_{age}=24.89, SD = 6.44) adult females were there in the experimental and the control group, respectively. A series of ANOVAs showed that participants' scores on depressive symptomatology and associated vulnerabilities and defences improved as compared to the baseline and the control group. The findings support the use of psychosocial community-based intervention in a non-specialized healthcare setting to manage depressive symptomatology, associated vulnerability and defences.
11.	Comparative study of Y_2O_3, SnO_2 and ZrO_2 as inhibitor to control high temperature corrosion of Ni-based superalloy G Goyal, N Bala, H Singh, S Prakash - Materials at High Temperatures, 2023 **Abstract:** High temperature corrosion of metals and alloys can be controlled by the use of inhibitors and fuel additives. In this work three different types of coatings namely Y_2O_3, SnO_2 and ZrO_2 coatings were superficially applied on Ni base superalloy Superni 718. Accelerated corrosion testing of the uncoated as well as the coated superalloy was done in a molten salt environment (Na_2SO_4-60%V_2O_5) at 900°C for 50 cycles. Each cycle consisted of 1 hour heating in a Silicon Carbide Tube furnace followed by 20 minutes cooling in ambient air. Weight change measurements after each cycle were taken by an electronic balance having an accuracy of 0.01 mg. XRD, SEM and EPMA analyses of the exposed specimens were carried out to characterise the oxide scales. The bare superalloy showed more overall weight gain, in comparison with all the coated counterparts. It was concluded that ZrO_2 was most effective in reducing corrosion rate in alloy A.
12.	Complexity results on cosecure domination in graphs Kusum, A Pandey - Conference on Algorithms and Discrete Applied Mathematics: Part of the Lecture Notes in Computer Science book series, 2023

	Abstract: Let G=(V,E) be a simple graph with no isolated vertices. A dominating set *S* of *G* is said to be a cosecure dominating set of *G* if for every vertex v∈S there exists a vertex u∈V\S such that uv∈E and (S\{v})∪{u} is a dominating set of *G*. The MINIMUM COSECURE DOMINATION PROBLEM is to find a minimum cardinality cosecure dominating set of *G*. Given a graph *G* and a positive integer *k*, the COSECURE DOMINATION DECISION PROBLEM is to decide whether *G* has a cosecure dominating set of cardinality at most *k*. The COSECURE DOMINATION DECISION PROBLEM is known to be NP-complete for bipartite, planar, and chordal graphs. In this paper, we show that the COSECURE DOMINATION DECISION PROBLEM remains NP-complete for split graphs, an important subclass of chordal graphs. On the positive side, we present a linear-time algorithm to compute the cosecure domination number of cographs. In addition, we also study the approximation aspects of the MINIMUM COSECURE DOMINATION PROBLEM. We show that the problem can be approximated within an approximation ratio of (Δ+1)(Δ+1) for perfect graphs with maximum degree ΔΔ. We also prove that the problem cannot be approximated within an approximation ratio of (1−ϵ)ln(|*V*|) for any ϵ>0, unless P = NP. Moreover, we prove that the MINIMUM COSECURE DOMINATION PROBLEM is APX-hard for bounded degree graphs.
13.	Computational insights into the superior efficiency of $Cs_2AgGa(Cl,Br)_6$ double halide perovskite solar cells M Kibbou, Z Haman…R Ahuja - Materials Chemistry and Physics, 2023 **Abstract:** Owing to their ecological integrity, non-toxicity, and outstanding performances, Double-Halide perovskites have been vigorously promoted as sustainable alternatives for thermoelectric and photovoltaic applications. In this context, we have systematically explored the structural and mechanical strength characteristics of $Cs_2AgGa(Cl,Br)_6$ materials through the tolerance factor analyses and Born stability criteria. Subsequently, a detailed study of their electronic, optical, and thermoelectric properties has been performed. As results, both $Cs_2AgGaCl_6$ and $Cs_2AgGaBr_6$ show semiconducting nature with a direct bandgap of about 2.57 eV and 1.42 eV, respectively. Additionally, with such desirable band gaps, the optical properties were examined based on the complex dielectric function. It has been derived that both materials exhibit a very high absorption spectrum in the order of 105 cm^{-1} and a low reflectivity not exceeding more than 18% in the visible and UV region. Furthermore, the $Cs_2AgGaBr_6$ has been taken into account as absorber to construct the planar p-intrinsic-n structure (FTO/TiO2/Cs2AgGaBr6/Spiro-OMeTAD/Au) and a high-record efficiency of 32.57% has been reached. The thermoelectric performance was also studied and revealed a very high Seebeck coefficient (thermo-power) and a sufficient figure of merit (ZT). Based on these results, we believe that the studied double-halide perovskites present outstanding performance for both optoelectronic and thermoelectric engineering devices. **Graphical Abstract:**

	
14.	[Copper-catalyzed regioselective remote C-H bond chalcogenation of aromatic amine derivatives without using any large template] B Paul, S Das, I Chatterjee - Organic Letters, 2023 **Abstract:** A mild and convenient strategy has been developed for the *para*-selective chalcogenation of anilide scaffolds via C–H bond functionalization. This methodology employs one of the most earth-abundant and inexpensive Cu(II) catalysts and a commercially available simple aryl chalcogen source without any complex directing template, exogenous ligand, acid/base, oxidant, or other additives. The key feature of this methodology is an impressive regioselectivity along with a wide range of functional group tolerance with good to excellent yields under aerobic conditions. 
15.	[Cosmological and black hole islands in multi-event horizon spacetimes] G Yadav, N Joshi – Physical Review D, 2023 **Abstract:** In this paper, we have analyzed the information paradox and its resolution using the island proposal in Schwarzschild de-Sitter black hole spacetime. First, we study the information paradox for the black hole patch by treating de-Sitter patch on both sides as a frozen background (by inserting thermal opaque membranes) and then carry out a similar study for de-Sitter patch. In both cases, when there is no island surface, the entanglement entropy has the linear time dependence as usual, whereas in the presence of an island surface, entanglement entropy becomes constant (equal to twice of thermal entropy of black hole/de-Sitter patch). Therefore, we obtain the Page curves for the black hole and de-Sitter patches consistent with the unitary evolution of black holes. In our case, we have found that the black hole island is located inside the black hole event horizon in contrast to the universal result for eternal black holes, and the cosmological island is also located inside cosmological event horizon. Further, we have studied the “effect of temperature” on Page curves and found that Page curves appear at late times for low-temperature black hole/de-Sitter patch and exhibit the opposite behavior for high-temperature. This implies that “dominance of islands” and “information recovery” takes more time for low-temperature black hole/de-Sitter patch in contrast to high-temperature black

	hole/de-Sitter patch. We also comment on the challenges of studying the information paradox in SdS spacetime without the thermal opaque membranes.
16.	Designing sulfonated polyimide-based fuel cell polymer electrolyte membranes using machine learning approaches T Rohilla, N Singh, NC Krishnan, DK Mahajan - Computational Materials Science, 2023 **Abstract:** Fuel cells are the efficient electrochemical energy conversion devices with wide-ranging applications. Polymer Electrolyte Membrane (PEM) is the primary component of a PEM fuel cell whose proton conductivity majorly determines the performance of the fuel cells. Due to the high cost and limited range of operating parameters, alternatives of perfluorinated ionomers based commercial PEMs are urgently required. Sulfonated polyimides (SPIs) based hydrocarbon PEMs, have exhibited better proton conductivity even at low hydration levels and high temperatures, making them possible candidates for replacing commercial PEMs. However, finding alternative SPI PEMs is a critical polymer discovery problem that requires enormous experimental efforts where Machine learning (ML) approaches can help to reduce such efforts. To this end, both supervised and unsupervised ML approaches are developed to predict the proton conductivity of SPIs. A hybrid dataset of 81 unique SPIs is generated that consists of collected chemical structure–properties data from reported literature and calculated quantitative structure–property and semi-empirical quantum chemical descriptors. Using simple and interpretable Decision Trees, rules that lead to a low or high class of proton conductivity labels with high accuracy are identified. The trained decision tree model can accurately predict the proton conductivity class labels with a prediction accuracy of 88% and a kappa statistic of 0.77. The random forest regression (RFR) model, on the other hand, identified additional set of features that can predict proton conductivity with reasonable error. Thus, high information-gain features have been identified and their correlation with the proton conductivity class labels have been explored. These findings are key to designing novel SPI PEMs while correlating proton transport at the ionomer level with factors such as the morphology of the microstructure and inter-chain interactions. **Graphical Abstract:** 
17.	Determinants of twisted generalized hybrid weaving knots S Joshi, M Prabhakar - Journal of knot theory and its ramifications, 2023 **Abstract:** This paper presents a formula for the determinant of the twisted generalized hybrid weaving knot $Q\hat{}3(m1,-m2,n,\ell)$ which is a closed 3-braid. As a corollary, we prove Conjecture 2 given in Singh and Chbili
18.	DFT study of bimetallic perovskite catalysts for steam reforming of bio-oil model oxygenates A Goyal, PP Singh, T Mondal - International Chemical Engineering Conference: Part of the AIJR Abstracts: Book of Abstracts Series, 2022 **Abstract:** Metal oxides have exhibited remarkable catalytic performance towards bio-oil steam reforming (SR) processes. Moreover, perovskite oxide (ABO_3) catalysts are promising owing to its combined impact of oxygen vacancies generated at A position (Lanthanide materials) and

