IIT Ropar
List of Recent Publications with Abstract
Coverage: May, 2021
A benzothiazole-based receptor for colorimetric detection of Cu2+ and S2-ions in aqueous media SM Park, S Saini, JE Park, N Singh, DO Jang - Tetrahedron Letters, 2021
<b>Abstract:</b> A benzothiazole-based azo compound was synthesized and evaluated as a probe for the selective sensing of cations and anions. The probe (PA) could detect Cu2+ ions in aqueous media selectively, without interference from other cations and with a limit of detection of 0.43 μM. The resultant complex, PA-Cu2+, could be used as a secondary probe for detecting S2– ions in aqueous media in the presence of other interfering anions through a cation displacement process.
Graphical Abstract:
Cus
A critical review on micro-and nanomotors: Application towards wastewater treatment
B Verma, SP Gumfekar, S Manigandan - The Canadian Journal of Chemical Engineering, 2021
Abstract: Micro-and nanomotors are synthetic devices that can transform various sources of energy into motion. These devices perform specialized tasks as they propel themselves in response to stimuli. The application of self-propelled micro-and nanomachines in wastewater treatment has been of prime importance in the last decade. Compared to static decontamination systems, micro-and nanomachines can remove or degrade water pollutants in a much more rapid way owing to higher diffusion rates and fluxes. The present review focuses on the recent progress of micro-and nanomachines in wastewater treatment and provides an overview of their structural features, synthesis procedures, and propulsion mechanisms. We reviewed the applications of micro-and nanomachines to remove heavy metals, dyes, and organic pollutants from wastewater. We also discussed the challenges micro-and nanomotors face during wastewater treatment, thus providing a holistic approach to the article. This article highlights the shortcomings as well as the opportunities for micro-and nanomotors-based technology in wastewater treatment.
A Signal Parameter Measurement Technique for Adversely Distorted Multifrequency Grid Signals K Chauhan, R Sodhi - Journal of The Institution of Engineers (India): Series B, 2021
Abstract: This paper proposes a simple yet effective signal parameter measurement technique (SPMT) for the accurate estimation of fundamental and harmonic parameters. The proposed method is evolved from the design of adaptive filter bank (AFB) on the basis of frequency spectrum of the input signal and is preceded by compressive sensing (CS). The AFB is capable to decompose the multifrequency signal into its respective modes and CS has got an excellent capability of providing an enhanced frequency resolution in a relatively shorter window. The accuracy of the proposed method is verified on various numerical simulated signal polluted by interharmonics, harmonics, noise, frequency offset, and real-time signal acquired from hardware setup. A comparison with existing approaches viz. empirical wavelet transform, improved adaptive filtering, Prony, exact model order-ESPRIT, sliding ESPRIT is also presented which

A Survey on Cache Timing Channel Attacks for Multicore Processors J Kaur, S Das - Journal of Hardware and Systems Security, 2021

Abstract: Cache timing channel attacks has attained a lot of attention in the last decade. These attacks exploits the timing channel created by the significant time gap between cache and main memory accesses. It has been successfully implemented to leak the secret key of various cryptography algorithms. The latest advancements in cache attacks also exploit other microarchitectural components such as hardware prefetchers, branch predictor, and replacement engine, in addition to the cache memory. Detection of these attacks is a difficult task as the attacker process running in the processor must be detected before significant portion of the attack is complete. The major challenge for mitigation and defense mechanisms against these attacks is maintaining the system performance while disabling or avoiding these attacks. The overhead caused by detection, mitigation and defense mechanism must not be significant to system's performance. This paper discusses the research carried out in three aspects of cache security: cache timing channel attacks, detection techniques of these attacks, and defense mechanisms in details.

A Three-Phase Quality Function Deployment Approach for Conceptualizing a Sustainable Product Life Cycle: Case Study of a Blower Heater

PK Singh, P Sarkar - International Conference on Research into Design: Part of the Smart Innovation, Systems and Technologies book series, 2021

Abstract: The increasing awareness and demand for producing environmentally sustainable products have stimulated the industries across the globe to implement eco-friendly practices in the development of various products. It is important to consider the environmental impact while conceptualizing a product, but at the same time, the choices of end users should not be overlooked. In this study, an ecodesign-based quality function deployment (QFD) approach is proposed for developing the sustainable products. The QFD approach used in this study consists of three different phases. The first phase, known as 'house of quality,' shows the relationship between the voice of customers and technical requirements of the product to be developed. In second phase, the relationship of the technical requirements with different part characteristics of the product is established. Third phase relates parts characteristics with various ecodesign practices spread across the entire life cycle of the product. The proposed methodology is applied for designing an environmentally conscious blower heater. The finding of this study shows that 'ensuring a higher durability,' 'reducing energy consumption during use' and 'ensuring easier maintenance and repair' are the most significant ecodesign practices that must be emphasized while designing a blower heater. The methodology developed in this research can assist the designers to develop eco-friendly products through the identification of the most relevant ecodesign practices for individual products.

Anomalous patterns of Saffman-Taylor fingering instability during a metastable phase separation

RX Suzuki, H Tada, S Hirano, T Ban...M Mishra... - Physical Chemistry Chemical Physics, 2021

**Abstract:** Phase separation is important in biology, biochemistry, industry, and other areas and is divided into two types: a spinodal decomposition type and a nucleation and growth type. The spinodal decomposition type phase separation occurs under the thermodynamically unstable conditions, and the nucleation and growth type phase separation occurs under thermodynamically metastable conditions. On the other hand, when a less viscous fluid displaces a more viscous one in porous media, the interface of the two fluids becomes hydrodynamically unstable and forms a finger-like pattern. The coupling of the hydrodynamic instability with the thermodynamic instability has been studied. It is reported that the hydrodynamic instability under thermodynamically unstable conditions, where spinodal decomposition type phase separation occurs, creates multiple moving droplets with a radius of 3–4 mm because of the

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spontaneous convection induced by the Korteweg force, which is driven by a compositional gradient during phase separation. However, the hydrodynamic instability under metastable conditions, where the phase separation of nucleation and growth type occurs, is still unrevealed. In this study, we applied fingering instability (hydrodynamic instability) under the metastable conditions, where the patterns are changed from fingering or droplets to anomalous patterns such as tip-widening or needle-like (top-pointed) fingering patterns when the initial concentration is metastable, which is considered near a binodal curve. These patterns are ubiquitous in nature, similar to dendrite crystals (snowflakes) or our body's cells. Thus, the patterns created can be controlled through hydrodynamic conditions such as the injection flow and thermodynamic conditions such as spinodal decomposition (thermodynamically unstable conditions) and metastable conditions.

