3.4.5 Number of research papers per teacher in the Journals notified on UGC website during the last five years: 3.648

3.4.5.1: Number of research papers in the Journals notified on UGC website during the last five years: 421

Supporting Documents

S. No.	Documents	Page No.
1.	Number of research papers in the Journals notified on UGC website during 2019-2020	01-99

Hydrothermally Assisted Synthesis of Porous Polyaniline@Carbon Nanotubes–Manganese Dioxide Ternary Composite for Potential Application in Supercapattery

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Abstract: In this study, ternary composites of polyaniline (PANI) with manganese dioxide (MnO_2) nanorods and carbon nanotubes (CNTs) were prepared by employing a hydrothermal methodology and in-situ oxidative polymerization of aniline. The morphological analysis by scanning electron microscopy showed that the MnO_2 possessed nanorod like structures in its pristine form, while in the ternary PANI@CNT/MnO_2 composite, coating of PANI over CNT/MnO_2, rods/tubes were evidently seen. The structural analysis by X-ray diffraction and X-ray photoelectron spectroscopy showed peaks corresponding to MnO_2, PANI and CNT, which suggested efficacy of the synthesis methodology. The electrochemical performance in contrast to individual components revealed the enhanced performance of PANI@CNT/MnO_2 composite due to the synergistic/additional effect of PANI, CNT and MnO_2 compared to pure MnO_2, PANI and PANI@CNT. The PANI@CNT/MnO_2 ternary composite exhibited an excellent specific capacity of 143.26 C g^{-1} at a scan rate of 3 mV s^{-1}. The cyclic stability of the supercapattery (PANI@CNT/MnO_2/activated carbon)—consisting of a battery type electrode—demonstrated a gradual increase in specific capacity with continuous charge–discharge over ~1000 cycles and showed a cyclic stability of 119% compared to its initial value after 3500 cycles.

Keywords: conducting polymer; polyaniline; MnO_2; CNT; supercapattery; energy storage device

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RESEARCH ARTICLE

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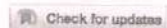
Copper oxide nanoparticles for the removal of divalent nickel ions from aqueous solution

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ABSTRACT

This study focused on the synthesis of copper oxide (CuO) nanoparticles by chemical precipitation method for the uptake of divalent nickel ions from aqueous media. The adsorption capacity was 15.4 mg/g under optimum conditions. The kinetic models were applied to find out the mechanism for the removal of nickel ions. The study indicated that the optimum conditions for nickel sequestration were pH = 7.0, initial concentration = 100 mg/L, nanoparticle dose = 0.2 g/L, contact time = 90 min, temperature = 26 ± 1 °C and rpm = 180. These results could be useful for the sequestration of Ni(II) ions from wastewater.

1. Introduction

Copper, chromium, cadmium, cobalt, zinc, lead, nickel, arsenic, and iron are the commonly occurring heavy metals in the industries and are toxic even at low concentrations (Anitha et al. 2015). Whereas, the heavy metals like copper, zinc, nickel, boron, iron, molybdenum are required in trace amounts in the form of micronutrients for the proper growth of the human beings and plants (Vardhan et al. 2019). But, if consumed in concentrations beyond permissible limits, they could be harmful as they are non-biodegradable and are quickly absorbed in human body through food chain (Kiruba et al. 2014). Nickel is a toxic heavy metal that is both environmentally and occupationally unsafe. It is a carcinogen, an embryotoxin and a teratogen. It causes various kind of ailments in human beings such as vomiting, nausea, headache, tightness in the chest, dizziness, dry cough, shortness of breath, chest pain, developmental effects in children, rapid respiration, cyanosis etc. (Pandey et al. 2007). Nickel causes nickel hypersensitivity in kids, particularly in developed countries (Vardhan et al. 2019). Its fumes cause irritation to respiratory system leading to pneumonitis and fibrosis (ATSDR 2005, Atkovska et al. 2018). Liver and kidney are also affected on exposure to nickel. A rare skin disease called dermatitis (nickel itch) is caused in humans due to contact with nickel and its compounds (WHO 2005).

Various industrial processes such as electroplating of nickel, ceramic industry, Ni-Cd batteries, stainless steel, catalysts and other chemicals, coinage, magnets, jewelry, foundry products, alloys, paint etc. are responsible for discharge of nickel in ambient environment (Jain et al. 2014). Nickel is found in the effluent of electroplating industry between the concentrations of 20–500 ppm. Maximum permissible limit for the discharge of Ni(II) containing effluent is 0.1 mg/L (Environment Protection (standards for effluent discharge) Regulation 2003). Nickel occurs as $Ni(H_2O)_6^{2+}$ ion in natural waters at pH ranging from 5.0 to 9.0 (WHO 2005).

Nickel laden wastewater can be treated using diverse conventional techniques such as chemical precipitation, chemical oxidation or reduction, electrochemical treatment, ion exchange, membrane filtration, solvent extraction, electrodialysis and adsorption (Jain et al. 2014, Nithya et al. 2018). However, these techniques are expensive and not effective. Hence, there is a need to search other suitable methods for the efficient uptake of heavy metals like nickel from wastewaters. Adsorption is one such method that can solve this problem because it is simple, cheaper, ecofriendly and no byproducts are released

Nanofillers-induced modifications in microstructure and properties of PBAT/PP blend: Enhanced rigidity, heat resistance, and electrical conductivity

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ARTICLE INFO

ABSTRACT

Carbon nanotube (CNT) and organoclay (15A) were introduced separately and simultaneously into the poly(butylene adipate-co-terephthalate) (PBAT)/polypropylene (PP) blend to fabricate PBAT-based nanocomposites with maleated PP played as a compatibilizer. SEM and TEM analyses confirmed the CNT and 15A were predominantly distributed in the PBAT matrix and in the dispersed PP phase, respectively. Addition of sole CNT or 15A developed a quasi-co-continuous PBAT-PP morphology. CNT assisted the nucleation for both PBAT and PP crystallization, while 15A facilitated the nucleation for PP only. The heat distortion temperature of the blend increased 20 °C at 3-phr CNT loading. Adding hybrid fillers of CNT and 15A improved Young's modulus and flexural modulus by up to 35% and 144%, respectively, compared with those of the parent blend. The impact strength increased by up to 33% after 2-phr CNT loading. The electrical resistivity of the blend reduced by more than 9 orders at 3-phr CNT loading.

1. Introduction

Polymer blends and composites are continuously drawing scientific and technical research interests owing to their potential in achieving superior properties compared with those of neat constituents. Hitherto, various polymer blends and composites designed with high performance are commercially available. As one of the commodity plastics that possess excellent processability and comprehensive properties, polypropylene (PP) has numerous applications, such as packaging, automobile parts, household appliances, textile fibers, and medical apparatus [1–3]. Nevertheless, the increase in the consumption of long life PP-based products has made them a solid waste management problem. In the past two decades, attempts were made to mitigate this problem and reduce the amount of PP used. One of the feasible approaches is to manufacture the blends/composites of PP with eco-friendly biodegradable polymers, such as poly(butylene succinate) (PBS), poly(lactic acid) (PLA) and so on [4–8].

Poly(butylene adipate-co-terephthalate) (PBAT), a copolymer of butylene adipate (BA) and butylene terephthalate (BT), is an emerging biodegradable polymer. It exhibits high impact strength and offers good mechanical properties similar to those of polyethylene. Thus, PBAT is a promising alternative material to several commodity plastics [9,10]. However, its high price has restricted its marketability. To extend its versatility and lower its cost, PBAT-based blends/composites were prepared and investigated [11–13]. Recently, Nakayama et al. [11] studied the properties of PBAT/PLA blends and composites with the presence of joncryl compatibilizer and silk fibroin powder. They reported that the processability and rigidity of PBAT significantly increased after the development of blends and composites. Moustafa et al. [13]. prepared and characterized PBAT composites filled with coffee grounds powder in the presence of poly(ethylene glycol) as a plasticizer. The hydrophobicity declined, and changes in thermomechanical properties of the prepared samples were revealed. In addition to the biodegradable polymers, commodity PP will be an ideal counterpart for fabricating PBAT blends and blend-based composites to improve the mechanical properties and effectively reduce the cost of PBAT.