	strong catalytic activity at B position (transition metals) correspondingly. In the present study, adsorption energies and their modes had been investigated to understand the catalytic trend for the SR reaction on the surface of three variant perovskite catalysts ($LaNiO_3$ (001), $LaNi_{0.8}Co_{0.2}O_3$ (001), and $LaNi_{0.8}Fe_{0.2}O_3$ (001)) using density functional theory (DFT). Furthermore, adsorption of primary bio-oil model oxygenates, steam, and key intermediates were studied on periodic slabs of perovskite catalysts. The synergistic effect of the bimetallic catalyst leads to variation in adsorption energies and enables an understanding of the relatively better catalytic behavior. The findings indicate that energies are sensitive to molecular orientation as well as surface interaction. Additionally, aromatic compounds like phenol, furfural, and benzaldehyde have more stable adsorption as compared to other molecules. On the other hand, CH was found as the major precursor for carbon deposition on the surface of perovskite catalysts because of its highest binding energy with catalyst surface. $LaNi_{0.8}Fe_{0.2}O_3$ (001) has shown the highest adsorption energy and shorter bond length of bio-oil model compounds and steam, while $LaNi_{0.8}Co_{0.2}O_3$ (001) possesses optimum energy and bond length values for all the investigated molecules. The binding energy for bio-oil model oxygenates and steam reduces in the following order: $LaNi_{0.8}Fe_{0.2}O_3$ (001) > $LaNi_{0.8}Co_{0.2}O_3$(001) > $LaNiO_3$ (001). Therefore, this study confirms that the cobalt doped $LaNiO_3$ (001) catalyst is the most efficient among the three distinct perovskites investigated for its optimal values of molecular binding.
19.	Distributed connected dominating sets in unit square and disk graphs B Gorain, K Mondal, S Pandit - International conference on theory and applications of models of computation: Part of the lecture notes in computer science book series, 2023 **Abstract:** The Minimum Dominating Set (MDS) and Minimum Connected Dominating set (MCDS) problems are well-studied problems in the distributed computing communities due to their numerous applications across the field. We study these problems in axis-parallel unit square and unit disk graphs. We exploit the underlying geometric structures of these graph classes and present constant round distributed algorithms in the $\mathcal{LOCAL}$ communication model. Our results are distributed constant factor approximation algorithms for the MCDS problem in unit square graphs that run in 18 rounds and in unit disk graphs that run in 44 rounds. The message complexity is linear for both the algorithms.
20.	Distributed dominating sets in interval graphs B Gorain, K Mondal, S Pandit - International computing and combinatorics conference: Part of the lecture notes in computer science book series, 2023 **Abstract:** The Minimum Dominating Set (MMDS) and Minimum Connected Dominating set (MMCDS) problems are well-studied in the distributed communities due to their numerous applications across the field. These problems are also crucial in wireless ad hoc networks, mainly for the particular type of geometric graphs. We study these problems in geometric graphs such as interval and unit interval graphs. We exploit the underlying geometric structures of these graph classes and present either constant factors distributed algorithms in constant rounds or algorithms with matching lower bounds in the $\mathcal{LOCAL}$ communication model.
21.	Drug repurposing: a new hope in drug discovery for prostate cancer JA Malik, S Ahmed, SS Momin, S Shaikh, A Alafnan… - ACS Omega, 2023 **Abstract:** Prostate cancer (PCA), the most common cancer in men, accounted for 1.3 million new incidences in 2018. An increase in incidences is an issue of concern that should be addressed. Of all the reported prostate cancers, 85% were detected in stages III and IV, making them difficult to treat. Conventional drugs gradually lose their efficacy due to the developed resistance against them, thus requiring newer therapeutic agents to be used as monotherapy or combination. Recent research regarding treatment options has attained remarkable speed and development. Therefore, in this context, drug repurposing comes into the picture, which is

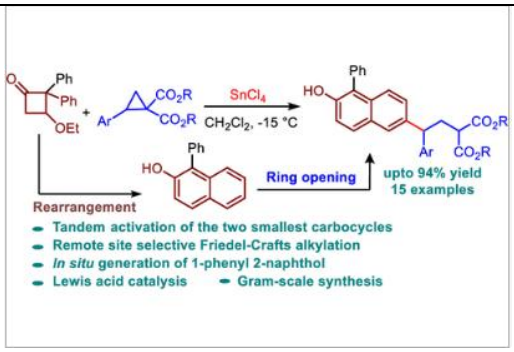
	defined as the "investigation of the off-patent, approved and marketed drugs for a novel therapeutic indication" which saves at least 30% of the time and cost, reducing the cost of treatment for patients, which usually runs high in cancer patients. The anticancer property of cardiac glycosides in cancers was tested in the early 1980s. The trend then shifts toward treating prostate cancer by repurposing other cardiovascular drugs. The current review mainly emphasizes the advantageous antiprostate cancer profile of conventional CVS drugs like cardiac glycosides, RAAS inhibitors, statins, heparin, and beta-blockers with underlying mechanisms. 
22.	Effect of fiber anisotropy and interphase on the stress jumps across the fiber/matrix interface in fuzzy fiber composites D Kaushik, M Saikia, HS Bedi, PK Agnihotri - National Academy Science Letters, 2023 **Abstract:** Designing the interphase region in conventional fiber-reinforced plastics is an efficient strategy to enhance their interfacial and interlaminar properties. The influence of the interphase region on stress concentration surrounding the fiber is systematically studied using finite element (FE) simulations in fuzzy fiber-reinforced composites. Two-phase (fiber/matrix) and three-phase (fiber/interphase/matrix) numerical models are used in FE simulation for comparative analysis. While the matrix is taken as isotropic material, both isotropic and transversely isotropic fibers are considered in numerical simulations. Two types of interphase regions: (1) interphase having a constant modulus and (2) graded interphase with varying modulus across the thickness are studied. The predictions from FE simulations are validated with the analytical results obtained from the rule of mixtures approach. FE simulations show that the presence of interphase increases the stiffness of the representative volume element (RVE) and reduces the stress concentration around the fiber. Moreover, the graded interphase is more effective in reducing the stress jump at the fiber/matrix interface in comparison with the interphase having a constant modulus.
23.	Energy-aware routing in SDN enabled data center network P Kamboj, S Pal - IEEE International Symposium on Network Computing and Applications (NCA), 2022 **Abstract:** Energy efficiency is considered a significant concern in the deployment and operation of data networks. The network devices need an enormous amount of energy to function, which leads to an increase in energy consumption in the data center networks (DCNs). Software-defined networking (SDN) solves the problem by adjusting the energy consumption proportionate to the amount of traffic. The network devices with low load can be turned into switch-OFF mode after transferring the traffic to another device. This energy-saving approach by analyzing the user's traffic demand increases the overall network utilization. In this work, we study the energy optimization problem using multipath routing in SDN-enabled data center networks (SD-DCN). We formulate the energy optimization as an integer linear program (ILP) problem to minimize the active Open vSwitch (OVS) switches in the network. To solve the problem in polynomial time, we propose a heuristic approach to route the traffic flows in the SD-