Antimonene Allotropes α-and β-Phases as Promising Anchoring Materials for Lithium–Sulfur Batteries

D Singh, SK Gupta, T Hussain, Y Sonvane, PN Gajjar, R Ahuja - Energy & Fuels, 2021

**Abstract:** In a quest to mitigate the undesirable shuttling effect that hampers the performance of Li–S batteries, we adopted first-principles calculations to study the anchoring mechanism of lithium polysulfides on antimonene phases, i.e., α-Sb and β-Sb. The anchoring mechanisms of LiPSs on α-Sb and β-Sb were studied through calculations of binding energy, charge transfer, and vertical binding distances from the monolayer to LiPSs. The results indicated that pristine α-Sb and β-Sb showed significant physisorption/chemisorption interactions toward LiPSs due to the considerable Eb values (0.71–1.68 and 0.96–2.07 eV, respectively). Meanwhile, with single Sb vacancy, the binding strength was enhanced (0.83–2.91 eV) for the β-Sb monolayer. Furthermore, we substituted the Sb atom with the Sn/Te atom and found stronger Eb (1.32–5.69 and 0.45–4.81 eV). All these bindings of LiPSs were much stronger than their interactions with those of electrolytes (DME/DOL) (Eb values: 0.20–1.16 and 0.17–1.07 eV). Also, we investigated the redistribution of electrons and the influence of electronic states near the Fermi level in DOS for LiPSs on α-Sb and β-Sb. Our findings suggest that pristine and defected β-Sb monolayers could be an excellent anchoring material for Li–S batteries.

Bendable ultra-high frequency radio-frequency identification tag antenna for retail garments using nonuniform meandered lines

M Kumar, A Sharma, IJ Garcia Zuazola - Engineering Reports, 2021

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**Abstract:** A bendable ultra-high frequency (UHF) radio-frequency identification (RFID) tag antenna using nonuniform meandered lines for retail garments in the textile industry is presented. Based on an earlier UHF RFID tag antenna using nonuniform meandered lines, the proposed tag is fully bendable and aimed to be embedded in retail garments for long-life cycles. As a result, a relatively low cost, wideband, compactness, and good conjugate matching with good dipole-like read range is presented. Results showed an antenna with a wide bandwidth of 900 MHz and a long read range of 10.1 m making the UHF RFID tag antenna using nonuniform meandered lines a potential candidate for retail garments in bendable applications of the textile industry. Simulations are corroborated by measurements and are in fairly agreement.

Combined experimental and computational study to unravel the factors of the Cu/TiO<sub>2</sub> catalyst for CO<sub>2</sub> hydrogenation to methanol

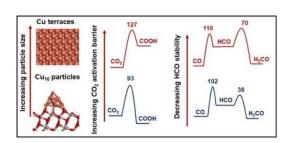
SK Sharma, A Banerjee, B Paul, MK Poddar... - Journal of CO2 Utilization, 2021

**Abstract:** The hydrogenation of CO<sub>2</sub> to methanol over Cu-nanoparticles supported on TiO<sub>2</sub> nanocrystals was studied at 30 bar pressure and 200–300 °C. 5 wt% Cu-TiO<sub>2</sub> catalyst was synthesized by a modified hydrothermal method (Cu-TiO<sub>2</sub>HT) and by incipient wetness impregnation method (Cu-TiO<sub>2</sub>IMP). TEM analysis of the Cu-TiO<sub>2</sub>HT catalyst revealed the formation of Cu-nanoparticles (3-5 nm), while larger Cu particle sizes were observed on the Cu-TiO<sub>2</sub>IMP catalyst. The Cu-TiO<sub>2</sub>HT catalyst showed superior catalytic activity (CO<sub>2</sub> conversion ~ 9.4 %) and methanol selectivity (~ 96 %) at 200 °C and 30 bar pressure. Low CO<sub>2</sub>

conversions ( $\sim$ 6%) and high CO selectivity ( $\sim$ 40 %) was obtained on the Cu-TiO2IMP catalyst. Density functional theory (DFT) calculations indicated the CO<sub>2</sub> activation to methanol to proceed via a reverse water gas shift pathway with a significantly lower (93 kJ/mol) CO<sub>2</sub> activation barrier on the Cu-nanoparticles, relative to the larger Cu particles (127 kJ/mol). In addition, the higher selectivity towards methanol over the Cu-TiO<sub>2</sub>HT catalyst was attributed to the higher CO and HCO stability on the Cu nanoparticles. Time of stream (TOS) study of the Cu-TiO2 catalysts showed no significant deactivation even after 150 h with molar feed ratio 1:3:1 (CO<sub>2</sub>:H<sub>2</sub>: N<sub>2</sub>) at 200 °C.

## **Graphical Abstract:**

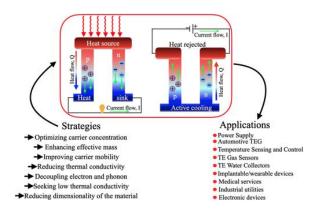
11.



<u>Dimensionality</u> effects in high-performance thermoelectric materials: Computational and experimental progress in energy harvesting applications

D Singh, R Ahuja – Wiley Interdisciplinary Reviews: Computational Molecular Science, 2021

Abstract: Thermoelectric (TE) materials can be used in the conversion of heat to electricity and vice versa, which can enhance the efficiency of the fuel, in addition to supplying solid alternative energy in several applications in accumulating waste heat and, as a result, help to find new energy sources. Considering the current environment as well as the energy crisis, the TE modules are a need of the future. The present review focuses on the new strategies and approaches to achieve high-performance TE materials including materials improvement, structures, and geometry improvement and their applications. Controlling the carrier concentration and the band structures of materials is an effective way to optimize the electrical transport properties, while engineered nanostructures and engineering defects can immensely decrease the thermal conductivity and significantly improved the power factor. The present review gives a better understanding of how the theory is affecting the TE field.