The properties of polymer blends can be further enhanced by the incorporation of nanofillers to obtain blend-based nanocomposites [4,14–16]. Among the commercially available nanofillers, carbon nanotube (CNT) and organoclay have drawn the interest of researchers owing to their potential in imposing synergistically improved properties for polymer matrices. The first CNT-added polymer nanocomposite was fabricated and studied by Ajayan et al. [17]. Meanwhile, the most promising pioneering work in fabricating polymer nanocomposites with organoclay as nanofiller was conducted on polyamide system by

Dr. DINESH K. VERMA

Article

Synergistic Tribo-Activity of Nanohybrids of Zirconia/Cerium-Doped Zirconia Nanoparticles with Nano Lamellar Reduced Graphene Oxide and Molybdenum Disulfide

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Abstract: Zirconia and 10%, 20%, and 30% cerium-doped zirconia nanoparticles (ZCO), ZCO-1, ZCO-2, and ZCO-3, respectively, were prepared using auto-combustion method. Binary nanohybrids, ZrO_2@rGO and ZCO-2@rGO (rGO = reduced graphene oxide), and ternary nanohybrids, ZrO_2@rGO@MoS_2 and ZCO-2@rGO@MoS_2, have been prepared with an anticipation of a fruitful synergic effect of rGO, MoS_2, and cerium-doped zirconia on the tribo-activity. Tribo-activity of these additives in paraffin oil (PO) has been assessed by a four-ball lubricant tester at the optimized concentration, 0.125% w/v. The tribo-performance follows the order: ZCO-2@rGO@MoS_2 > ZrO_2@rGO@MoS_2 > ZCO-2@rGO > ZrO_2@rGO > MoS_2 > ZrO_2 > rGO > PO. The nanoparticles acting as spacers control restacking of the nanosheets provided structural augmentation while nanosheets, in turn, prevent agglomeration of the nanoparticles. Doped nanoparticles upgraded the activity by forming defects. Thus, the results acknowledge the synergic effect of cerium-doped zirconia and lamellar nanosheets of rGO and MoS_2. There is noncovalent interaction among all the individuals. Analysis of the morphological features of wear-track carried out by scanning electron microscopy (SEM) and atomic force microscopy (AFM) in PO and its formulations with various additives is consistent with the above sequence. The energy dispersive X-ray (EDX) spectrum of ZCO-2@rGO@MoS_2 indicates the existence of zirconium, cerium, molybdenum, and sulfur on the wear-track, confirming, thereby, the active role played by these elements during tribofilm formation. The X-ray photoelectron spectroscopy (XPS) studies of worn surface reveal that the tribofilm is made up of rGO, zirconia, ceria, and MoS_2 along with Fe_2O_3, MoO_3, and SO_4^{2-} as the outcome of the tribo-chemical reaction.

Keywords: doped nanoparticles; nanohybrids; X-ray photoelectron spectroscopy; friction; wear; tribo-activity

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Dielectric Relaxation Behavior of Silver Nanoparticles and Graphene Oxide Embedded Poly(vinyl alcohol) Nanocomposite Film: An Effect of Ionic Liquid and Temperature

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Abstract: This paper presents the dielectric characteristics of nanocomposite films of poly(vinyl alcohol) (PVA) embedded with silver (Ag) nanoparticles and graphene oxide(GO). The nanocomposite films were fabricated by using the solvent casting approach. The morphological analysis was carried out through scanning electron microscopy (SEM) and transmission electron microscopy (TEM). The dielectric relaxation behavior of nanocomposite films was analyzed in the frequency range of 10^1 to 10^6 Hz, by varying GO loading. The temperature effect was investigated over the temperature range of 40 to 150 °C. The effect of ionic liquid (IL) was also explored by comparing the dielectric behavior of films fabricated without using ionic liquid. The conductive filler loading variation showed a significant effect on dielectric permittivity(ε'), complex impedance (Z^*) and electric conductivity (σ_{ac}). The obtained results revealed that the dielectric permittivity (ε') increased by incorporating Ag nanoparticles and increasing GO loading in PVA matrix. An incremental trend in dielectric permittivity was observed on increasing the temperature, which is attributed to tunneling and hopping mechanism. With an increase in nanofiller loading, the real part of impedance (Z') and imaginary part of impedance (Z'') were found to decrease. Further, the semicircular nature of Nyquist plot indicated the decrease in bulk resistivity on increasing GO loading, temperature and incorporating ionic liquid. On the basis of above findings, the obtained GO-Ag-PVA nanocomposite films can find promising applications in charge storage devices.

Keywords: dielectric permittivity; graphene oxide; poly(vinyl alcohol); polymer nanocomposite

1. Introduction

Nanocomposites play an important role in the technological advancement of the 21st century. Nanocomposite is a multiphase material made up of matrix phase and the reinforcing phase, having enhanced thermal, mechanical, electrical, optical properties, as compared to individual phases. Due to the versatile nature of nanocomposites, they find numerous potential applications in various fields. [1–4]. Polymer nanocomposites are the combination of polymers as the matrix phase and the nanofillers like carbon-based nanoparticles, metal nanoparticles, etc. [5–7]. Polymer nanocomposites have attracted great interest of scientific communities due to their encouraging properties and widened applications, such as conductive coatings, sensors, energy storage devices, microwave

Cellulose Nanocrystal Reinforced Chitosan Based UV Barrier Composite Films for Sustainable Packaging

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Abstract: In this study, green composite films based on cellulose nanocrystal/chitosan (CNC/CS) were fabricated by solution casting. FTIR, XRD, SEM, and TEM characterizations were conducted to determine the structure and morphology of the prepared films. The addition of only 4 wt.% CNC in the CS film improved the tensile strength and Young's modulus by up to 39% and 78%, respectively. Depending on CNC content, the moisture absorption decreased by 34.1–24.2% and the water solubility decreased by 35.7–26.5% for the composite films compared with neat CS film. The water vapor permeation decreased from 3.83×10^{-11} to 2.41×10^{-11} gm^{-1} s^{-1} Pa^{-1} in the CS-based films loaded with (0–8 wt.%) CNC. The water and UV barrier properties of the composite films showed better performance than those of neat CS film. Results suggested that CNC/CS nanocomposite films can be used as a sustainable packaging material in the food industry.

Keywords: nanocomposite; chitosan; cellulose nanocrystal; UV barrier; mechanical properties

1. Introduction

Petrochemical-based polymeric materials are extensively used in various applications ranging from packaging materials to aircraft components. The broad application of these materials had led to severe environmental challenges due to improper disposal in the environment. In this regard, researchers have focused on biodegradable sustainable packaging materials from scientific and technical sectors [1–3]. Hence, bio-based packaging materials based on polysaccharides, proteins, and lipids are increasingly used [4,5]. However, the inferior mechanical and poor barrier properties of natural polymers often hinder their application in food packaging. Reinforcing nanofillers are incorporated into biopolymer formulations to effectively enhance their thermal and physio-chemical properties and fabricate high-performance polymer nanocomposite films [6–8]. Nanocomposite films can also serve as water and UV light barriers to improve the shelf-life and quality of preserved food products [9].

Chitosan (CS) is a natural cationic polysaccharide containing numerous reactive amino groups (β-1,4-linked glucosamine and N-acetylglucosamine) that can participate in several chemical reactions [10,11]. CS is yielded by the partial deacetylation (to varying degrees) of chitin, which is the second most abundant naturally occurring polysaccharide next to cellulose. CS is very useful in various fields, such as food, agriculture, and wastewater treatment [12]. CS can also be applied to prevent the dehydration of meat, which is the most important diet to sustain human life [13].