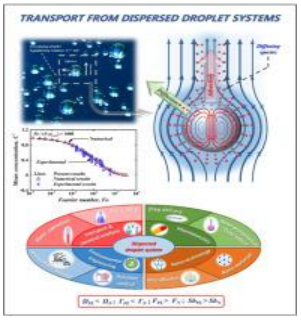
	DCN. The proposed approach is tested over data center network topologies – Fat-Tree and BCube. The simulation results show that our proposed approach presents an enhancement of 24%, 16%, and 15% in average delay, throughput, and energy savings in the Fat-Tree topology compared to the benchmark schemes. Further, our proposed approach achieves 17%, 19%, and 17% enhancement in average delay, throughput, and energy savings in the BCube topology compared to the benchmark schemes.
24.	Energy Efficient Wireless Communication Utilizing Reinforcement Based Learning S Chakravarty, M Banerjee, S Agarwal - IEEE 19th International Conference on Smart Communities: Improving Quality of Life Using ICT, IoT and AI, 2022 **Abstract:** IoT devices and battery technology have come to the forefront of a society that acknowledges the need for better, cleaner power management and generation. As these technologies improve, better and more efficient means of wireless communication can extend the longevity of battery power devices and networks. The use of reinforcement learning can spur an even greater improvement in these protocols than traditional means. Experiments show the efficacy of the approach as well as the efficiency achieved using the RL process.
25.	Experimental investigation of cycle-to-cycle variations in homogeneous charge compression ignition engine fuelled with methanol using wavelets RK Yadav, MR Saxena, RK Maurya – SAE Technical Paper, 2023 **Abstract:** The development of automotive engines continues to be determined by gradually more stringent emissions norm including CO2 emissions and fuel consumption. To fulfil the simultaneous emission requirements for near zero pollutant and low CO2 levels, several research studies are currently being carried out world over on new engine combustion process, such as Homogeneous Charge Compression Ignition (HCCI). In HCCI engines, combustion rates and ignition timing are dominated by physical and chemical properties of fuel/air/residual gas mixtures, boundary conditions including ambient temperature, pressure, and humidity and engine operating conditions such as load, speed etc. Higher cycle-to-cycle variations are observed in HCCI combustion engines due to large variability of these factors. The cyclic variations in HCCI engine are investigated on a modified four-stroke, four-cylinder engine. The HCCI combustion mode is tested with gasoline, ethanol and methanol fuels. This study presents the cyclic combustion analysis of HCCI engine using statistical and Wavelet Transform techniques. The cyclic variations are characterized under different operating conditions such as relative air-fuel ratios (λ), intake air temperatures (T_i) and engine speeds (N). Results indicate that combustion instability is more prone to lean charge operation, and the variations are significantly higher for higher λ and lower T_i. The wavelet analysis indicates that cyclic variations in IMEP, CA10 and CA50 occurs at different frequencies. The peak power in global Wavelet spectrum shifted from low frequency to high frequency period as engine mode shifted toward leaner operation.
26.	Experimental investigation on combustion characteristics of novel preheated air swirl burner operating on the heavy oil fired furnace for reducing NOx emission P Singh, H Singh, AK Singh - Energy Sources, Part A: Recovery, Utilization, and Environmental Effects, 2023 **Abstract:** This paper presents an experimental study carried out to evaluate the influence of air swirl vane angles on pollutants in a heavy oil fuel fired furnace with a recuperator. A novel burner system with a range of concentric air swirl generators (vane angles of 15°, 20°, 30°, 45°, 60°, and 90°) was ultimately incorporated to the combustion chamber of a 250 kg crucible furnace. This study examined the thermal efficiency and the polluting emission parameters of CO_2, HC, CO, and NOx. According to the results, preheated air-fuel and air swirl generators with vane angles of 45° and 30° emit the least HC and CO, whereas air swirl vane angles of 90° emit the most. A preheated primary air swirl vane angle of 45° results in the lowest NOx emission (25 ppm) value. Furthermore, with larger air swirl vane angles of 45° results in increased

	temperature and premixed combustion, as well as a raise in NOx emission. To ensure accurate airflow for complete combustion, secondary air entry area kept twice the primary air entry area in the novel burner. The results showed that when the temperature of the preheated primary and secondary air and heavy oil fuel combination increased, so did the mean effective temperature of the combustion gases. Conversely, when the vane angle is reduced and no preheated air-fuel combination is present, the mean temperature of the combustion gas drops dramatically.
27.	Facile fabrication of NiFeB deposited flexible carbon cloth electrode towards overall water splitting in alkaline and saline solutions A Kafle, D Gupta, TC Nagaiah - Electrochimica Acta, 2023 **Abstract:** Water electrolysis has boomed as a sustainable tool for greener production of hydrogen, nonetheless the expensive technology is dragging its flourishment. Although it is being addressed by the development of cost effective and efficient electrocatalyst for the electrolytic cell, the use of pure water feed stock and lack of reactor friendly electrode is still challenging. Meanwhile the development of the reactor friendly corrosion resistive flexible electrode capable of sea water splitting can further reduce the overall production cost. Herein, we have demonstrated a straightforward and activation-free electroless deposition approach to fabricate the reactor friendly self-standing flexible electrode. The NiFeB deposited carbon cloth electrode was obtained by the sonication assisted metal ion adsorption and reduction dip and coat method without the use of expensive activators or sensitizers. The as fabricated NiFeB@OCC exhibit a promising oxygen evolution reaction (OER) and hydrogen evolution reaction (HER) by achieving 20 mA cm^{-2} at an overpotential of 255 mV and 241 mV respectively with high durability (24 h). Moreover, the electrode retains the activity under various deformation conditions as well as in alkaline saline electrolyte. Additionally, it exhibits appreciable activity towards overall water splitting as it requires 1.69 V for 10 mA cm^{-2} current density. Consequently, its encouraging activity and high stability even in harsh condition could carry forward the great potential for practical saline water splitting.
28.	Fatigue response of glass-filled epoxy composites: A crack initiation and propagation study A Arora, A Sharma, M Singh, DK Mahajan, V Kushvaha - International Journal of Fatigue, 2023 **Abstract:** This paper presents a comprehensive experimental investigation on the fatigue response of glass-filled epoxy composites when subjected to cyclic loading. Rod-shaped particulate glass fibers in a volume fraction of 0%, 5%, 10% and 15% are reinforced in the epoxy matrix. The mechanical behavior of the resulting composite is studied under monotonic tensile loading and tension–tension cyclic fatigue loading. The undergoing damage mechanisms leading to the crack initiation and its propagation are studied using the in-situ low cycle fatigue testing. The crack initiation behavior and the crack initiation life are found to be affected by different crack initiation sites such as the epoxy-fiber interface, the matrix and the fiber itself. Fractography reveals that the crack coalescence, crack propagation and the failure are largely affected by the varying volume fraction of glass fibers. The specimen with 10% volume fraction is found to exhibit the maximum fatigue life under the applied cyclic loading.
29.	Generic multispectral demosaicking using spectral correlation between spectral bands and pseudo-panchromatic image V Rathi, P Goyal - Signal Processing: Image Communication, 2023 **Abstract:** Single imaging sensor-based multispectral imaging systems (MSISs) facilitate snapshot imaging with a multispectral filter array (MSFA). These single sensor-based MSISs need an effective image demosaicking method to generate the full-multispectral image from the mosaicked image captured by an imaging sensor with MSFA help. This paper proposes an effective and generic multispectral image demosaicking (MSID) method based on the concept of the pseudo-panchromatic (PPAN) image. The proposed MSID method accepts the mosaicked image capture with the help of preferred binary tree-based MSFA patterns. We estimate the