Effect of graphene on thermal conductivity of laser cladded copper G Singh, V Ghai, S Chaudhary, S Singh, PK Agnihotri, H Singh - Emergent Materials, 2021

**Abstract:** A thick copper coating on the triangular plates of vacuum vessels has been proposed for plasma passivation and vertical stability in tokamak. Laser cladding technique is utilized to develop such coatings. However, the process leads to a drastic decrease in the thermal conductivity of the copper coating. Regaining the thermal conductivity of laser cladded copper is a challenging task. In this work, we have verified that graphene deposition can improve the

thermal conductivity of laser cladded copper. Graphene layers have been grown on a 3-mm-thick laser cladded copper at 900 °C under methane, argon, and hydrogen atmosphere inside a thermal chemical vapor deposition system. The thermal conductivity of the laser cladded copper was found to be improved from 140 W/mK for as-deposited cladding to 309 W/mK after graphene growth. Further, structural morphology and thermal conductivity of graphene-coated laser cladded copper remained intact after irradiation tests with high-energy prompt gamma-rays and heavy nuclei exposure, which depicted its sustainability in actual environmental conditions.

Effect of polymer additives and viscous dissipation on natural convection in a square cavity with differentially heated side walls

A Chauhan, PM Sahu, C Sasmal - International Journal of Heat and Mass Transfer, 2021

Abstract: This study presents an extensive numerical investigation on how the addition of polymer molecules into a Newtonian solvent would tend to influence the natural convection heat transfer phenomena in a differentially heated square cavity. The rheological behaviour of the resulting polymer solution is modelled based on the FENE-P viscoelastic constitutive equation, which along with other governing equations, namely, mass, momentum, and energy equations, have been solved using the open source CFD code OpenFOAM over the following ranges of conditions: Rayleigh number,  $10^3 \le \text{Ra} \le 10^6$ ; Weissenberg number,  $1 \le \text{Wi}$ <100; polymer extensibility parameter,  $10 \le L^2 \le 500$ , polymer viscosity ratio,  $0.5 \le \beta \le 0.9$  and for a fixed value of the Prandtl number of Pr=7. At low values of the Rayleigh number, the average Nusselt number gradually increases with the Weissenberg number. However, at high values of it, the average Nusselt number first increases steeply up to a critical value of the Weissenberg number, and beyond that, it remains almost constant as the Weissenberg number further increases. The average Nusselt number is seen to decrease with the increasing values of both the polymer extensibility paramter and polymer viscosity ratio. The viscous dissipation tends to deteriorate the heat transfer rate in comparison to that seen in the absence of it; however, the extent of this deterioration is found to be independent on the values of Wi,  $L^2$  and  $\beta$ . Furthermore, detailed discussion of the results in terms of the streamline a profiles, isotherm contours, distribution of local Nusselt number, variation of velocity components, etc., is also presented. Finally, from an application standpoint, a simple correlation for the average Nusselt number is presented, which can be used for the interpolation of the present results for the intermediate values of the governing parameters in a new application.

Effect of structural characteristics on damping modification factors for floor response spectra in RC buildings

M Surana, Y Singh, DH Lang - Engineering Structures, 2021

**Abstract:** Floor response spectra (FRS) are used to compute the design floor accelerations for seismic design of acceleration-sensitive non-structural components (NSCs) in a building. In the present study, the elastic FRS at different floor levels are investigated for a set of linear and nonlinear models of both low- and mid-rise reinforced concrete (RC) frame structures. The damping modification factors (DMFs) for the elastic FRS are derived for seven different damping ratios of the NSC's (i.e. 0.1%, 0.2%, 0.5%, 1%, 2%, 5%, and 10%), and six different levels of inelastic response in the building structure. It is observed that DMFs for the elastic FRS are influenced by both NSC and building structure characteristics. The factors affecting the DMFs for the elastic FRS include the damping ratio of the NSC, the tuning ratio (i.e. the ratio between the period of vibration of the NSC, Ts, to the fundamental period of vibration of the building structure, T1), the modal periods (T1 and T2), and the level of the building structure's inelasticity. Conversely, the vertical location of the NSC in the building structure does not affect DMFs significantly. Further, in the case of a tuned response of the NSC, the DMFs for elastic FRS are significantly higher for NSC damping ratios less than 5% and lower for NSC damping ratios greater than 5%, than those conventionally used for the elastic ground response spectra (GRS). This is true for the elastic response as well as for low levels of inelasticity in the building structure. On the other hand, at high levels of the building structure's inelasticity, the DMFs for elastic FRS approach to the conventional DMFs derived for the elastic GRS. Considering these observations, a design-oriented multilinear model is proposed to compute DMFs for the elastic FRS, accounting for the specific characteristics of the NSC (i.e. the period and the damping ratio of the NSC) and the building structure (i.e. the modal periods and the level of the inelasticity). The proposed model for computing the DMFs for elastic FRS is validated by comparing the model predictions with those obtained by time-history analyses, using a different RC frame building and an entirely different suite of ground-motion records than those that were used to develop the proposed model. The proposed model to compute DMFs for the elastic FRS can be used with both the current code-based and the performance-based seismic design of NSCs located in the inelastic building structures.

<u>Failure Behavior of Cemented Tungsten Carbide Materials: A Case Study of Mining Drill Bits</u> PK Katiyar, R Maurya, PK Singh - Journal of Materials Engineering and Performance, 2021

Abstract: The present work is mainly focused on the macroscopic and microscopic examination of failed tungsten carbide (WC-Co) drill bits to find the root cause of the insert's failure. Different failed WC-Co tool bits have been observed macroscopically and found that the inserts have failed due to shear-off, cracks, and gradual wear. The FE-SEM and AFM micrographs have been used to understand the different degradation and the tribocorrosion mechanisms of WC-Co inserts. Typical shape change mechanisms of individual WC grains have also been studied in detail with the help of FE-SEM micrographs, which have been influenced by the tribocorrosion in the presence of the mining environment. Ultrasonic cleaning method has been used to clean the inserts for the microscopic examinations. Various morphologies of fragmented WC grains have been examined to understand the shape change mechanisms of WC grains. The different electrode potential between the Co binder and the WC grains is the primary cause of the microgalvanic form of corrosion. Hence, in the present study the wear and corrosion mechanisms of WC-Co insert along with the possible approaches to reduce the tribocorrosion have been discussed in detail. It was found that the proper understanding of tribocorrosion mechanisms is essential for the selection, development, and advancement of the suitable WC-Co tool materials.