Polyamide 6/Poly(vinylidene fluoride) Blend-Based Nanocomposites with Enhanced Rigidity: Selective Localization of Carbon Nanotube and Organoclay

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Abstract: Polyamide 6 (PA6)/poly(vinylidene fluoride) (PVDF) blend-based nanocomposites were successfully prepared using a twin screw extruder. Carbon nanotube (CNT) and organo-montmorillonite (30B) were used individually and simultaneously as reinforcing nanofillers for the immiscible PA6/PVDF blend. Scanning electron micrographs showed that adding 30B reduced the dispersed domain size of PVDF in the blend, and CNT played a vital role in the formation of a quasi-co-continuous PA6-PVDF morphology. Transmission electron microscopy observation revealed that both fillers were mainly located in the PA6 matrix phase. X-ray diffraction patterns showed that the presence of 30B facilitated the formation of γ-form PA6 crystals in the composites. Differential scanning calorimetry results indicated that the crystallization temperature of PA6 increased after adding CNT into the blend. The inclusion of 30B retarded PA6 nucleation (γ-form crystals growth) upon crystallization. The Young's and flexural moduli of the blend increased after adding CNT and/or 30B. 30B exhibited higher enhancing efficiency compared with CNT. The composite with 2 phr 30B exhibited 21% higher Young's modulus than the blend. Measurements of the rheological properties confirmed the development of a pseudo-network structure in the CNT-loaded composites. Double percolation morphology in the PA6/PVDF blend was achieved with the addition of CNT.

Keywords: polyamide 6; poly(vinylidene fluoride); blend; nanocomposites; physical properties

1. Introduction

Polymer blends filled with nanofillers have attracted considerable attention in academia and in the industry because of their superior properties compared with conventional blends. Polyamide 6 (PA6) is an essential crystalline engineering plastic with good chemical stability, high strength, excellent wear resistance, and oil resistance. The crystal structures in PA6 are mainly α- and γ-morphism [1–4]. The α-form is composed of a fully extended planar zigzag chain conformation, while the γ-form consists of pleated sheets of parallel chains joined by hydrogen bonds [5]. The polar functional groups (amide) of PA6 tend to absorb moisture, resulting in poor stability after prolonged exposure to air environment. Poly(vinylidene fluoride) (PVDF), another crystalline engineering plastic, possesses high mechanical strength, excellent thermal/chemical stability, and good hydrolysis resistance and weatherability [6,7]. PVDF has five distinct polymorphs (α, β, γ, δ, ε). The polar β-structure-induced piezo- and pyroelectric characteristics of PVDF allows for applications in sensors and actuators [8,9].
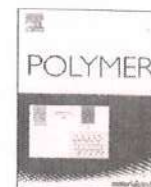
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Enhanced thermal stability, toughness, and electrical conductivity of carbon nanotube-reinforced biodegradable poly(lactic acid)/poly(ethylene oxide) blend-based nanocomposites

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ARTICLE INFO

ABSTRACT

Carbon nanotube (CNT) was incorporated into the miscible poly(lactic acid)/poly(ethylene oxide) (PLA/PEO) blend to successfully fabricate biodegradable nanocomposites. Scanning electron microscope images revealed the well dispersion of as-received CNT within the blend through the melt-mixing process. Thermogravimetric analysis showed that the CNT significantly improved the thermal stability of the blend (up to 68 °C increase at 3-phr CNT addition compared to the blend at 10 wt% loss) in air. Differential scanning calorimetry data showed the nucleation effect of CNT on the crystallization of individual PLA and PEO; the presence of CNT increased the melting temperature of PLA crystals. Measurement of rheological behavior confirmed the formation of CNT (pseudo-)network structure in the composites. The impact strength of the composite with 3-phr CNT loading was three times higher than that of the blend. The electrical resistivity of the blend reduced by up to nine orders of magnitude at 3-phr CNT loading. The electrical and rheological percolation thresholds were both achieved at 1-phr CNT loading for the nanocomposites.

1. Introduction

Polymer-based (nano)composites have received significant interest in academia and industry during the last three decades [1,2]. Different mixtures of polymer matrices and nanofillers were designed to study their potential in enhancing the thermal stability, flame retardance, electrical and mechanical properties of their neat polymers with the least addition of nanofillers [3–5]. Among the nanofillers widely studied, carbon nanotube (CNT) is one of the candidates that may evidently improve the performance of parent components. A low concentration of CNT (ca. <3 wt%) can drastically increase the electrical and thermal conductivity of the polymer matrices, given that CNT has excellent conductivity and large aspect ratio [6,7]. The conductivity of CNT-loaded nanocomposites depends on the tunneling regions between CNT rather than the physical networking of CNT.

Considering economic growth, non-renewable and petroleum-based chemical consumption of polymers in various applications has caused considerable environmental pollution calamity. In recent years, environment-friendly biodegradable polymers have been extensively investigated and validated as excellent materials for the substitution of conventional polymers to alleviate environmental issues [8–10]. Poly (lactic acid) (PLA) is a bio-based/biodegradable polymer that shows promising stiffness comparable to some commodity plastics [11]. PLA also possesses good transparency, oil resistance, and low toxicity. It is used in various applications, including drug delivery, tissue engineering, food packaging, and bottle container [10,12,13]. However, PLA has distinctive deficiencies, such as low flexibility, brittleness, poor thermo-mechanical properties, and slow crystallization rate that restrict its further applications. To overcome these disadvantages and retain PLA biodegradability, studies have been carried out to manufacture the PLA blends with biodegradable counterparts, such as poly(butylene succinate), poly(ε-caprolactone), and poly(ethylene oxide) (PEO) [14–17]. For the same reason, PLA-based (nano)composites have been fabricated and examined to increase the versatility of PLA [18–23]. The crystallization rate and crystallinity of PLA in the blends and composites indeed play significant roles in determining the properties and

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Synthesis, thermal, photo-physical, and biological properties of mononuclear Yb^{3+}, Nd^{3+}, and Dy^{3+} complexes derived from Schiff base ligands

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ABSTRACT

Six new lanthanide complexes, $[Ln(NO_3)_2(L_1H_2)](NO_3).xCHCl_3.yH_2O$ $\{Ln = Yb$ (1), $x = 1$, $y = 2$; Nd (3), $x = 2$, $y = 3$ and Dy (5), $x = 2$, $y = 2\}$ and $[Ln(NO_3)_2(L_2H_2)](NO_3).xCHCl_3$ $\{Ln = Yb$ (2), $x = 1$; Nd (4), $x = 2$ and Dy (6), $x = 2\}$, were prepared by NNNOO-donor pentadentate Schiff base ligands N,N'-bis(3-methoxysalicylidene)$-2,2'$-diaminoethylamine (L_1H_2) and N,N'-bis(2-hydroxynaphthalidene)$-2,2'$-diaminoethylamine (L_2H_2). These synthesized complexes were characterized by elemental analysis, FT-IR, ^{1}H NMR, UV-vis spectroscopy, and mass spectrometry. The thermal characteristics of complexes were studied by TGA technique. The observation of the fluorescence emission properties of ligands L_1H_2 and L_2H_2 and its Ln(III) complexes in DMSO solution at excitation wavelength of 320 nm shows that the ligands favor energy transfers to the emitting energy level of Ln(III) complexes. The computational calculations using density functional theory of ligands and its Yb((III) complexes were performed to obtain optimized molecular geometry, the highest occupied molecular orbital, the lowest unoccupied molecular orbital and other parameters. The Schiff bases, metal salts, and its Ln(III) complexes were screened for their in vitro antibacterial studies against Staphylococcus aureus, Enterococcus faecalis, Escherichia coli, and Salmonella typhi bacterial strains. The results of the antibacterial investigation show that the lanthanide complexes possess more potent bactericide properties than ligands and metal salts.