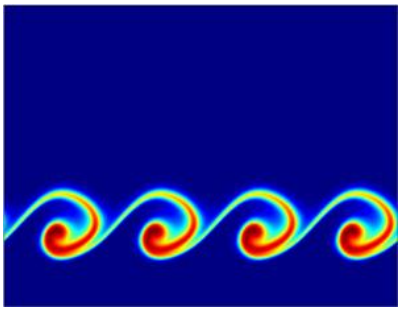
	PPAN image from the mosaicked image by utilizing the spatial filters developed carefully based on the spectral band's relative placement in the binary tree-based MSFA pattern. Our proposed MSID method utilizes the spectral correlation between the PPAN image and the mosaicked image to generate the multispectral image. The proposed generic MSID method surpasses the existing generic MSID methods in different image quality parameters on the multispectral images from two benchmark multispectral datasets.
30.	Hoop compression driven instabilities in spontaneously formed multilayer graphene blisters over a polymeric substrate M Pandey, R Ahuja, R Kumar - Nanotechnology, 2022 **Abstract:** The blistering of elastic membranes is prone to elastic-solid as well as substrate-based mechanical instabilities. The solid-based instabilities have been well-explored in the mechanically indented blisters of elastic membranes over the rigid/ solid substrates, but an integrated study illustrating the underlying mechanism for the onset of solid as well as substrate-based instabilities in the spontaneous blistering of a 2D material is still lacking in the literature. In this article, an extensive experimental as well as analytical analysis of the spontaneous blister-formation in the multilayer graphene (MLG) flakes over a polymeric substrate is reported, which elucidates the involved mechanism and the governing parameters behind the development of elastic-solid as well as viscoelastic-substrate based instabilities. Herein, a 'blister-collapse model' is proposed, which infers that the suppression of the hoop compression, resulting from the phase-transition of the confined matter, plays a crucial role in the development of the instabilities. The ratio of blister-height to flake-thickness is a direct consequence of the taper-angle of the MLG blisters and the thickness-dependent elasticity of the upper-bounding MLG flakes, which shows a significant impact on the growth-dynamics of the viscous fingering patterns (viscoelastic-substrate based instabilities) under the MLG blisters.
31.	Hypoxia-induced miR-210-3p expression in lung adenocarcinoma potentiates tumor development by regulating CCL2-mediated monocyte infiltration L Arora, D Patra, S Roy, S Nanda, N Singh, AK Verma…D Pal – Molecular Oncology, 2022 **Abstract:** In most cancers, tumor hypoxia downregulates the expression of C-C motif chemokine 2 (*CCL2*), and this downregulation has been implicated in monocyte infiltration and tumor progression; however, the molecular mechanism is yet not clear. We compared non-cancerous and lung-adenocarcinoma human samples for hypoxia-inducible factor 1-alpha (HIF-1A), *microRNA-210-3p* (*mir-210-3p)* and CCL2 levels. Mechanistic studies were performed on lung adenocarcinoma cell lines and 3D tumor spheroids to understand the role of hypoxia-induced miR-210-3p in the regulation of *CCL2* expression and macrophage polarization. HIF-1 A stabilization increases miR-210-3p levels in lung adenocarcinoma and impairs monocyte infiltration by inhibiting *CCL2* expression. Mechanistically, miR-210-3p directly binds to the 3'untranslated region (UTR) of *CCL2* mRNA and silences it. Suppressing miR-210-3p substantially downregulates the effect of hypoxia on *CCL2* expression. Monocyte migration is significantly hampered in miR-210-3p mimic-transfected *HIF-1A* silenced cancer cells. In contrast, inhibition of miR-210-3p in *HIF-1A*-overexpressed cells markedly restored monocyte migration, highlighting a direct link between miR-210-3p level and tumor monocyte burden. Moreover, miR-210-3p inhibition in 3D tumor spheroids promotes monocyte recruitment and skewing towards an anti-tumor M1 phenotype. Anti-hsa-miR-210-3p-locked nucleic acid (LNA) delivery in a lung tumor xenograft zebrafish model caused tumor regression, suggesting that miR-210-3p could be a promising target for immunomodulatory therapeutic strategies against lung adenocarcinoma.
32.	Laser transmission welding of polycarbonate sheets using electrolytic iron powder absorber DK Goyal, R Yadav, R Kant - Optics and Laser Technology, 2023 **Abstract:** This paper presents Laser Transmission Welding (LTW) of polycarbonate sheets

	using electrolytic iron powder as an absorber to obtain a clean and high-strength joint without any gap between the sheets. Surface temperature is measured to analyze the bubble morphology and relate them with the heat absorbed at the interface. The lap shear test is performed to evaluate the weld strength, and fracture modes of the welded joints. The results show that maximum weld strength is achieved with smaller bubbles. Scanning electron microscope (SEM) micrograph of the fractured surface shows micro-fibrils at the inter-bubble space, enhancing the weld strength. The iron particles present inside the bubble increase the size of the bubbles, and the presence of cleavage facets reveals the brittle failure of the joint. The weld joints are fractured mainly by interfacial and substrate fractures. The optimum process parameters are obtained using a genetic algorithm (GA), and the confirmation test shows an improvement of 36.32 % in weld strength compared with Taguchi parameters.
33.	Limit cycle oscillation dynamics in a MLDI combustor Y Nanda, A Saurabh, L Kabiraj, RV Gomez, E Gutmark - AIAA SCITECH Forum, 2023 **Abstract:** Thermoacoustic oscillations in a high-pressure Multi-Nozzle Lean Direct Injection combustor with fuel staging have been examined. The combustor consists of three independently controlled fuel stages, i.e., the pilot, intermediate and outer fuel stages. Limit cycle oscillations have been identified for two cases with different fuel supply to the three stages of the combustor, operating at different equivalence ratios. The oscillation dynamics of the two cases has been characterized and quantified by employing non-linear time series analysis tools. Phase portraits, recurrence plots and recurrence quantification methods were used by phase space reconstruction of the scalar pressure measurements. Further comparisons between the two cases were made by correlating the time resolved OH* Chemiluminescence images to the pressure oscillations. Phase averaging and spectral proper orthogonal decomposition were used for understanding the flame dynamics between the three fuel stages.
34.	Mechanism of bonding during laser transmission welding using EIP absorber DK Goyal, R Kant - Materials and Manufacturing Processes, 2023 **Abstract:** This paper aims to investigate the bonding mechanism during laser transmission welding of polycarbonate sheets using an electrolytic iron powder (EIP) absorber. The experiments are performed at different scan speeds and laser powers. The mechanical strength is determined by the lap shear test. The influence of line energy, interface temperature, and absorptivity on weld strength is discussed. The weld characteristics, bond morphology, and elemental distribution at the cross-section and fracture interface of the welded samples are analyzed. The results show that the maximum breaking strength of 1180 N is obtained at the 400 mm/min scan speed and 100 W laser power. The iron particles are observed mechanically interlocked at the lowest line energy with partial chemical bonding. However, the chain diffusion and chemical bonding have been increased with line energy. Thermal degradation and burning of the polycarbonate at the interface restrict the bonding and reduces the weld strength.
35.	Merging two strained carbocycles: lewis acid catalyzed remote site-selective friedel–crafts alkylation of in situ generated β-naphthol A Hazra, T Kanji, P Banerjee - The Journal of Organic Chemistry, 2022 **Abstract:** Lewis acid catalyzed tandem activation of the two smallest carbocycles, 3-ethoxy cyclobutanones, and donor–acceptor cyclopropanes has been demonstrated. The diphenyl-substituted 3-ethoxy cyclobutanone rearranges itself by intramolecular cyclization for the *in situ* generation of 1-phenyl 2-naphthol, which further undergoes remote site-selective Friedel–Crafts alkylation with donor–acceptor cyclopropane to synthesize a series of γ-naphthyl butyric acid derivatives. Further control experiments for mechanistic investigations and synthetic applications have also been carried out.