Fundamentals of ATR-FTIR Spectroscopy and Its Role for Probing In-Situ Molecular-Level Interactions

H Kaur, B Rana, D Tomar, S Kaur, KC Jena - Modern Techniques of Spectroscopy: Part of the Progress in Optical Science and Photonics book series, 2021

**Abstract:** Infrared (IR) vibrational spectroscopy is the most reliable technique to determine the molecular composition and structure of chemical compounds. In the past two decades, with the advancement in the IR instrumentation, attenuated total reflectance Fourier transform infrared (ATR-FTIR) vibrational spectroscopic tool have taken an invaluable position in the field of chemistry, physics, material and biological sciences. It readily probes the molecular structure, chemical interactions and dynamics of the molecular species. Owing to its higher sensitivity with the surrounding fluctuations, ATR-FTIR aids in extracting the information about the molecular configuration and the local interactive framework of different analytes existing in diverse morphological states. ATR-FTIR can be employed for interfacial studies at distinct levels by varying the incident angle and the material used for ATR crystal to obtain a required penetration depth of the IR beam in the sample medium at the ATR crystal/sample interface. The current chapter introduces the background, modern theoretical, and practical aspects of the ATR-FTIR spectroscopy descriptively. The chapter also previews a considerable amount of research currently pursued in different application domains including bio-nano model systems, biomolecular assembly, binary solvents, forensics and electrochemical devices, covering the molecular-scale perspectives using the ATR-FTIR vibrational spectroscopy.

GIS-Based Landslide Hazard Zonation and Risk Studies Using MCDM

A Tyagi, RK Tiwari, N James - Local Site Effects and Ground Failures: Part of the Lecture Notes in Civil Engineering book series, 2021

**Abstract:** In India, landslides are the most frequently occurring disaster in the regions of the Himalayas and the Western Ghats. They are mainly triggered either by rainfall or earthquake or the combination of both, causing severe damage to human life and infrastructure. This study presents a comprehensive use of the multi-criteria decision-making (MCDM) method in landslide risk assessment for the Tehri area in the state of Uttarakhand, India. The Tehri area is situated in the Lesser Himalaya of Garhwal hills which lies in zone IV of seismic zoning map of India. Because of the large-scale slope instability in the area, it has received the special attention of the researchers. In the recent past,—many landslide hazards and risk zonation is carried out for different regions in the Uttarakhand state. However, limited work is done considering temporal factors such as seismic ground shaking, rainfall, and seismic amplification at surface level. The DEM data is used to produce topographic characteristics such as slope, aspect, and relative relief. DEM data is also used for the detailed drainage analysis which includes topographic wetness index (TWI), stream power index (SPI), drainage buffer, and reservoir buffer. Seismic hazard analysis is performed using the deterministic methodology to estimate the peak horizontal acceleration. The amplification factor is calculated using the non-linear site amplification method. In this study, the analytical hierarchy process (AHP) is used to evaluate the landslide hazard index which is used to generate landslide hazard zonation (LHZ) map. Further, the landslide vulnerability assessment is done for the study area. The vulnerability map of the study area is derived in terms of landuse/landcover (LULC) using remote sensing data of Landsat 8 which can provide useful information that helps people to understand the risk of living in an area.

Impact of channel correlation on network coded cooperation with two sources P Kumar, S Darshi, S Shailendra - Physical Communication, 2021

Abstract: In this paper, we consider Digital Network Coded Cooperation (DNCC) with Decode-and-Forward (DF) relaying scheme in correlated environment. In order to quantify the performance of DNCC network, analytical closed form expression of the outage probability for Non-Line of Sight (NLoS) correlated environments is derived. For the sake of completeness and comparison, investigation of uncorrelated environments is also presented. Unlike existing investigations, it is observed that spatial correlation among channels considerably improves the performance of such networks. In particular, detrimental effects of the Digital Network Coding (DNC) noise is abated by the channel correlation. Additionally a discussion on various deterministic geometries for such networks is also presented to get further insights about node placement. Cumulative Distribution Function (CDF) obtained for Signal to Noise Ratio (SNR) of relay path can be utilized for performing diversity calculations. Outage closed form expressions derived may be used to choose network parameters judiciously in different NLoS correlated scenarios for achieving better Quality of Service (QoS) in next generation wireless networks.

<u>Introduction to New Research Directions in Solar Energy Technologies</u>
H Tyagi, PR Chakraborty, S Powar... - New Research Directions in Solar Energy Technologies:
Part of the Energy, Environment, and Sustainability book series, 2021

**Abstract:** The overall theme of this book is related to the topics of solar energy. This book has been divided into four parts. The first part relates to the general issues of clean and sustainable energy. The second part of this book deals with the topic of power generation using solar energy.

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<u>Investigation of Mechanical, Material, and Compositional Determinants of Human Trabecular Bone Quality in Type 2 Diabetes</u>

P Sihota, RN Yadav, R Dhaliwal... V Mehandia...N Kumar - The Journal of clinical endocrinology and metabolism, 2021

#### **Abstract:**

### Context

Increased bone fragility and reduced energy absorption to fracture associated with type 2 diabetes (T2D) cannot be explained by bone mineral density alone. This study, for the first time, reports on alterations in bone tissue's material properties obtained from individuals with diabetes and known fragility fracture status.

# Objective

To investigate the role of T2D in altering biomechanical, microstructural, and compositional properties of bone in individuals with fragility fracture.

## Methods

Femoral head bone tissue specimens were collected from patients who underwent replacement surgery for fragility hip fracture. Trabecular bone quality parameters were compared in samples of 2 groups, nondiabetic (n = 40) and diabetic (n = 30), with a mean duration of disease  $7.5 \pm 2.8$  years.

#### Results

No significant difference was observed in aBMD between the groups. Bone volume fraction (BV/TV) was lower in the diabetic group due to fewer and thinner trabeculae. The apparent-level toughness and postyield energy were lower in those with diabetes. Tissue-level (nanoindentation) modulus and hardness were lower in this group. Compositional differences in the diabetic group included lower mineral:matrix, wider mineral crystals, and bone collagen modifications—higher total fluorescent advanced glycation end-products (fAGEs), higher nonenzymatic cross-link ratio (NE-xLR), and altered secondary structure (amide bands). There was a strong inverse correlation between NE-xLR and postyield strain, fAGEs and postyield energy, and fAGEs and toughness.

## Conclusion

The current study is novel in examining bone tissue in T2D following first hip fragility fracture. Our findings provide evidence of hyperglycemia's detrimental effects on trabecular bone quality at multiple scales leading to lower energy absorption and toughness indicative of increased propensity to bone fragility.