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Dr. Mitesh Jaiswal

Antimony(III) complexes with N-phenylthiourea derivative ligands: Design, Synthesis, Characterization and Computational studies

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Abstract: The reactions of antimony(III)chloride with N-phenylthiourea derivative ligands gives antimony(III) complexes of type, $[SbCl_2L]$. The reaction was performed in 1:1 molar ratio. The newly synthesized complexes were characterized by melting point, elemental analysis, FT-IR, UV–Vis, ^1H and ^{13}C NMR spectroscopy and Mass spectrometry. The computational calculations using density functional theory (DFT) of ligands and complexes were also performed to obtained optimized molecular geometry, the highest occupied molecular orbital (HOMO), the lowest unoccupied molecular orbital (LUMO) and other parameter. The spectroscopic data and computational studies suggest five coordination around antimony atom.
Keywords: Antimony(III) complex, N-phenylthiourea, DFT, HOMO-LUMO energy.
Graphical Abstract. The ground state optimized geometry of antimony(III) complex

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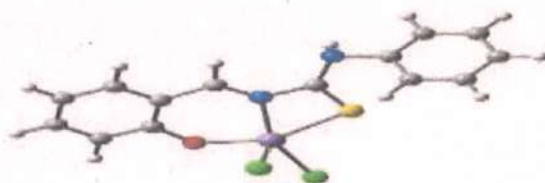
Research paper

An experimental and theoretical investigation of lanthanide complexes [Ln = Nd, Yb, Eu, Dy and tb] with 4-((2-hydroxy-naphthalen-1-yl) methylene amino)benzenesulfonamide ligand

Sikandar Paswan[a], Nitesh Jaiswal[b], Vishnu Kumar Modanawal[a], Manoj Kumar Patel[a], Rana Krishna Pal Singh[a,*]

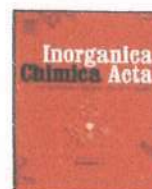[a] Synthetic Inorganic and Metallo-Organic Research Laboratory, Department of Chemistry, University of Allahabad, Prayagraj 211002, Uttar Pradesh, India
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ABSTRACT

Reaction of lanthanide(III) salts with N, O donors 4-((2-hydroxynaphthalen-1-yl) methyleneamino)benzenesulfonamide (L) Schiff base ligand afforded five new mononuclear lanthanide complexes of type $[Ln(NO_3)_2(L)(H_2O)_2](H_2O)_x$ {where Ln = Nd (1), x = 2, Yb (2), x = 1, Eu (3), x = 2, Dy (4), x = 1, Tb (5), x = 2}. These newly synthesized complexes were characterized by elemental analysis, molar conductance, FT-IR, UV–Vis spectroscopy and mass spectrometry. The thermal behavior of complexes was studied by TGA technique. The computational calculations using density functional theory (DFT) of ligand and their lanthanide complexes were performed to obtain optimized molecular geometry, the highest occupied molecular orbital (HOMO), the lowest unoccupied molecular orbital (LUMO) and other parameters. The fluorescence studies reveal that emission spectra of lanthanide complexes show the characteristic luminescence due to lanthanide ions which indicates that Schiff base ligand can sensitize the Ln(III) ions. The Schiff base and their lanthanide complexes were screened for their in vitro antibacterial studies against Escherichia coli (ATCC 25922), Staphylococcus aureus (ATCC 29213), Klebsiella pneumoniae (BAA 1705), Acinetobacterr baumannii (BAA 1605) and Pseudomonas aeruginosa (ATCC 27853). The results exhibit that the antibacterial activity of Ln(III) complexes was greater than the free Schiff base ligand.

1. Introduction

The growing demand of luminescent materials for different societal applications has been witnessed in recent times. The luminescence and magnetic features of lanthanide complexes motivated the researcher for its exploration. The design and synthesis of lanthanide complexes with organic ligands including Schiff bases emerged as an important research area in recent times [1–4]. The existence of long-lived excited states of trivalent lanthanide ions (Ln^{3+}) produces the luminescence properties in lanthanide complexes. These photophysical properties of lanthanide complexes could be tuned and enhanced with the help of rationally designed ligands. The emerging interest of chemists towards research in the lanthanide complexes is due to their interesting structures [5,6] and a wide range of potential applications in biological sectors, catalysis, luminescence and magnetic properties [7–10].

Sulfonamides were the first drugs used as preventive and therapeutic agents against different diseases [11–14]. Sulfur donor Schiff base ligands play an important role in metal coordination chemistry due to its important biological properties including antibacterial, anti-toxicity, antifungal and antitumor properties [15,16]. The biological activities of metal complexes in several cases improved significantly on the addition of sulfonamide derivative ligands to metal salts rationally. The metal complexes of sulfonamide derivatives ligands have shown significant potential against cancer cell lines and other biological activities [17]. The interesting coordination chemistry of lanthanide metals with N, O donor Schiff base ligands and their applications in different scientific areas including chemical, medical and industrial sectors make enough for their importance and fascinate the chemist for the synthesis of new complexes [18].

Due to the above promising facts and our continued interest [19], an attempt was made to investigate the synthesis, characterization and antimicrobial properties of lanthanide (III) Schiff base complexes of

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Amino Borate-Functionalized Reduced Graphene Oxide Further Functionalized with Copper Phthalocyanine Nanotubes for Reducing Friction and Wear

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ABSTRACT: Covalent functionalization of graphene oxide (GO) was performed by 2-aminoethyl diphenyl borate (ADB) to overcome the demerits of plain GO/reduced GO (rGO) during lubrication such as the agglomeration and restacking of nanosheets, poor dispersibility in the base lube, poor adhesion to the steel surface, inadequate friction and wear-reducing characteristics, and last abysmal load-carrying ability. ADB was deliberately chosen to outreach the benefits of the enhanced lubrication by in situ formed boron nitride during tribological testing due to boron–nitrogen synergy. Nucleophilic attack of the $-NH_2$ group of ADB opened epoxide rings of GO, forming $-NH-C-C-OH$ and simultaneously reducing GO to rGO. The product, therefore, is represented as ADB–rGO. For the betterment of lubricity, further noncovalent functionalization was also considered using triboactive phthalocyanine (Pc) or copper(II) phthalocyanine (CuPc). Based on the results of molecular dynamics and tribological tests in paraffin oil (PO), CuPc was preferred over Pc. Configurations of the adsorbate CuPc on the surface reveal that CuPc tends to fold/unfold upon adsorption. Thus, the CuPc nanotubes (NTs) were used for the noncovalent functionalization of ADB–rGO. The techniques FTIR, p-XRD, SEM/HR-SEM, TEM/HR-TEM, EDX, and XPS were applied to characterize the additives. The tribological activity of different additives evaluated on a four-ball tester based on ASTM D4172 and ASTM D5183 tests reveals the order for antiwear/antifriction efficiencies and reduction in wear rates as CuPc–(ADB–rGO) > CuPc NTs > Pc > ADB–rGO > GO > PO. Thus, CuPc–(ADB–rGO) overpowered the demerits of GO. The morphology of the surface lubricated with GO, ADB–rGO, was studied using SEM and AFM (contact mode). EDX analysis of the steel surface in the presence of CuPc–(ADB–rGO) divulges the additional elements boron, nitrogen, and copper in the in situ formed tribofilm, highlighting their active role in improving the tribological activity. XPS studies of the tribofilm show boron nitride, boron oxide, iron oxides, cupric oxide, and graphitic compounds. The synergic performance of layered structures rGO, CuPc, and in situ formed boron nitride validated the spectacular tribological performance of CuPc–(ADB–rGO).

KEYWORDS: CuPc MD simulations, covalent and noncovalent functionalized reduced graphene oxide, nanotubes, antiwear lubricant additives, boron nitride
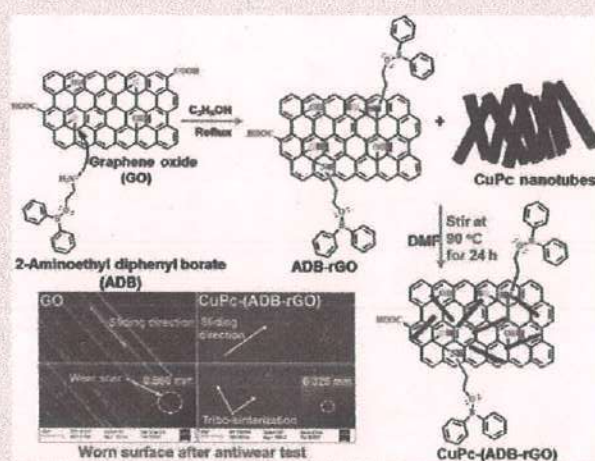
1. INTRODUCTION

Friction and wear are inherently inimical to the mechanical systems. The proximity of the rubbing surfaces in such systems eventually brings disastrous effects to the machine components. A lubricant is imposed between the rubbing surfaces to curb the menace of friction and wear. Antiwear and antifriction additives are blended with the base lubricant for promoting lubrication.[1–3] These additives are generally conventional organic compounds[2–7] or nanomaterials.[8–11] Nanomaterials, mainly inorganic nanoparticles,[8] nanosheets,[9–11] and carbon-based materials,[9–15] are well-acknowledged in the field of

tribology because their fast action at the interface increases the efficiency and their high chemical stability reduces emissions. Carbon-based materials, including graphene,[9–11] fullerenes,[12] carbon nanotubes (CNTs),[13] and carbon spheres,[14,15] are