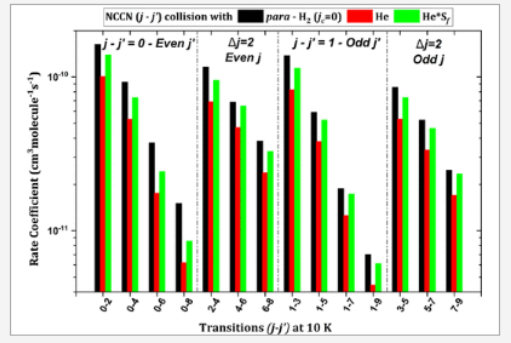
	
36.	Microwave ablation trocar for ablating cancerous tumors: a numerical analysis V Satish, R Repaka - Medical & biological engineering & computing, 2023 **Abstract:** Microwave ablation (MWA) is a newly developing minimally invasive thermal therapies technology. The ablation region obtained during MWA mainly depends on the type and efficiency of the trocar as well as the energy transfer from the generator to the biological tissue. In the present article, a novel trocar for MWA therapies has been proposed. A 3-dimensional tumor-embedded hepatic gland ablated with the novel MWA trocar has been numerically analyzed using finite element method–based software. The novel trocar consists of a flexible dual tine supplied with a microwave power of 15 W at 2.45/6 GHz for an ablation time of 10 min for all the cases. Various combinations of supplied energy and deploying lengths result in tumor ablations ranging from 2.7 to 4 cm in diameter. Supplying energy at high frequency (6 GHz) to the trocar results in ablating tumors (> 4 cm) with spherical ablation region. The novel trocar generated large ablation regions which are 2–3 times bigger than the tumors obtained using existing single-slot non-cooled trocars. This research on novel trocar may help clinicians in treating large size tumors of symmetric and asymmetric shapes by overcoming the problem associated with precise position of trocar into the tissue.
37.	Mitigation of wave impact on sea wall by a floating elastic plate and a porous structure G Sahoo, S Singla, SC Martha - Journal of offshore mechanics and arctic engineering, 2023 **Abstract:** The purpose of the present study is to reduce the high wave load on a sea wall by utilizing an elastic plate (EP) kept at fixed distance from a porous structure (PS). Thin plate theory is used to model the flow past EP, while Sollit and Cross theory is used to model the flow past PS. A linear potential theory-based analytical solution to the current problem is developed using the eigenfunction expansion technique. To understand the effect of PS and EP in creating tranquility zone and minimum wave loads on the rigid wall, horizontal wave force on the wall, reflection coefficient, dissipation coefficient and free surface elevation are computed and analyzed for different values of width and friction factor of PS, flexural rigidity and length of EP, angle of incidence, and distance between PS and EP, and the distance between EP and rigid wall. The study demonstrates that both structures considerably reduce the stress on the rigid wall and the wave reflection. It is found that the force on the wall shifted to the left as the width and frictional factor of PS increased. It is observed that PS effectively minimises the free surface elevation in the region between EP and the wall. It is also found that an effective tranquility zone may be produced, which will put less wave force on the rigid wall, with sufficient spacing between PS and EP, and EP and wall. The given model is expected to assist in preserving various coastal assets significantly.
38.	On enhancing interfacial mass transport through microextraction in dispersed droplet systems M Trivedi, A Sharma, K Agarwal, RP Chhabra, N Nirmalkar - International Journal of Heat and Mass Transfer, 2023 **Abstract:** The physio-chemical hydrodynamics and the solute transport around a translating

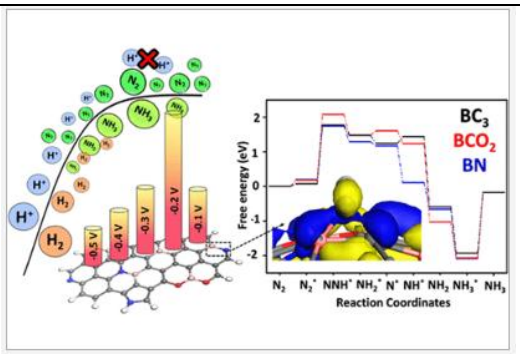
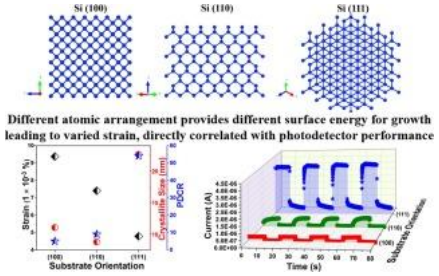
	dispersed drop are often multicomponent and multiphase systems. When such a dispersed droplet system is out of the thermodynamic equilibrium, steep momentum and concentration gradients are developed around the interface leading to rapid flow and solute transport. In broader perspectives, the dispersed droplet system has direct/indirect relevance to addressing the technological challenges in the 21^{st} century, namely, energy storage, hydrogen production, CO_2 capture, biofuel production, chemical analysis, diagnosis extraction, and drug delivery. Environmental engineering challenges include flotation and separation technology, inkjet printing, coatings, and paints. The most challenging issue in such applications is enhancing the transport rate from the droplet to the bulk of the fluid. In this work, we have proposed a novel method to foster the transport of solute from the drop to the bulk fluid by altering the viscosity of the bulk fluid. We have exploited the shear-thinning behavior of the fluid in bulk to reduce the viscous losses and resistances to the mass transfer. A linear thermodynamic equilibrium relation at the fluid-fluid interface is considered. The scant prior experimental results were observed to agree with the present findings. Therefore, the extensive numerical findings are presented for the ranges of pertinent parameters such as Reynolds number, ($1 \le R_e \le 75$) Peclet number, ($10 \le P_e \le 103$), internal to external fluid diffusivity ratio, ($0.5 \le d_{ratio} \le 4$), dispersed to continuous fluid viscosity ratio, ($0.25 \le u_{ratio} \le 4$) and power-law index, ($0.4 \le n \le 1$). The drag coefficient exhibits an increase of 180% with the increase in the u_{ratio} as well as with the n at the maximum convective regime. The Sherwood number exhibits a positive dependence on the Reynolds number, Peclet number, and the diffusivity ratio. On the contrary, the viscosity ratio lowers the transport of species from the droplet to the fluid due to the reduced internal circulations inside the droplet. Shear-thinning fluid behavior offers a higher extraction efficiency than the Newtonian fluid (upto 30% increase in at low Pe). Finally, simple predictive correlative equations have been proposed for the drag coefficient and the average Sherwood number over the conditions considered here. **Graphical Abstract:** 
39.	One-dimensional consolidation test with pore pressure measurements — An accelerated procedure R Moozhikkal, RG Robinson - Geotechnical Testing Journal, 2023 **Abstract:** Consolidation properties of cohesive soils are often determined using the controlled-strain loading (CSL) consolidation test. It was well recognized in the literature that the consolidation properties, such as compression index (C_c), coefficient of consolidation (c_v), and preconsolidation pressure (σ_c'), depend on the axial strain rate adopted for conducting the CSL test. Fixing the appropriate axial strain rate is often a challenge in CSL tests. The conventional incremental load (IL) consolidation test suffers from the limitation that it takes long time to complete the test. In the present study, an accelerated IL consolidation testing procedure with pore water pressure measurements is developed in an attempt to overcome the limitations of the CSL and conventional IL consolidation tests. The duration of the IL is controlled such that the subsequent IL is applied once the excess pore pressure dissipates to 15 % of the total applied stress (pore pressure ratio, R_u, is 0.15). The testing procedure is validated by performing a series

	of experiments on six reconstituted and four intact soil samples. The consolidation parameters obtained from the proposed method compares very well with conventional IL test as well as with the CSL consolidation test, suggesting its validity. The proposed method is about 3 times faster when compared with the standard CSL test. Therefore, the proposed method is a viable alternative to the CSL consolidation test.
40.	Online shopping fake reviews detection using machine learning A Moqueem, F Moqueem, CV Reddy, D Jayanth… - International conference on cognition and recognition: Part of the communications in computer and information science book series, 2023 **Abstract:** Online shopping has drastically reduced the tiresome job of reaching out to offline stores and selecting goods in a limited product range. Almost everything is available online, right from the basic essential goods to costlier electrical appliances in today's world. The sellers increasingly misuse these massive online platforms for increasing their product sales by posting false reviews. Consumer engagement reports suggest that around 82% of customers read online reviews before purchasing a product online. So these reviews are crucial for them to decide if the product suits them and is reliable. So, in this paper, we propose various machine learning models for detecting fake reviews and delineate and do a comparative analysis of each model to determine the best algorithm. This work plays a vital role in reducing and checking fake reviews.
41.	Optimization of slew mitigation capacitor in passive charge compensation based delta-sigma modulator MA Saeed, M Kumar, B Umapathi, DM Das - IEEE Transactions on Circuits and Systems II: Express Briefs, 2023 **Abstract:** In this paper we propose a scheme of optimizing the size of charge compensation (CC) capacitor in a delta-sigma modulator (DSM) using a passive charge compensation (PCC) based switched capacitor integrator (SCI). The slewing behavior of a PCC based SCI is analyzed in both integration phase (IP) and sampling phase (SP) to optimize the size of CC capacitor. The effectiveness of the proposed scheme is demonstrated by implementing a 2-1 cascaded DSM using PCC based SCI with optimized value of CC capacitor in 0.18-µm CMOS technology. The DSM operates at a frequency of 5-MHz and achieves a peak SNDR of 103.1-dB in the audio bandwidth of 20-kHz. The power consumption of DSM is 220-µW at a supply voltage of 0.85-V and it consumes 1.3 mm of area. Post-layout simulations show an improvement of 10.8-dB in the SNDR of DSM by using the optimized value of CC capacitor in PCC based SCI.
42.	Oscillating rheological behavior of Turbatrix aceti nematodes N Ali, S Nand, A Kiran, M Mishra, V Mehandia - Physics of Fluids, 2023 **Abstract:** We present an experimental investigation of the rheological aspects of collective motion by the swimming *Turbatrix aceti* nematodes. We discover that these nematodes can significantly change the rheological properties of the suspension due to their body oscillations and form synchronized waves, which produce strong fluid flows. The strength of the collective state changes the shape of the interface where they swim in synchronization. We unravel that the effective viscosity of the nematode suspension at higher shear rates shows steady viscous behavior with time, where no significant effect of nematode activity is observed. For the first time, we have reported that at low shear rates, the activity effect is significant enough to generate oscillating viscous effects. In addition, we also measured the influence of the nematode concentration on suspension viscosity. This work opens a new way for understanding the rheological aspects of active matter under low and high shear rates. We illustrate these dynamics by showing that the force generated by these nematodes is sufficient to change the suspension rheology. The various aspects of nematodes, especially their large size and ease of culturing, make them a good model organism for experimental investigation as active fibers with oscillations. The oscillating behavior regulates the interfacial phenomenon and produces oscillatory rheological dynamics at low shear rates. The results of our work can be utilized to