<u>Low and Medium Carbon Alcohol Fueled Dual-Fuel Compression Ignition Engine</u>

MR Saxena, RK Maurya - Alcohol as an Alternative Fuel for Internal Combustion Engines: Part of the Energy, Environment, and Sustainability book series, 2021

**Abstract:** Dual-fuel operation in CI-engine is an emerging strategy to improve engine efficiency along with the simultaneous in-cylinder reduction of  $NO_x$  and PM emissions. In dual-fuel operation, low-reactivity fuel (such as methanol, ethanol) and high-reactivity fuel (such as diesel) are used in the same engine cycle. This chapter presents a detailed analysis of performance, combustion, and emission characteristics of low and medium carbon alcoholdiesel fueled dual-fuel CI-engine. This chapter also briefly explains the production of alcohol fuel and the benefits of their inimitable properties. The influence of engine operating parameters on the heat release rate, combustion duration, and cyclic combustion variations has been discussed in this chapter. Additionally, the effect of the operating parameters on CO, unburnt hydrocarbon,  $NO_x$ , soot, particle emissions, and unregulated emissions is also presented. Results depict that with an increase in engine load, the combustion characteristics changed from partial

burn to misfire to proper combustion and to knocking (at full engine load). The dual-fuel operation has higher HC, CO, HCHO, CH<sub>3</sub>OH, HCOOH, C<sub>6</sub>H<sub>6</sub>, 1,3-C<sub>4</sub>H<sub>6</sub>, and C<sub>7</sub>H<sub>8</sub> emissions, whereas NO<sub>x</sub> and soot emissions are lower than conventional diesel operation.

Metal Phosphate Catalysts to Upgrade Lignocellulose Biomass into Value-Added Chemicals and Biofuels

A Shivhare, A Kumar, R Srivastava - Green Chemistry, 2021

Abstract: Alternative and green sources of energy are needed to replace rapidly depleting and non-renewable fossil fuels. Abundant and renewable lignocellulose biomass can be transformed into value-added chemicals and biofuels that are currently derived from non-renewable fossil fuels. The conversion of lignocellulose biomass has been extensively investigated over heterogeneous catalysts via various catalytic processes. In particular, solid acid catalysts possessing both Lewis and Brønsted acid sites have drawn significant research interest. Among these catalysts, metal phosphates are of particular interest due to their relatively facile synthesis routes, low cost, environmental friendliness, and tunable Lewis and Brønsted acid sites. In this tutorial review, we have provided a brief overview of the synthesis methodologies and have summarized several catalytic processes involved in biomass upgrading, including dehydration, oxidation, transfer hydrogenation, transesterification, hydrogenolysis, and hydrodeoxygenation over metal phosphate catalysts to produce value-added chemicals and biofuels. The main emphasis is to highlight the relationship between the textural properties of the catalysts and their catalytic performances and to elucidate future research opportunities available in this exciting area.

Modulation of Ru and Cu nanoparticle contents over CuAlPO-5 for synergistic enhancement in the selective reduction and oxidation of biomass-derived furan based alcohols and carbonyls A Kumar, R Bal, R Srivastava - Catalysis Science & Technology, 2021

**Abstract:** Furfural (FAL) and 5-hydroxymethylfurfural (HMF) are important and sustainable platform chemicals. They are produced from lignocellulose biomass and attract significant attention as precursors for producing value-added chemicals and fuels. The selective conversion of these chemicals requires precise modulation of reaction parameters, solvent, and catalyst. In this study, FAL is selectively reduced to furfuryl alcohol (FOL), and HMF is selectively oxidized to 2,5-diformylfuran (DFF) over a Cu and Ru decorated copper aluminophosphate (CuAlPO-5) catalyst. A high FAL conversion (99.5%) and FOL selectivity (99.6%) are obtained in water under mild reaction conditions of 353 K and 1 MPa H2 pressure. On the other hand, 94.0% HMF conversion and 99.9% DFF selectivity are obtained at 1 atm O<sub>2</sub> flow at 413 K. Both these processes are efficiently conducted over Cu and Ru nanoparticles supported CuAlPO-5 at optimized Cu and Ru contents and under different reaction conditions. The calculated activation energies for these processes are 21.5 kJ mol<sup>-1</sup> (for FAL hydrogenation) and 34.5 kJ mol<sup>-1</sup> (for HMF oxidation). The temperature-programmed reduction/oxidation (TPR/TPO) and adsorption results suggest the synergy between Cu and Ru, resulting in higher catalytic activity. Systematic and precise modulation of active metal contents and minimizing the Ru content in the Cu-Ru bimetallic catalyst system would be desirable from the industrial and academic perspective, especially for achieving oxidation/reduction capabilities in biomass conversion using a single catalyst.

FAL

Reduction

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FOL

October 100

<u>Moment-based estimation for parameters of general inverse subordinator</u>
A Grzesiek, R Połoczański, A Kumar... - Physica A: Statistical Mechanics and its Applications, 2021

**Abstract:** In recent years the processes with anomalous diffusive dynamics have been widely discussed in the literature. The classic example of the anomalous diffusive models is the continuous time random walk (CTRW) which is a natural generalization of the random walk model. One of the fundamental properties of the classical CTRW is the fact that in the limit it tends to the Brownian motion subordinated by the so-called -stable subordinator when the mean of waiting times is infinite. One can consider the generalization of such subordinated model by taking general inverse subordinator instead of the -stable one as a time-change. The inverse subordinator is the first exit time of the non-decreasing Lévy process also called subordinator. In this paper we consider the Brownian motion delayed by general inverse subordinator. The main attention is paid to the estimation method of the parameters of the general inverse subordinator in the considered model. We propose a novel estimation technique based on the discretization of the subordinator's distribution. Using this approach we demonstrate that the distribution of the constant time periods, visible in the trajectory of the considered model, can be described by the so-called modified cumulative distribution function. This paper is an extension of the authors' previous article where a similar approach was applied, however here we focus on moment-based estimation and compare it with other popular methods of estimation. The effectiveness of the new algorithm is verified using the Monte Carlo approach.