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Original Article

Tribological activity of ionic liquid stabilized calcium-doped ceria nanoparticles

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Rashmi B Rastogi[1]

Abstract

10% Calcium-doped ceria (CCO) nanoparticles have been synthesized by sol–gel method. Their surface has been modified by surfactants, sodium dodecyl sulfate and 1-decyl-3-methyl imidazolium bis(trifluoromethyl sulfonyl) imide to yield SCCO and IL-CCO respectively. Powder X-ray diffraction patterns of nanoparticles and surface modified nanoparticles are indicative of cubic phase of ceria. Fourier transform infrared spectra confirm the surface modification of nanoparticles, particularly with ionic liquid. Morphology of the as-prepared nanoparticles investigated by field emission scanning electron microscopy, transmission electron microscopy/high-resolution transmission electron microscopy reveals that there is decrease in size of nanoparticles from CCO followed by SCCO and then IL-CCO. Wrapping of nanoparticles by ionic liquid is apparent in the scanning electron microscopy (SEM) and transmission electron microscopic (TEM) images. The tribological activity of the well-characterized nanoparticles has been evaluated at the optimized concentration, 0.2% w/v in paraffin oil under ASTM D4172 and ASTM D5183 test conditions using a four-ball tester. Based on tribological parameters, mean wear scar diameter, average friction coefficient, load-carrying capacity, and loss of frictional power, their relative performance followed the order – IL-CCO > SCCO > CCO. Worn surface analysis by scanning electron microscopy/energy-dispersive X-ray spectroscopy, atomic force microscopy corroborated the tribological performance. The order of the activity could be correlated with the size of the nanoparticles. Moreover, lubricating properties of ionic liquid have been instrumental for the exalted activity of IL-CCO. The presence of heteroatoms of ionic liquid, nitrogen, oxygen, fluorine, sulfur along with calcium and cerium of nanoparticles in energy-dispersive X-ray (EDX) spectroscopy analysis of the wear scar surface lubricated with IL-CCO confirms the vital role of ionic liquid towards the tribological activity.

Keywords

Nanoparticles, surface modification, ionic liquid, triboactivity, surface analysis

Introduction

Ionic liquids, possessing inherent polar character, are mainly considered as green solvents due to extremely low vapor pressure and almost nonvolatile behavior.[1] Because of high thermal and chemical stability, ionic liquids themselves may be used as synthetic lubricants. Since these are expensive chemicals, it is better to use them as an additive to a base lubricant rather than as lubricant itself.[2,3] Some reports are available in literature where ionic liquids have been used for functionalization of graphene,[4,5] stabilization of nanoparticles/quantum dots/carbon nanotubes.[6–11] Properties of ionic liquids may be regulated by selection of appropriate cation or anion in ionic liquid. Several ionic liquids, cation based like imidazolium, ammonium, pyridinium, phosphonium[12–21] etc.,

anion based such as tetrafluoro borate $[BF_4]^-$, hexafluoro phosphate $[PF_6]^-$, [Sulfonate], (trifluoromethylsulfonyl) imide $[Tf_2N]^-$, (2-ethylhexyl) phosphate [DEHP], etc. and mixed ionic liquid have been used in the field of tribology.[2]

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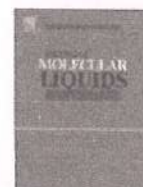
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Ionic liquid stabilized Ag@C composite for improvement of triboactivity

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ARTICLE INFO

ABSTRACT

Synthesis of carbon spheres and their composite Ag@C was accomplished by the hydrothermal method. The composite Ag@C was stabilized by the ionic liquid, 1-decyl 3-methyl imidazolium boron tetrafluoride (DMIM BF_4) to yield (IL-Ag@C). The Fourier Transform Infrared(FT-IR) spectra approved the formation of composites. The powder XRD patterns of the composites matched with JCPDS files. Examination of morphological characteristics of Ag@C by scanning electron microscopy/high-resolution scanning electron microscopy(SEM/HR-SEM), transmission electron microscopy/high-resolution transmission electron microscopy(TEM/HR-TEM) revealed spherical nanoparticles of about 30-40 nm size embedded on carbon spheres of 1.2-1.6 μm. Upon addition of ionic liquid, the composite appears to be wrapped in it. Energy-dispersive X-ray(EDX) analysis associated with SEM exhibited the presence of additional elements of ionic liquid, fluorine and nitrogen, besides silver and carbon in IL-Ag@C confirming its formation. The binding energy data obtained from X-ray photoelectron spectroscopy (XPS) corroborated the formation of IL-Ag@C. Triboactivity of the carbon nanospheres and the composites were assessed in base lube PEG-200 at 0.5% w/v concentration on a four-ball tester under ASTM D4172 and ASTM D5183 conditions. Based on tribological data namely coefficient of friction(COF), mean wear scar diameter(MWD), load-carrying capacity and loss of frictional power, the relative order of activity of different additives could be established as:

IL—Ag@C > Ag@C > IL > C spheres > PEG—200

The above order was authenticated by morphological studies of the wear scar by SEM and AFM(Atomic Force Microscopy) techniques. The EDX analysis of the wear scar surface lubricated with IL-Ag@C showed iron also in addition to the constituent elements of the composite. Thus, active participation of the adsorbed additive towards tribofilm formation is validated. The XPS studies of the same surface, further confirm the presence of boron nitride, boron carbide along with iron oxide. These boron compounds have, indeed, enriched the tribofilm for improved triboactivity.

1. Introduction

Ionic liquids are a class of organic compounds that exist as liquids at room temperature. They possess distinctive properties such as non-volatility, innate polarity and high chemical and thermal stability. These are referred to as green solvents owing to negligible vapour pressure. Therefore, ionic liquids find pertinence in synthetic chemistry, specifically nanostructures. Enormous applications of ionic liquids have been realized in various fields, in general, but catalysis [1–3] and lubrication, in particular. In the field of lubrication, these have been used as base lubricants [4–6] or as additives to the lubricants [7–9]. Their applications in amelioration of lubricating behaviour of the nanomaterials, for example, functionalization of graphene [10–12], stabilization of the

surface of metal nanoparticles/quantum dots [13–16] and metal nanoparticles-carbon nanotubes hybrid leading to a reduction in size and change in their morphology, etc. are pivotal in making them the most captivating materials of research today.

Carbonaceous materials in the form of graphene oxide [17–19], graphene [20–23] or carbon nanotubes [24,25] have been widely acknowledged as antifriction and antiwear lubricant additives. On the other hand, as per literature reports, carbon spheres though appropriate for rolling action, have been sparsely studied. The main impediment in their frequent use is distortion in their shape under working conditions. Since metal nanoparticles have been invariably employed as friction and wear modifiers to the base oil, it appears fascinating to invigorate carbon spheres by nanoparticles. Considering the high thermal conductivity of copper, we have reported Cu@C possessing excellent triboactivity [26]. H. Song et al. have considered low shear strength and high ductility of environmentally benign silver nanoparticles to

Ternary Composite of Methionine-Functionalized Graphene Oxide, Lanthanum-Doped Yttria Nanoparticles, and Molybdenum Disulfide Nanosheets for Thin-Film Lubrication

Nivedita Shukla, Dinesh K. Verma, Alok K. Singh, Bharat Kumar, Kavita, and Rashmi B. Rastogi*