	further study the novel metamaterials with negative viscosity, which have applications in healthcare and energy systems.
43.	Reaction-induced Kelvin–Helmholtz instability in a layered channel flow SN Maharana, KC Sahu, M Mishra - Journal of Fluid Mechanics, 2023 **Abstract:** We show that a vertical viscosity stratification at a localized region caused by a chemical reaction yields an inconspicuous shear layer. A chemo-hydrodynamic Kelvin–Helmholtz instability or cat-eye-shaped morphology develops at one reaction front, while the other front diffuses steadily over time. Through linear stability and nonlinear simulations, the existence of such instabilities is established if the log-mobility ratio exceeds a critical value. We find unique scalings between the stable and unstable zones that demonstrate how the influence of variations in solute diffusion on instability can be eliminated. The observed unstable patterns agree with existing experimental results. 
44.	Recent escalations in MXenes: from fundamental to applications J Jyoti, BP Singh, M Sandhu, SK Tripathi – Nanomaterials: Book Chapter, 2023 **Abstract:** Enormous efforts have been devoted towards the development of various advanced materials with long cycle life, high power density and high energy density for energy storage and conversion applications. From the discovery of MXene, the family of two-dimensional (2D) transition metal nitrides, carbides and carbonitrides has attained significant research focus due to their outstanding properties. MXene has drawn significant attention because they have tunable layered structures, controllable interfacial chemistry, high mechanical strength, excellent electronic conductivity, superior specific surface area, magnetic properties, hydrophilic features, multiple possible surface terminations and the ability to accommodate intercalates. In this chapter, we reported the synthesis techniques and properties of MXene and MXene-based hybrid materials and their potential applications. The MXene has been synthesized by various routes such as chemical vapor deposition (CVD), sputtering, pulse laser plasma deposition and etching techniques. Generally, etching technique has been used for the synthesis of MXene. Different etchants have been used for the synthesis of MXene such as hydrofluoric acid, lithium fluoride, hydrochloric acid, ammonium hydrazine, etc. After etching, the surface termination groups such as –F, –OH and–O presents on the MXene influence their properties. The surface termination groups on 2D MXene have been significantly used in various applications such as rechargeable batteries, supercapacitors, electromagnetic interference shielding, sensors and so on. In summary, a widespread overview of the synthesis of MXene with the current challenges and encouraging technologies for the preparation of large scale MXene and its usefulness in several applications are provided.
45.	Resonant column and cyclic torsional shear tests on Sutlej river sand subjected to the seismicity of Himalayan and Shivalik hill ranges: A case study S Rohilla, R Sebastian - Soil Dynamics and Earthquake Engineering, 2023 **Abstract:** The study of site-specific dynamic properties of soil holds vital importance in many

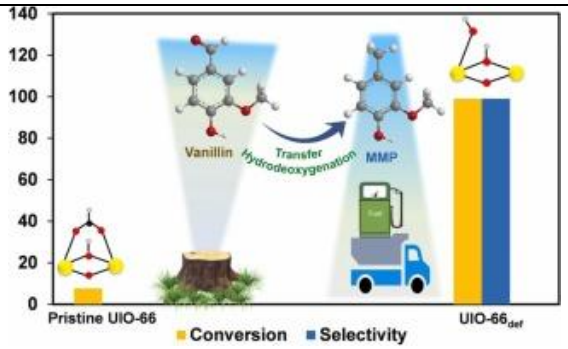
	geotechnical engineering problems for the region holding high active seismicity. The Sutlej River basin, a valley and high-risk seismic zone in the north-eastern part of the Punjab state, has been considered for the study. The site-specific shear modulus reduction curves and material damping ratio curves for a range of shear strain amplitudes have been developed under varying experimental conditions of confining pressure, relative density, and loading frequency using the resonant column (RC) tests and cyclic torsional shear (CTS) tests. The study addresses the usage of two testing approaches, i.e., resonant column test (RC) and cyclic torsional shear test (CTS), for the estimation of shear modulus and damping ratio values at varying shear strain amplitudes. The regression analysis has been performed for the two testing techniques viz. RC and CTS to study the sensitivity of shear modulus values and material damping ratio values towards varying experimental conditions. The shear modulus and damping ratio values determined from cyclic torsional shear tests were observed to have great dependency on the frequency of loading. The knowledge of site-specific dynamic properties will support practical interpretation for the geotechnical engineering problems in the region.
46.	Risk factors for developing pressure ulcers in neonates and novel ideas for developing neonatal antipressure ulcers solutions AN Mallick, M Bhandari, B Basumatary, S Gupta, K Arora, AK Sahani - Journal of Clinical Neonatology, 2023 **Abstract:** Pressure Ulcers (PU) are highly prevalent iatrogenic occurrences among hospitalized adults and neonatal patients. These decubitus ulcers are progressive in nature and are mostly seen in patients that are immobile for prolonged periods, either by virtue of being bedridden or chair bound. The continual pressure on the skin surfaces disrupts blood supply from the subcutaneous regions and leads to the development of PUs. Several treatment and prevention protocols have been defined for adult patients. However, there is a dearth of literature available for critically ill pediatrics or neonates and often adult practices are used to treat pressure injuries in them. There is a significant physiological and anatomical difference between the skin of newborns and adults or even older children. The dermal layer of a preterm neonate is <60% of the thickness of an adult and has a much higher susceptibility for developing pressure ulcers. The immune system of premature infants lacks an efficient antigenic specificity, diversity or immunologic memory, making them prone to lethal infections. The study was performed using search engines like PubMed, EMBASE and Google Scholar, with the focus of the search strategy being the breadth rather than the details of the study. Selected keywords were used alone or in combination with each other to retrieve relevant articles. This review focuses on the risk of developing PUs in neonates, explains the currently available solutions of PU prevention in adults, emphasizes the need for neonatal specific solutions and presents novel ideas for developing antisore bed for neonates.
47.	Role of site-wise dynamic defects in a resource-constrained exclusion process N Bhatia, AK Gupta - Chaos, Solitons & Fractals, 2023 **Abstract:** We study an exclusion process with site-wise dynamic disorder in a resource constrained environment. The dynamic defects that hinder the particle flux on the lattice stochastically appear and disappear throughout the lattice with a constrained binding rate and a constant unbinding rate, respectively. The effect of constrained resources on the stationary properties of the system has been comprehended in the form of the filling factor. The analytical results replicated by naive mean-field theory accord quite well with the Monte Carlo simulation for faster defects irrespective of the affected hopping rate and slower defects with a large affected hopping rate. For slower defects with a small affected hopping rate, some correlations are observed in the system, leading to the adoption of an enhanced mean-field approach which provides reasonably better approximations than the usual naive-mean field. These correlations slowly fade away with an increase in the affected hopping rate. Our theoretical calculations unify the parameters – the affected hopping rate, defect binding (unbinding) rate, and defect density –