<u>Performance Projection of 2-D Material-Based CMOS Inverters for Sub-10-nm Channel Length</u> A Rawat, AK Gupta, B Rawat - IEEE Transactions on Electron Devices, 2021

**Abstract:** In this work, we comprehensively investigate the performance of CMOS inverters based on 2-D materials (2DMs), such as MoS<sup>2</sup>, WSe<sup>2</sup>, WSe<sup>2</sup>, black phosphorus (BP), WSe<sup>2</sup>-MoS<sup>2</sup>, and benchmark against their silicon (Si) counterpart for sub-10-nm channel length. The performance evaluation of the 2DM-based CMOS inverters is done using an in-house developed multiscale modeling approach, which translates the atomistic device model into the professional circuit simulation using the Verilog-AMS interface. Among 2DM-based inverters, heterogeneous WSe<sup>2</sup>-MoS<sup>2</sup> inverter configuration exhibits excellent switching characteristics for 5.6 nm and beyond channel length with a larger static noise margin, nanowatt-order power dissipation, and comparative speed to Si-based inverter. Despite lower noise margins and higher power dissipation, Si-based inverter, with lower gate capacitance, allows marginally higher speed than that of 2DM-based inverters. Furthermore, at 3-nm channel length, static and dynamic performance metrics of inverter degrade significantly due to more pronounced short-channel effects; however, MoS2-based inverter demonstrates a good functionality. The performance analysis and benchmarking show promise and opportunities with 2DM-based devices for future logic applications; however, optimizing the contact resistance, parasitic capacitances, and channel length are the key device design parameters in developing the high-performance CMOS inverter.

<u>Prediction of mechanical properties of Trabecular Bone in Patients with type 2 diabetes using damage based Finite Element Method</u>

RN Yadav, P Sihota, P Uniyal, D Neradi, JC Bose...S Kumar...N Kumar - Journal of Biomechanics, 2021

Abstract: Type-2 diabetic (T2D) and osteoporosis (OP) suffered patients are more prone to fragile fracture though the nature of alteration in areal bone mineral density (aBMD) in these two cases are completely different. Therefore, it becomes crucial to compare the effect of T2D and OP on alteration in mechanical and structural properties of femoral trabecular bone. This study investigated the effect of T2D, OP, and osteopenia on bone structural and mechanical properties using micro-CT, nanoindentation and compression test. Further, a nanoscale finite element model (FEM) was developed to predict the cause of alteration in mechanical properties. Finally,

a damage-based FEM was proposed to predict the pathological related alteration of bone's mechanical response. The obtained results demonstrated that the T2D group had lower volume fraction (-18.25%, p = 0.023), young's modulus (-23.47%, p = 0.124), apparent modulus (-37.15%, p = 0.02), and toughness (-40%, p = 0.001) than the osteoporosis group. The damage-based FE results were found in good agreement with the compression experiment results for all three pathological conditions. Also, nanoscale FEM results demonstrated that the elastic and failure properties of mineralised collagen fibril decreases with increase in crystal size. This study reveals that T2D patients are more prone to fragile fracture in comparison to OP and osteopenia patients. Also, the proposed damage-based FEM can help to predict the risk of fragility fracture for different pathological conditions.

<u>Probing the defects and trap distribution in  $MgAl_2O_4$  nanocrystals through electron spin resonance and thermoluminescence</u>

S Dani, S Kumar, F Singh, A Vij, A Thakur - Journal of Physics D: Applied Physics, 2021

Trap distribution in MgAl2O4 nanocrystals has been investigated by analyzing thermoluminescene (TL) glow curves upon UV-irradiation. To probe various defects and trap distribution with the growth of spinel phase and crystallinity, three different fuels viz. monoethanolamine (MEA), glycine and urea, were employed in the combustion synthesis and annealing was performed at 700 °C and 900 °C. MEA and glycine resulted in crystalline spinel phase in annealed samples, however, urea resulted in minor secondary phase of MgO with the spinel phase in pristine as well as annealed samples. The X-ray photoelectron spectroscopy informed the presence of minor concentration of C and N in addition to Mg, Al and O, which are expected to influence the various defects of MgAl<sub>2</sub>O<sub>4</sub> samples. The TL glow curve broadening in pristine and 700 °C annealed samples inferred the presence of multiple closely distributed traps. Shallow traps were more populated with urea, while higher concentration of deep traps was observed with MEA and glycine. Computerized glow curve deconvolution of the TL glow curves revealed various trapping parameters. The observed shallow and deep traps have been attributed to various electron and hole centres such as antisite defects, O- and F+ centres. The significant high temperature shift of glow curve maxima in 700 °C annealed samples, synthesized using MEA and glycine, might be due to the reorganization of the local energy levels with the growth of spinel phase. Quenching of TL intensity at 900 °C anticipated the defect annealing accompanied by clustering of existing defects. Electron spin resonance analysis probed the existence of F+, V- centres and the spin-spin interaction of electron/hole spin trapped at these centres with the nearby cations, and estimated the formation of paramagnetic defect clusters at 900 °C annealing. A schematic band model is proposed to illustrate the TL behavior in MgAl<sub>2</sub>O<sub>4</sub> nanocrystals.

Psychological impacts of COVID-19 pandemic on the mode choice behaviour: A hybrid choice modelling approach

B Aaditya, TM Rahul - Transport Policy, 2021

Abstract: The COVID-19 pandemic is a pivotal moment in the history of mankind, which had a huge impact on the fast-paced world. The uncertainty associated with the plight of the pandemic, pushed the world towards a sense of insecurity and panic. Apart from the disease, the psychological problems connected to the lockdowns has caused an unprecedented change in the thought process of people towards travel. In the present study, we aim to statistically illustrate the change, the pandemic and lockdowns brought upon the travel mode choice behaviour. An Integrated choice and latent variable (ICLV) framework was adapted to understand the impact of the novel behavioural constructs, such as awareness of the disease and people's perception of the strictness of lockdown towards the mode choice in the post pandemic scenario. Different trip types were characterized according to the nature of the trip and their mode choice were assessed separately for the impact of the latent constructs. The results suggest that the awareness of the disease and the perception of strictness of the lockdown implemented play a major role in affecting the change of the mode choice of people. Further, the perception of safety in public

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transport, characterized by the social distancing and sanitization measures, determine the willingness of people towards the choice of public transit systems. The study concludes with a focus on the policies, which could be implemented for a safe travel in the post lockdown stage.