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ABSTRACT: For enhancement of the tribological activity of nanolamellar graphene oxide (GO), its nucleophilic substitution was performed by methionine to yield methionine-functionalized reduced graphene oxide (M-rGO). Further, noncovalent functionalization of another tribo active material, nanolamellar MoS_2, was accomplished by lanthanum (7%)-doped yttria nanoparticles (NPs), resulting in the formation of a nanocomposite, (La-Y_2O_3)-MoS_2. The doped NPs were deliberately chosen for this purpose because there was a clear increase in the wear/friction-reducing tendencies of yttria after doping with lanthanum. For further advancement of the tribological activity, a ternary nanocomposite (La-Y_2O_3)-MoS_2-(M-rGO) was synthesized con-

taining lanthanum-doped yttria NPs, M-rGO, and MoS_2 nanosheets. The NPs, nanosheets, and composites have been characterized by powder X-ray diffraction, high-resolution scanning electron microscopy (HR-SEM), transmission electron microscopy, and Raman spectroscopy. X-ray photoelectron spectroscopy (XPS) was employed to study the chemical states of different elements in (La-Y_2O_3)-MoS_2-(M-rGO). The tribological properties of well-characterized composites were evaluated in paraffin oil (PO) using a four-ball tester according to ASTM D4172 and ASTM D5183 standards at the optimized concentration, 0.20% (w/v). There was incremental evolution in the tribological properties from plain PO through Y_2O_3, MoS_2, M-rGO, La-Y_2O_3, and (La-Y_2O_3)-MoS_2 and finally to (La-Y_2O_3)-MoS_2-(M-rGO). Here functionalization of GO has invigorated its structure. Both nanosheets coordinated to control agglomeration of the NPs. The NPs prevented the nanosheets from restacking. SEM and atomic force microscopy images of the wear scar validated the results of tribological tests. The presence of yttrium, lanthanum, sulfur, and molybdenum besides carbon, nitrogen, and oxygen in the energy-dispersive X-ray spectrum of the worn surface in the presence of PO blended with (La-Y_2O_3)-MoS_2-(M-rGO) is indicative of its strong adsorption on the surface. On the basis of XPS studies of the wear track, the constituents of the tribofilm could be identified as adsorbed rGO, yttria, lanthanum oxide, and MoS_2, in addition to tribochemically produced Fe_2O_3, MoO_3, and SO_4^{2-}. The mutualistic approach of the constituents has yielded splendid results.

KEYWORDS: *lanthanum-doped yttria nanoparticles, MoS_2, functionalized graphene nanosheets, nanocomposite, tribological properties*
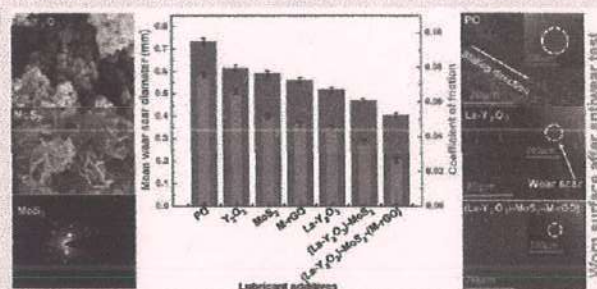
1. INTRODUCTION

Wear and friction between moving surfaces have to be overcome for endurance of the machine components. Additives with antifriction and antiwear properties are, therefore, blended with the base lubricant. Because of their small size, nanosized materials are beneficial for quick response at the interface.[1−3] Various types of nanosheets, nanoparticles (NPs), and nanocomposites are available in the literature for their tribological properties.[4−7] Among the nanosheets, MoS_2,[8,9] graphene,[10−12] and boron nitride[13] have specifically drawn attention because of the existence of weak van der Waals forces between the proximal layers, which facilitates shearing under a sliding motion.[13−15]

Graphene is a two-dimensional (2D) hexagonal lattice of sp^2-hybridized carbon atoms. Each carbon atom is bonded to its three neighbors by a σ bond and one π bond perpendicular

to the plane.[9] Graphene oxide (GO),[11,12] an oxidized form of graphene, consists of oxygen-containing functional groups like epoxide, hydroxy, and carboxylic acid; therefore, it has less sp^2 character/less graphitic nature[16] or more defects. The load-bearing capacity and wear/friction-reducing characteristics of GO/reduced graphene oxide (rGO) are not very commendable. Apart from moderate tribological activity, some drawbacks are also associated with lubrication like agglomerating
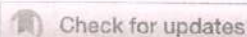
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PAPER

Tetrahydropyrazolopyridines as antifriction and antiwear agents: experimental and DFT calculations†

Kavita,‡[a] Pratibha Verma,‡[a] Dinesh K. Verma,[ab] Bharat Kumar,[a] Alok K. Singh,[a] Nivedita Shukla,[a] Vandana Srivastava[a] and Rashmi B. Rastogi ⓘ *[a]

Some tetrahydropyrazolopyridines (THPP-H) with the methoxy (THPP-OMe) and methyl (THPP-Me) substituents were synthesized by a one-pot multi-component reaction. NMR spectroscopy (^{1}H and ^{13}C) was used to authenticate the synthesis. According to the results of tribological tests ASTM D4172, and ASTM D5183 on a four-ball tester in paraffin oil (PO) at a concentration of 0.25% w/v, their relative tribo-activity along with a reference additive, zinc dialkyldithiophosphate (ZDDP) could be figured out as mentioned below-THPP-OMe > THPP-Me. > THPP-H > ZDDP. The calculation of frictional power loss from the coefficient of friction data of the tested additives supports the given order. As is apparent from AFM and SEM micrographs of the wear scar surface for plain oil with and without different tetrahydropyrazopyridines, surface evenness endorses the above trend. Proof for strong adsorption of the synthesized additives is provided by EDX analysis of the steel ball surface after performing the tribological test, where nitrogen and oxygen are vividly seen as heteroatoms. XPS studies reveal the composition of the *in situ* formed tribofilm. The moieties containing carbon bonded to oxygen/nitrogen as decomposed products of the additive together with oxides of iron in +II or +III oxidation states are perceptible in the tribofilm, the tribofilm interferes with the proximity of the surfaces keeping them far apart. Consequently, friction and wear are remarkably reduced. Findings from Density Functional Theory (DFT) calculations are in full agreement with the results obtained from tribological experiments.

1. Introduction

Friction and wear together have been immanent adversaries to mechanical systems. Lubrication stands as the only remedial measure to safeguard such systems.[1-5] Sundry lubricant systems with numerous types of additives, therefore, have been fabricated to address this issue. Among them, heterocyclic organic compounds,[6] nanomaterials,[7,8] inorganic lamellar structures[9] and metal complexes[10] find paramount significance. Zinc dialkyldithiophosphates (ZDDP) have been employed, very often, as multifaceted antiwear additives.[11,12] However, their incessant use is prohibited because of their susceptibility to attenuating the efficacy of exhaust emission catalytic converters, thus enhancing air pollution.[13] From an environmental perspective, various standards have been put forth to control sulphated ash, sulphur and phosphorus (SAPS) contents in an additive.[14]

Nanolubricants[15,16] are well appreciated for their dexterous antiwear behavior but their agglomeration poses a great problem for the stability of their dispersions. In contrast, the use of conventional organic compounds is everlasting owing to their comparatively higher solubility in base oils. From the viewpoint of adsorption over the metal/alloy surface, heterocyclic compounds containing heteroatoms specifically, nitrogen and oxygen are categorically advocated for their friction/wear lowering disposition. The lone pair of electrons at heteroatoms and the aromatic ring electrons are basically involved in the process of adsorption.[17-20] A comprehensive literature survey reveals that several groups of workers have chosen to investigate the tribological efficiency of different types of heterocyclic compounds. Kamano *et al.* have patented several pyridines, pyridazines, pyrazines, pyrimidines, pyrroles, pyrazoles, imidazoles as antiwear agents.[21] Friction and wear-reducing behavior of indole, indazole and benzotriazole in liquid paraffin oil have been reported by Zhongyi and co-workers.[22] Tribological properties of the benzimidazoles[23] and tetrazole derivatives[24] have been investigated in liquid paraffin oil. The antiwear and antifriction properties of imidazoline derivatives[25] in water–glycol mixture and triazine in poly-alpha olefin base

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† Electronic supplementary information (ESI) available. See DOI: 10.1039/d0ra00794c

‡ These authors contributed equally to this work.