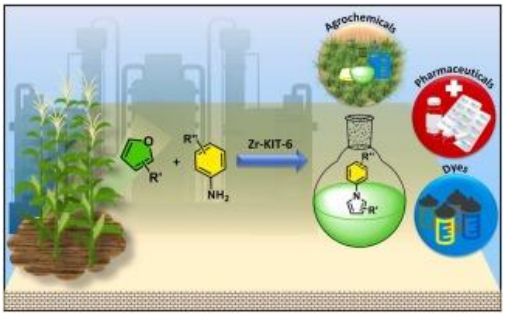
	that control defect kinetics on the lattice into a single parameter known as the obstruction factor. The repercussions of the obstruction factor have been thoroughly examined by discussing its limiting cases. The phase boundaries that are yielded through different mean-field approaches are uniquely impacted by their corresponding obstruction factor.
48.	Rotational excitation of NCCN by p-H_2(j_c = 0) at low temperatures A Kushwaha, Ritika, P Chahal, TJD Kumar - ACS Earth and Space Chemistry, 2023 **Abstract:** NCCN is a potential candidate for detection in interstellar space, but to model its emission spectra, accurate collisional rates are required. Here, we present a first truncated *ab initio* four-dimensional potential energy surface of NCCN–H_2, generated using explicitly correlated coupled-cluster singles and doubles with the perturbative triple excitations [CCSD(T)-F12b] method and aug-cc-pVTZ basis set. The surface allows NCCN to rotate in the *x*–*z* plane, and H_2 is restricted to three orientations [(a) parallel to the *z* axis, (b) perpendicular to the *z* axis but still in the *x*–*z* plane, and (c) perpendicular to the *z* axis and also perpendicular to the *x*–*z* plane] and averaged to obtain a reduced two-dimensional (2D) surface. To augment data points, the surface is fitted into a neural networks model. Multipole expansion coefficients for this reduced 2D surface of NCCN–H_2 have been calculated and utilized in determining collisional cross sections using the close-coupling method for collision energies until 1500 cm^{-1}. Finally, the rate coefficients for reduced NCCN–H_2 have been computed. These rate coefficients closely approximate the collision of NCCN with *p*-H_2(j_c = 0), and they are greater by 1.8–2.8 times than the rates of NCCN–He previously investigated. 
49.	Selective electrochemical conversion of N_2 to NH_3 in neutral media using B, N-containing carbon with a nanotubular morphology D Gupta, A Kafle, S Kaur, TS Thomas, D Mandal, TC Nagaiah - ACS Applied Materials & Interfaces, 2023 **Abstract:** Electrochemical dinitrogen reduction (NRR) has riveted substantial attention as a greener method to synthesize ammonia (NH_3) under ambient conditions. Here, B, N-containing carbon catalysts with a discrete morphology were synthesized from the metal–organic framework-ionic liquid (MOF-IL) composite for NRR in a neutral electrolyte medium (pH = 7). Morphology-dependent activity is witnessed, wherein C-BN@600 with a nanotubular morphology is able to achieve a high NH_3 yield rate of 204 μg h^{-1} mg_{cat}^{-1} and an F.E. of 16.7% with a TOF value of 0.2 h^{-1} at −0.2 V *vs* RHE. Further, a rigorous protocol is put forward for true NH_3 estimation by tracing/eliminating any source of contamination in catalysts, electrolytes, or gas supply *via* ultraviolet–visible (UV–vis) spectroscopy, gas-purification methods, and isotope labeling experiments. Density functional theory predicts BN to be the favorable active site for N_2 adsorption with a reduced energy barrier in the first reduction step and sequential stabilization of the B–N bond by an adjacent carbon atom.

	
50.	Strain effects on the optoelectronic performance of ultra-wide band gap polycrystalline β-Ga_2O_3 thin film grown on differently-oriented Silicon substrates for solar blind photodetector D Kaur, S Debata, DP Singh, M Kumar - Applied Surface Science, 2023 **Abstract:** β-Ga_2O_3 based photodetectors are being intensively researched as possible substitutes to conventional Silicon deep-UV PDs. However, high cost of single-crystalline Ga_2O_3 poses hindrance towards commercialization by semiconductor industry still monopolized by Si. An easier integration with existing technology can be achieved by growing Ga_2O_3 thin films on Si directly, but growth of lattice mismatched substrates is often tricky and complicated with various parameters such as interfacial energies, surface energies, etc. playing important roles. Thus, it becomes imperative to investigate the role of each of these on film growth and devices thereof. Herein, polycrystalline β-Ga_2O_3 thin films are grown on different orientations of Si namely (1 0 0), (1 1 0) and (1 1 1), offering varied surface energies for film growth even under identical conditions. Best growth is observed on Si (1 1 1) substrate, deduced by largest crystallite size and lowest strain using Williamson-Hall method. This leads to devices of Ga_2O_3 on Si (1 1 1) having improved performance compared to other orientations. To validate effect of strain on device performance, a well-known method of reducing strain further – introduction of seed layer – is utilized, leading to further enhancement. This implies that PD performance is highly dependent on orientation of substrate used as the strain induced ultimately affects film growth. **Graphical Abstract:** 
51.	Strong effect of fluid rheology on electrokinetic instability and subsequent mixing phenomena in a microfluidic T-junction F Hamid, C Sasmal - Physics of Fluids, 2023 **Abstract:** When two fluids of different electrical conductivities are transported under the influence of an electric field, the electrokinetic instability (EKI) phenomenon often triggers in a microfluidic device once the electric field strength and conductivity gradient exceed some critical values. This study presents a detailed numerical investigation of how the rheological behavior of a fluid obeyed by the non-Newtonian power-law constitutive relation could influence this EKI phenomenon in a microfluidic T-junction. We find that as the fluid rheological behavior changes from shear-thickening ($n>1$) to shear-thinning ($n<1$), the EKI phenomenon is significantly influenced under the same conditions. In particular, the intensity of this EKI

	phenomenon is found to be significantly higher in shear-thinning fluids than in Newtonian and shear-thickening fluids. Also, the critical value of the applied electric field strength for the inception of this EKI phenomenon gradually increases as the fluid rheological behavior progressively moves from shear-thinning to shear-thickening. The corresponding mixing phenomenon, often achieved using this EKI phenomenon, is also notably higher in shear-thinning fluids compared to Newtonian and shear-thickening fluids. A detailed analysis of both the flow dynamics and mixing phenomena inside the microdevice is presented and discussed in this study. To perform so, we also employ the data-driven dynamic mode decomposition technique, considered one of the widely used reduced-order models to analyze a dynamical system. This analysis facilitates a better understanding of the EKI-induced chaotic convection and mixing phenomena inside the microdevice. We observe that the spatial expanse and intensity of the coherent flow structures differ significantly as the power-law index changes, thereby providing valuable insight into certain aspects of the underlying flow dynamics that, otherwise, are not apparent from other analyses.
52.	Synthesis, drug-likeness evaluation of some heterocyclic moieties fused indole derivatives as potential antioxidants A Kumari, RK Singh - Combinatorial Chemistry & High Throughput Screening: Book Chapter, 2023 **Abstract:** Background: Indole and its derivatives have a wide range of pharmacological effects, including analgesic, antimicrobial, antidepressant, anti-diabetic, anti-convulsant, anti-helminthic, and anti-inflammatory properties. They are crucial structural components of many of today's powerful antioxidant medications. Objective: Using the Schotten–Baumann reaction, the indole ring was linked to other key heterocyclic moieties such as morpholine, imidazole, piperidine, and piperazine at the active 3rd position and then tested for antioxidant activity. Method: Synthesis of derivatives was accomplished under appropriate conditions and characterized by IR, NMR (1H and 13C), and mass spectrum. Using the Swiss ADME online application, ADME properties were also determined. In vitro antioxidant activity using DPPH method and Reducing power method was used. Results: In the DPPH assay, compounds 5a (IC50=1.01±0.22 µg/mL), 5k (IC50=1.21±0.07µg/mL), whereas compounds 5a (EC50=23±1.00 µg/mL), 5h (EC50=26±2.42 µg/mL) in the reducing power assay were most potent as compared with standard Ascorbic acid. Compounds 5a, 5h, and 5k demonstrated maximal potency equivalent to standard. Lipinski's rule was followed in ADME outcomes. Conclusion: The synthesis and evaluation of indole derivatives to investigate their antioxidant action has received a lot of attention. These discoveries could lead to more effective antioxidant candidates being designed and developed.
53.	TPPD: Targeted pseudo partitioning based defence for cross-core covert channel attacks J Kaur, S Das - Journal of Systems Architecture, 2023 **Abstract:** Contemporary computing employs cache hierarchy to fill the speed gap between processors and main memories. In order to optimise system performance, Last Level Caches (LLC) are shared among all the cores. Cache sharing has made them an attractive surface for cross-core timing channel attacks. In these attacks, an attacker running on another core can exploit the access timing of the victim process to infiltrate the secret information. One such attack is called a cross-core Covert Channel Attack (CCA). Timely detection and then prevention of cross-core CCA is critical for maintaining the integrity and security of users, especially in a shared computing environment. In this work, we have proposed an efficient cross-core CCA mitigation technique. We propose a way-wise cache partitioning on targeted sets, only for the processes suspected to be attackers. In this way, the performance impact on the entire LLC is minimised, and benign applications can utilise the LLC to its full capacity. We have used a