<u>Pulse compression favorable frequency modulated thermal wave imaging for non-destructive</u> testing and evaluation: an analytical study

A Rani, R Mulaveesala - IOP SciNotes, 2021

Abstract: InfraRed Thermography (IRT) is one of the non-destructive testing and evaluation (NDT&E) approach widely used for testing and evaluation of wide verity of materials such as metals, semiconductors and composites. Among the widely used Thermal NDT&E (TNDT&E) approaches for better depth resolution and sensitivity for detection of defects located at different depths inside the test specimen recently proposed correlation based approach gained importance due to its enhanced defect detection capabilities. The present paper introduces a novel one-dimensional analytical solution for the frequency modulated excitation scheme under adiabatic boundary conditions for detection of flat bottom holes as defects in a mild steel sample. The performance of the Pulse Thermography (PT), Lock-in Thermography (LT) and Frequency Modulated Thermal Wave Imaging (FMTWI) methods are highlighted their defect detection capabilities have been compared by adopting the recently introduced correlation based post-processing approach. Finally, the proposed analytical method has been validated with the results obtained from the commercially available finite element based software.

 $\frac{Recent\ Developments\ in\ the\ Design\ of\ Cd_xZn_{1-x}S\text{-}Based\ Photocatalysts}\ for\ Sustainable}{Production\ of\ Hydrogen}$ 

B Debnath, S Dhingra, CM Nagaraja - Solar RRL, 2021

Abstract: Photocatalytic production of clean fuel hydrogen (H2) from water using semiconductor nanomaterials as photocatalysts aided by natural sunlight represents a promising means to fulfill the growing energy demand and for mitigating increasing concentration of atmospheric CO2 due to the burning of fossil fuels. Among the widely studied semiconductor nanomaterials, the CdxZn1-xS ternary system has gained significant interest due to its tunable band edge, optical and electronic properties by merely varying the Cd2+/Zn2+ content. Consequently, CdxZn1-xS-based nanostructures have been extensively studied as promising visible-light-active photocatalysts for H2 production from water and other photocatalytic transformations. Herein, a comprehensive account of the research progress in the development of CdxZn1-xS-based photocatalysts for the production of solar fuel, H2 from water is provided. Further, various strategies used in enhancing the photocatalytic activity of CdxZn1-xS photocatalysts, like control of the morphology (0D, 1D, 2D, and 3D), bandgap engineering, and fabrication of various heterostructures have been discussed in detail. Furthermore, opportunities and future perspectives of CdxZn1-xS-based photocatalysts for practical applications have also been discussed. Overall, the importance of CdxZn1-xS-based photocatalysts is showcased for efficient visible-light-driven hydrogen production and can be beneficial for the design of sustainable photocatalytic systems.

Securing IoT with Blockchain

V Agarwal, S Pal – Book Chpater: Securing IoT and Big Data, 2020

**Abstract:** The Internet of Things (IoT) interconnects billions of diverse devices delivering remarkable services ranging from smart homes, industries, and finance to healthcare. However, the connected IoT devices are facing the problem of security due to decentralized storage and vulnerability of private data. Blockchain, integrated with IoT, can help in solving issues related to security by storing the data in an immutable and distributed manner. Blockchain is a tamper-proof distributed ledger that stores data in the form of transactions encrypted through cryptographic approaches. This chapter aims to outline a comprehensive and sweeping study of the current research endeavours in the area of blockchain-based IoT. We initially start with the issues in IoT, then present the fundamentals of blockchain and how it can be used to mitigate the

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risks associated with IoT devices. From there, we proceed to explain the real-life applications of blockchain-based IoT structures, followed by a review of the existing techniques for combining these two technologies in an efficient manner to provide a secure IoT.

<u>Site Characterization Using Satellite Data and Estimation of Seismic Hazard at Ground Surface</u> N James, S Kolathayar, TG Sitharam - Local Site Effects and Ground Failures: Part of the Lecture Notes in Civil Engineering book series, 2021

Abstract: This paper presents the seismic site characterization carried out for Karnataka (state level) as well as for India (country level) using topographic slope map derived from Digital Elevation Model (DEM) data. Two DEM data, SRTM, and ASTER were used to derive the slope maps. For Karnataka (state level), the slope map was generated from ASTER DEM considering a grid size of 5 × 5 km and for India (country level), the slope map was generated from SRTM DEM considering the grid size of 10 × 10 km. Based on the slope value, every grid point was characterized into various NEHRP site classes, and spatial variation of average shear wave velocity for top 30 m (Vs30) value throughout the study areas is presented in this paper. Peak horizontal acceleration (PHA) at bedrock level was evaluated for the same grid points using deterministic as well as probabilistic methodologies. The amplification factor for every grid point was obtained from the site coefficients corresponding to NEHRP site class. The surface level peak horizontal acceleration (PHA) was then evaluated for every grid point by multiplying bedrock level PHA with the corresponding amplification factor. Spatial variation of seismic hazard at the surface for the state of Karnataka as well as for entire India is presented in this paper.

Sustainability in supply networks: finding the most influential green interventions using interpretive structural modeling technique

RK Sharma, PK Singh, P Sarkar, H Singh - International Journal of Sustainable Engineering, 2021

Abstract: Manufacturing organisations adopt various kinds of green interventions to make their operations more environment friendly. However not all interventions have a similar impact on enhancing the environmental efficiency of supply networks. The present study aims to identify the most effective green interventions for effective green supply chain management (GSCM) using the interpretive structural modelling (ISM) technique. GSCM includes the implementation of green interventions to enhance the environmental viability of their products and processes. First, a set of green interventions is identified through literature and expert opinions, and then these are analysed using the ISM technique. The green interventions 'developing environmental strategies, policies and procedures' and 'performance review and long term action plan' are identified as the most influential green interventions as they have low dependence and high driving power, which means that it is important to give emphasis on these interventions for effective green supply chain management. Additionally, the study identifies that 'adoption of cutting edge technology', 'cleaner production', and others are the interventions with high dependence and high driving power. Among all the interventions analysed none has an independent character. Sustainability managers can use this technique and the results in improving sustainability in their SCM.