# Theoretical and experimental studies of pyranopyrazoles and their tribological compatibility with a borate ester

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GRAPHICAL ABSTRACT
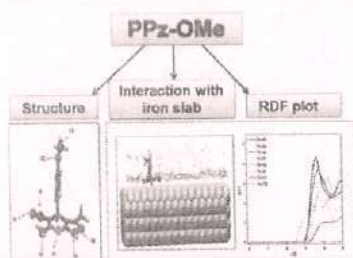
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ABSTRACT

The tribological properties of fused heterocyclic ring systems have been scarcely studied. Generally, increased heteroatoms in such molecules should make them better additives. Accordingly, antiwear behavior of substituted pyranopyrazoles (PPz-R, where R = H, methyl and methoxy), compounds with fused heterocyclic rings, have been investigated in the present research. These compounds were characterized by FTIR and NMR (^{1}H and^{13}C) spectroscopy. Their tribological activity followed the order PPz-OMe > PPz-Me > PPz-H > ZDDP (standard). Atomic force microscopy (AFM) and scanning electron micrographs (SEM) of wear scar lubricated with pyranopyrazoles exhibited surface smoothness according to tribological results. The energy-dispersive X-ray (EDX) spectroscopy analysis revealed the heteroatoms nitrogen and oxygen of additive on the surface. XPS analysis showed that interaction of the best additive, PPz-OMe with a borate ester (Van lube 289), increased the efficiency synergistically. Results of DFT calculations on the interaction between adsorbent and substituted pyranopyrazoles are in agreement with the experimental data. The order of adsorption energies found using molecular dynamics (MD) simulations, correlated very well with the additive activity order. Furthermore, MD studies gave the conformation of the additive molecules on the adsorbing surface, paving the way to an understanding of the mechanism of adsorption and triboactivity.

Mechanical and Thermophysical Properties of ScM (M: Ru, Rh, Pd, Ag) Intermetallics

Jyoti Bala[1] · Devraj Singh[2] · D. K. Pandey[3] · C. P. Yadav[3]

Abstract

In this paper, we have investigated the elastic, mechanical, ultrasonic, and thermophysical properties of B2 structured scandium based intermetallic compounds ScM (M=Ru, Rh, Pd, Ag) at 300 K. Initially, the elastic constants were determined under potential model approach considering the interaction up to second nearest neighbors defined by Coulomb and Born–Mayer potential. The second order elastic constants (SOECs) were used to find the mechanical parameters such as shear modulus, bulk modulus, Poisson's ratio, Young's modulus, Pugh's indicator, Zener ratio, Vicker's hardness, Cauchy's pressure, and Lame modulus in ScM intermetallic compounds. Further, SOECs were applied to compute the ultrasonic velocities and Debye velocity for wave transmission through ScM along $\langle 100 \rangle$ orientation. We have also evaluated thermal conductivity, thermal expansion coefficient, melting point, and thermal relaxation time of the chosen compounds. Finally, the ultrasonic attenuation was estimated using thermo-elastic relaxation and phonon–phonon interaction mechanisms at room temperature. The mechanical properties of ScM were discussed and analyzed on the basis of obtained elastic constants while their ultrasonic properties were discussed in connection with elastic and thermal properties.

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Sudhanshu Tripathi*, Rekha Agarwal and Devraj Singh

Size-Dependent Ultrasonic and Thermophysical Properties of Indium Phosphide Nanowires

Abstract: The present work explores the diameter- and temperature-dependent ultrasonic characterization of wurtzite indium phosphide nanowires (WZ-InP-NWs) using a theoretical model based on the ultrasonic non-destructive evaluation (NDE) technique. Initially, the second- and third-order elastic constants (SOECs and TOECs) were computed using the Lennard-Jones potential model, considering the interactions up to the second nearest neighbours. Simultaneously, the mechanical parameters (Young's modulus, shear modulus, elastic anisotropy factor, bulk modulus, Pugh's ratio and Poisson's ratio) were also estimated. Finally, the thermophysical properties and ultrasonic parameters (velocity and attenuation) of the InP-NWs were determined using the computed quantities. The obtained elastic/mechnical properties of the InP-NWs were also analyzed to explore the mechanical behaviors. The correlations between temperature-/size-dependent ultrasonic attenuation and the thermophysical properties were established. The ultrasonic attenuation was observed to be the third-order polynomial function of the diameter/temperature for the InP nanowire.

Keywords: Elastic Constants; Indium Phosphide Nanowires; Thermal Conductivity; Ultrasonic Attenuation.

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1 Introduction

Rigorous investigations carried out in the last decade have exhibited the applicability of indium phosphide (InP) at the nanoscale. InP is a III-V group semiconductor material that exists in the wurtzite (WZ) and zinc blende (ZB) crystalline forms at room temperature (300 K) [1–3]. The observation of the WZ phase in the crystal lattice of the InP nanostructure is an important finding that cannot be found at the bulk scale, where the zinc blende form is pervasive. Recent investigations have shown that the suitability of the InP nanowires (InP-NWs) for high-speed digital circuits, opto-electronic devices, and high-frequency and high-power electronics applications due to its high electron mobility, high degree of covalent bonding, large excitation diameter and less ionic characteristics in comparison to the I-VII and II-VI semiconductors [4–7]. Figure 1 shows the hexagonal WZ structure of the InP nanowire and its cross-sectional view. The figure clearly indicates that very few InP atoms are lying on the surface of nanowire in comparison to the volume.

The experimental study of mechanical and fracture mechanisms in the InP-NWs shows that the fracture strain of the InP-NWs is like that of the ZnO-NWs but lesser than that of the GaAs-NWs. A density function theory (DFT)-based investigation on InP has shown that pressure variation can also affect the chemical bonding leading to modification in crystal structure and physical properties of InP [3]. The two forms (ZB and WZ) of the InP-NWs structure differ due to stacking along $<111>/<001>$ growth directions [8]. The band gap difference between WZ- and ZB-InP-NWs can be described as $\Delta E_g = 0.79/d$ and $\Delta E_g = 0.88/d^{1.32}$, respectively, as a function of diameter (d) [9]. The study on piezoelectric and elastic properties along the $<111>/<001>$ directions of ZB- and WZ-structured NWs with three different forms of hetero-structures reveals that the piezoelectric field along the unique axis of nanowires is more prominent in the WZ crystalline form [10]. The variations in the shear strains in both forms of the nanowires' crystalline structures influence their mechanical properties. However, it has been reported that the principal shear strain is independent of crystalline structure variations and that the piezoelectric field/piezoelectric potential of the nanowires depends on the crystalline structures [10].

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Rapid removal of lead(II) ions from water using iron oxide–tea waste nanocomposite – a kinetic study

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Abstract: Lead (Pb) ions are a major concern to the environment and human health as they are contemplated cumulative poisons. In this study, facile synthesis of magnetic iron oxide–tea waste nanocomposite is reported for adsorptive removal of lead ions from aqueous solutions and easy magnetic separation of the adsorbent afterwards. The samples were characterised by scanning electron microscopy, Fourier transform-infrared spectroscopy, X-ray diffraction, and Braunner–Emmet–Teller nitrogen adsorption study. Adsorptive removal of Pb(II) ions from aqueous solution was followed by ultraviolet–visible (UV–Vis) spectrophotometry. About 95% Pb(II) ion removal is achieved with the magnetic tea waste within 10 min. A coefficient of regression $R^2 \simeq 0.99$ and adsorption density of 18.83 mg g^{-1} was found when Pb(II) ions were removed from aqueous solution using magnetic tea waste. The removal of Pb(II) ions follows the pseudo-second-order rate kinetics. External mass transfer principally regulates the rate-limiting phenomena of adsorption of Pb(II) ions on iron oxide–tea waste surface. The results strongly imply that magnetic tea waste has promising potential as an economic and excellent adsorbent for the removal of Pb(II) from water.

1 Introduction

Owing to extensive globalisation and industrialisation across the world, environmental contamination has become a major problem, threatening the wellness of humans and animals. A number of industrial processes are responsible for the release of heavy metals in ground and aquatic water resources. The health effects on humans due to heavy metals are quite life threatening. These heavy metals reach the environment through various processes. Some processes that can be mentioned are the agriculture, smelting and mining industries, manufacturing, and vehicles, power plants, aircrafts, and ships that use fossil fuels [1].

Among heavy metals, lead (Pb) compounds are of immense concern as they are contemplated as cumulative poisons and may cause neurological disorders in children. Both natural and anthropogenic origin of lead in the environment leads to detrimental effects on living beings [2]. A wide spectrum of health problems may arise due to drinking water contaminated even with a very low concentration of Pb(II) ions for the long term. Damage caused to the reproductive system, central nervous system, liver, and kidney along with loss of basic cellular processes and brain functions is some of the severe health effects of lead [3]. Source of lead ions in the water bodies is generally from corrosion of lead incorporated pipes, paints, and other household materials. Lead concentrations in water in some industrial areas are very high, nearly 500 mg l^{-1}. Recommended levels are below 0.01 mg l^{-1} [1].