	cycle-accurate simulator (gem5) to analyse the performance of the proposed method and its security effectiveness. It has been successful in abolishing the cross-core covert timing channel attack with no significant performance impact on benign applications. It causes 23% less cache misses in comparison to existing partitioning based solutions while requiring ≈0.26% storage overhead.
54.	Understanding translational research in schizophrenia: A novel insight into animal models JA Malik, Z Yaseen, L Thotapalli, S Ahmed, MF Shaikh… - Molecular Biology Reports, 2023 **Abstract:** Schizophrenia affects millions of people worldwide and is a major challenge for the scientific community. Like most psychotic diseases, it is also considered a complicated mental disorder caused by an imbalance in neurotransmitters. Due to the complexity of neuropathology, it is always a complicated disorder. The lack of proper understanding of the pathophysiology makes the disorder unmanageable in clinical settings. However, due to recent advances in animal models, we hope we can have better therapeutic approaches with more success in clinical settings. Dopamine, glutamate, GABA, and serotonin are the neurotransmitters involved in the pathophysiology of schizophrenia. Various animal models have been put forward based on these neurotransmitters, including pharmacological, neurodevelopmental, and genetic models. Polymorphism of genes such as dysbindin, DICS1, and NRG1 has also been reported in schizophrenia. Hypothesis based on dopamine, glutamate, and serotonin are considered successful models of schizophrenia on which drug therapies have been designed to date. New targets like the orexin system, muscarinic and nicotinic receptors, and cannabinoid receptors have been approached to alleviate the negative and cognitive symptoms. The non-pharmacological models like the post-weaning social isolation model (maternal deprivation), the isolation rearing model etc. have been also developed to mimic the symptoms of schizophrenia and to create and test new approaches of drug therapy which is a breakthrough at present in psychiatric disorders. Different behavioral tests have been evaluated in these specific models. This review will highlight the currently available animal models and behavioral tests in psychic disorders concerning schizophrenia.
55.	Unveiling and understanding the remarkable enhancement in the catalytic activity by the defect creation in UIO-66 during the catalytic transfer hydrodeoxygenation of vanillin with isopropanol AK Kar, R Sarkar, AK Manal, R Kumar, S Chakraborty, R Ahuja, R Srivastava - Applied Catalysis B: Environmental, 2023 **Abstract:** The catalytic transfer hydrodeoxygenation of vanillin is generally achieved using noble metal-based catalysts. Herein, we report a mechanistic investigation of the catalytic transfer hydrodeoxygenation (CTHDO) of vanillin over a defect-induced UIO-66 MOF. The remarkable enhancement in the CTHDO of vanillin was due to the unique structural features of the defect-induced UIO-66 MOF. The defect creation was confirmed using PXRD, N_2-sorption, FT-IR, XPS, HRTEM, dissolution ^{1}H NMR, and quantified by TGA. The linker deficiency created Lewis acid and dynamic Bronsted acid and was confirmed by the NH_3-TPD and CD_3CN drift FT-IR. The periodic density functional theory calculations were conducted to elucidate the reaction pathway and mechanism. Density function theory, poisoning studies, control reactions, and quantified defect sites elucidate the active sites of the UIO-66_{def} involved in the CTHDO of vanillin with isopropanol. The catalyst was efficiently recycled and retained its activity and structural features after multiple recycles. **Graphical Abstract:**

	 The catalytic transfer hydrodeoxygenation of vanillin to 2-methoxy-methyl phenol was achieved using the defect-induced (UIO-66_{def}). The modulated structural features (Lewis acidity and Bronsted acidity) after the defect generation led to the development of the active sites for this transformation.
56.	Variable node higher-order XFEM for fracture modeling in orthotropic material K Dwivedi, H Pathak, S Kumar - Proceedings of the Institution of Mechanical Engineers, Part C: Journal of Mechanical Engineering Science, 2023 **Abstract:** A novel computational approach presented in this work to improve the accuracy and efficiency of fracture modeling in an orthotropic material medium. Extended finite element method (XFEM) with higher-order enrichment functions was employed at the different scale mesh topology. The approach combined variable node element concepts for different scale mesh connections and higher-order XFEM for accuracy and completeness of discontinuity domain. The proposed computational methodology was employed with in-house developed MATLAB code. Further, stochastic fracture studies were discussed for reliability of the cracked structures. Few numerical examples with multiple geometrical discontinuities were simulated to check the computational efficiency and accuracy.
57.	Wafer-scale controlled growth of MoS_2 by magnetron sputtering: from in-plane to inter-connected vertically-aligned flakes R Wadhwa, S Thapa, S Deswal, P Kumar, M Kumar - Journal of Physics: Condensed Matter, 2023 **Abstract:** Recently, Molybdenum disulfide (MoS_2) has attracted great attention due to its unique characteristics and potential applications in various fields. The advancements in the field have substantially improved at the laboratory scale however, a synthesis approach that produces large area growth of MoS_2 on a wafer scale is the key requirement for the realization of commercial two-dimensional (2D) technology. Herein, we report tunable MoS_2 growth with varied morphologies via radio frequency magnetron sputtering by controlling growth parameters. The controlled growth from in-plane to vertically-aligned (VA) MoS_2 flakes has been achieved on a variety of substrates (Si, Si/SiO_2, sapphire, quartz, and carbon fiber). Moreover, the growth of VA MoS_2 is highly reproducible and is fabricated on a wafer scale. The flakes synthesized on the wafer show high uniformity, which is corroborated by the spatial mapping using Raman over the entire 2-inch Si/SiO_2 wafer. The detailed morphological, structural, and spectroscopic analysis reveals the transition from in-plane MoS_2 to VA MoS_2 flakes. This work presents a facile approach to directly synthesize layered materials by sputtering technique on wafer scale. This paves the way for designing mass production of high-quality 2D materials, which will advance their practical applications by integration into device architectures in various fields.
58.	Zr-KIT-6 catalyzed renewable synthesis of N-aryl pyrroles for producing bioactive synthetic compounds AK Manal, R Srivastava - Applied Catalysis A: General, 2023

	Abstract: The sustainable synthesis of bioactive compounds using biomass-derived platform chemicals is essential to meet future chemical demand. Herein a mild and eco-friendly route is presented for structurally diverse pyrrole derivatives from biomass-derived furan. The furans react with aryl amines to construct N-aryl pyrroles in high yields over a robust Lewis acid Zr-KIT-6. Among the synthesized catalysts of this study, Zr-KIT-6 (20) exhibited excellent performance. The same protocol provides a broad utility to synthesize diverse functional pyrrole derivatives. Mechanistic study over Lewis acid Zr-KIT-6 and Bronsted acid KIT-6-SO_3H catalysts indicate that the Lewis acid Zr-KIT-6 follows the direct nucleophilic substitution pathway and Bronsted acid KIT-6-SO_3H follows the traditional Pall-Knorr reaction pathway. In addition, the co-catalyst-free straightforward domino process requires mild reaction conditions. The broad synthetic utility of the presented methodology was successfully applied to synthesizing biologically active and pharmaceutically relevant antitubercular and antibacterial active N-aryl pyrrole derivatives from renewable furans. **Graphical Abstract:**  Lewis acid Zr-KIT-6 followed the direct nucleophilic substitution pathway to produce structurally diverse pyrroles from biomass-derived furans.

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