<u>Sustainable Design and Development of Stubble Removing Agricultural Machine for Stopping the Burning of Paddy Stubble</u>

H Singh, P Sarkar, H Singh, F Singh - International Conference on Research into Design: Part of the Smart Innovation, Systems and Technologies book series, 2021

**Abstract:** India is an emerging economy and has shown a great increase in the production of crops particularly after the green revolution. New kinds of seeds, fertilizers, machinery, and sowing techniques have helped a lot in meeting the needs of the country in terms of grains produced per hectare. Due to the rapid development, there is an increase in the overall pollution giving rise to greenhouse gases, and ultimately depleting the ozone layer along with the rise in

the seawater level causing various problems. Air pollution is particularly increasing various respiratory diseases in small children, which is a major concern for society. Rice and wheat are the most popular cultivation in India, which produced stubble. However, wheat stubble can be used as fodder for the cattle, but rice stubble is avoided as it has high silica content. To reduce the ever-increasing pollution, the stubble removing machine (SRM) is designed and developed for fully controlling the pollution due to the burning of paddy stubble. Earlier the only method to clear the agriculture land was to burn the paddy stubble after the harvesting or use machines designed for different applications. Burning of stubble creates a lot of harmful gases like COx ,NOx, and their derivatives. Various other machines were developed including stubble management system (SMS) and its higher version called super SMS but were not so promising according to their application procedure. The present developed machine works on the principle of cutting, collecting, and managing the paddy stubble and clears the fields instantaneously for the next crop and also vanishing the problem of pollution due to the burning of stubble. We propose a system-level solution for the same.

<u>Towards Row Sensitive DRAM Refresh through Retention Awareness</u>
T Goel, D Maura, K Goswami, S Das, DS Banerjee - 22nd International Symposium on Quality Electronic Design, 2021

**Abstract:** Dynamic Random Access Memory (DRAM) is the de-facto choice for main memories in modern day computing systems. It is based on capacitor technology, which is volatile in nature. Hence, these memories require periodic refreshing, usually at 64 ms, in order to ensure data persistence. Refreshing results in blocking of the memory device for performing normal read or write operations. However, it has been found that not all cells of the device requires uniform refreshing at 64 ms. Due to shrinking of technologies, deviations are observed in nominal parameters which causes variations in retention and restoration time. In this paper, we propose a retention aware DRAM refreshing model, which is operated in auto-refresh (AR) mode of a DRAM device. We call the proposed model Lightweight Retention Time Aware Refreshing, or simply LRAR, which can be operated either in a deterministic or an approximate mode while consuming a constant amount of hardware space. The former ensures consumption of least possible area in comparison to previously proposed works. While the latter is aimed to incorporate periodic refreshing for a newly emerged DRAM phenomenon called Variable Retention Time, or, VRT, which uses the basics of approximation. After extensive evaluation, we find that our proposed model reduces execution time of programs up to 11% (9.4% on average). The memory system's energy consumption is also reduced by an average of 11.5%, and refresh energy by an average of 73.6%. We achieve the aforementioned gains at a modest area overhead of 7,240µm<sup>2</sup> (0.0018% of a 400mm<sup>2</sup> die) and storage overhead.

Tuning polyoxometalate composites with carbonaceous materials towards oxygen bifunctional activity

TC Nagaiah, D Gupta, SD Adhikary, A Kafle, D Mandal - Journal of Materials Chemistry A, 2021

**Abstract:** Oxygen electrochemistry plays an imperative role in renewable energy systems. Development of non-precious metals and efficient bifunctional catalysts for the oxygen reduction reaction and oxygen evolution reaction (ORR & OER) is highly demanded for metal—air batteries. Herein, a conjugate of tetra-cobalt sandwich polyoxometalate  $[\text{Co}_4(\text{H}_2\text{O})_2(\text{PW}_9\text{O}_{34})_2]^{10-}$  (CoPOM) and polyvinyl butyl imidazolium (PVIM) (PVIM—CoPOM) supported on carbonaceous materials was explored as an oxygen bifunctional catalyst in alkaline media. The PVIM—CoPOM/NCNT composite is highly active towards ORR and OER. The novel composite exhibits a low overpotential  $(\eta_{j10})$  of 0.28 V vs. RHE for OER, outperforming the state-of-the-art RuO<sub>2</sub> catalyst (0.35 V), and a comparable ORR activity to Pt/C with similar overall oxygen electrode activity to the benchmark precious metal catalyst. A conventional Zn—air battery with the PVIM—CoPOM/NCNT air cathode shows high energy density and a low charge—discharge potential gap.

<u>Unruh-DeWitt detector responses for complex scalar fields in de Sitter spacetime</u> M Ali, S Bhattacharya, K Lochan - Journal of High Energy Physics, 2021

**Abstract:** We derive the response function for a comoving, pointlike Unruh-DeWitt particle detector coupled to a complex scalar field  $\phi$ , in the (3+1)-dimensional cosmological de Sitter spacetime. The field-detector coupling is taken to be proportional to  $\phi \dagger \phi$ . We address both conformally invariant and massless minimally coupled scalar field theories, respectively in the conformal and the Bunch-Davies vacuum. The response function integral for the massless minimal complex scalar, not surprisingly, shows divergences and accordingly we use suitable regularisation scheme to find out well behaved results. The regularised result also contains a de Sitter symmetry breaking logarithm, growing with the cosmological time. Possibility of extension of these results with the so called de Sitter  $\alpha$ -vacua is discussed. While we find no apparent problem in computing the response function for a real scalar in these vacua, a complex scalar field is shown to contain some possible ambiguities in the detector response. The case of the minimal and nearly massless scalar field theory is also briefly discussed.

<u>Use of Phase Change Materials for Energy-Efficient Buildings in India</u>
P Patil, KVS Teja, H Tyagi - New Research Directions in Solar Energy Technologies: Part of the Energy, Environment, and Sustainability book series, 2021

Abstract: A large amount of energy is being used worldwide to maintain the ambient temperature conditions inside buildings. Most of this energy is generated from the combustion of fossil fuels. Also, air conditioning units used in buildings emit harmful greenhouse gases. For these reasons, we must find some alternate passive designs that can be implemented for the conservation of energy within the premises. As phase change materials (PCM) have large energy storage capacity due to its high values of latent heats, PCMs can be efficiently used to reduce the surge in energy demands. Incorporating PCM within building components enhances their thermal heat capacity as well as improves the energy efficiency of the buildings. Numerous researchers are experimenting with PCMs for their use in energy-efficient buildings. In this study, numerical modeling has been carried out for a PCM incorporated model that can be used depending on different climatic zones in India. The dimensions and boundary conditions used in numerical modeling are kept near the realistic weather conditions in various climate zones. The PCM selection has been carried out by taking into consideration the desirable thermophysical properties, operating temperature, availability, and weather conditions in different locations. From the results, it can be concluded that this model is beneficial in reducing the cooling loads of buildings in extremely hot places as well as for decrementing the heating loads in cold weather zones.

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