Numerous conventional methods such as oxidation, reduction, precipitation, membrane filtration, ion exchange, and adsorption have been explored for the removal of metal ions from aqueous solutions. Adsorption, among all, is the most economical and promising technique for the removal of heavy metal ions from their aqueous solutions [4, 5]. Activated carbon is generally used for the removal of heavy metals in water. However, its extensive application as an adsorbent is limited due to high cost and cumbersome disposal. Carbon-based nanomaterials such as

graphene oxide and reduced graphene oxide have also shown promising results [6]. Fe$_3$O$_4$ nanoparticles have emerged as an extremely effective material for adsorptive removal of heavy metal ions [7–9]. A combination of electrostatic attraction and ligand exchange has been reported to facilitate metal ion adsorption by magnetite [10–12]. Fe$_3$O$_4$ nanoparticles can be instantly separated from aqueous solutions with the aid of an external magnetic field and have advantages of high efficiency. The magnetic separation process is economically viable as it is rapid, highly efficient and not affected by temperature or pH change of the aqueous solutions [13]. Despite several advantages, there are a few challenges presented by Fe$_3$O$_4$ nanoparticles. Firstly, Fe$_3$O$_4$ nanoparticles tend to break down and dissolve. The small size of nanoparticles hinders the recycling process. Secondly, the nanoparticles co-aggregate in the solution due to high-surface energy. This reduces the effective surface area, thereby reducing adsorption efficiency. To evade the co-aggregation of nanoparticles, the use of metal, polymer, clay, and silica has been reported [14, 15]. Low-cost alternative adsorbents based on agricultural waste materials such as husk from rice, egg shells, peanut shells, saw dust, corn cobs, tree barks, dried leaves, tea waste and coffee grounds, rice and wheat bran [16, 17] have been popularly researched upon for their potential properties in the elimination of heavy metal ions from water. The use of these low-cost adsorbents along with Fe$_3$O$_4$ nanoparticles may also minimise the co-aggregation of the Fe$_3$O$_4$ nanoparticles and improve their adsorption characteristics.

Tea is a popularly consumed beverage around the world. An enormous quantity of untreated tea wastes is frequently dumped into the environment. In addition, annually larger amounts of tea leaves are added to the environment by natural processes such as defoliation or pruning. Such tea wastes may lead to environmental issues during their decomposition process and pollute water by releasing dissolved organic substances. The reuse of these tea wastes, on the other hand, will not only benefit the farmers but also

Elastic and ultrasonic properties of fermium monopnictides

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Abstract

Determinations of higher order elastic constants, thermal properties, mechanical properties and ultrasonic behavior have been done for fermium monopnictides. Initially, the lattice and non-linearity parameters were used to compute the higher order elastic constants at temperatures of 0K, 100K, 200K and 300K by means of the Born potential mode. Variation of Cauchy's relations has been found at higher temperature due to weak atomic interactions. The second order elastic constants (SOECs) were used to estimate mechanical parameters such as the Young's modulus, bulk modulus, Pugh's ratio, shear modulus, Zener's anisotropy factor, hardness, and Poisson ratio. On the basis of the values of these parameters, we found a brittle nature of fermium monopnictides. Furthermore, the SOECs were applied to compute the wave velocities for shear and longitudinal modes of propagation along <100>, <110> and <111> crystallographic orientations. Properties such as the lattice thermal conductivity, acoustic coupling constant, thermal relaxation time and attenuation of ultrasonic waves due to thermo-elastic and phonon-phonon interaction mechanisms have been calculated at room temperature. The results of present investigation have been analysed with available findings on other rare-earth materials.

Keywords: Fermium monopnictides, Higher order elastic constant, Thermal conduction, Ultrasonic attenuation

1. Introduction

Ultrasonics is an important branch of acoustics, which have tremendous applications in medical science [1], engineering [2] and materials science [3]. Actinide monopnictides have gained more research interest due to the presence of their partially filled electrons. Much research has been done to explain the role of f electrons in actinide monopnictides. We have found a variety of theoretical studies on Th, Np, U and Pu monopnictides/monochalcogenides that explain their mechanical and thermophysical properties with temperature and pressure in the available literature [4-11]. These studies considered their bulk moduli and phase transition properties at high pressures. Also they examined lattice dynamic properties, which are further used to evaluate specific heat of the compounds. The electronic and elastic parameters of fermium monopnictides were study with first principles calculations by Amine Monir et al. [10]. These first principles computations with discussion of the phase-structure and magnetic phase as well as the magnetic and electronic properties of the FmP were presented by Bahnes et al. [11]. In these studies, the authors did not consider the temperature dependent ultrasonic attenuation for fermium monopnictides (FmP, FmAs and FmSb). So we extended the thermophysical and ultrasonic studies on FmPn to fill this gap in the literature.

In the present investigation, we compute the second and third order elastic constants (SOECs and TOECs) of fermium monopnictides and ultrasonic velocity, Debye temperature, Debye average velocity, the acoustical coupling constant and attenuation loss due to thermoelastic relaxation and phonon viscosity phenomena along <100>, <110> and <111> orientations. The computational results are compared with other types of materials having a similar nature.

2. Theory

A theoretical approach for the computation of elastic constants and other thermo-physical properties was done to compute the temperature dependent SOECs and TOECs and ultrasonic properties along the <100>, <110> and <111> directions. It has been divided into six parts, which follow below.

2.1 Higher order elastic constants

For a crystal structure, the theory of elasticity [12-13] describes the relationship of stress and strain as

$$Y = (I + \varepsilon)X \qquad (1)$$

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Ultrasonic attenuation in intermetallics HfX(X=Os, Ir and Pt)

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Ultrasonic study of B_2-structured hafnium based compounds HfX(X=Os, Ir and Pt) along <110> direction were evaluated at room temperature. Initially, the Coulomb and Born-Mayer potential model was used to find out the higher order elastic constants of HfX at room temperature. We have used the second order elastic constants (SOECs) to compute the mechanical properties such as bulk modulus, Young's modulus, shear modulus, Pugh's ratio, Poisson's ratio, Zener anisotropic factor, Vicker's hardness, Lame's modulus of chosen materials. Further, the SOECs and third order elastic constants (TOECs) were applied to compute ultrasonic velocities and Debye temperature. The thermal conductivity and thermal relaxation time of chosen monopnictides compounds have also been computed at room temperature. We have found that HfOs is strongest and most fit material for crystallographic study in B_2 phase. In addition to above evaluated parameters, energy density, specific heat per unit volume, thermal conductivity, acoustic coupling constants and ultrasonic attenuation for longitudinal and shear modes propagation along <110> direction have been estimated. The ultrasonic attenuation was least in case of HfOs. Obtained results have been discussed and justified with available findings for their future prospects.

Keywords: Elastic constants, mechanical properties, thermal conductivity, ultrasonic attenuation.

Introduction

The hafnium based compounds have large applications in medical field due to their outstanding mechanical and corrosion properties[1]. Most of the hafnium based compounds exhibit in B_2 crystalline structure. The most of the features of hafnium based compounds HfX (X=Os, Ir and Pt) have been reported experimentally in the literature[2]. Various properties of hafnium based compounds were investigated by many researchers[3-6]. Out of which, Guo et al.[3] reviewed experimental studies of the standard enthalpies of formation of the binary intermetallic compounds of early transition metals with the transition metals. Novakovic et al.[4] investigated electronic structures, cohesive energies and enthalpies of formation for Hf-TM (TM = Fe, Co, Rh, Ru) by using the ab initio Full-Potential Linearized Augmented Plane Waves calculations of the most stable Hf and TM elemental phases and HfTM compounds of the CsCl

and CuAu structure types. Xing et al.[5] calculated the ground-state structural phase stabilities and enthalpies of formation of thirty-six binary transition-metal refractory TM and TM_3 compounds formed by Group IV elements T (T = Ti, Zr, Hf) and platinum group elements M (M = Ru, Rh, Pd, Os, Ir, Pt) using first-principles local density functional approach. The electronic structure, elastic, and phonon properties of OsM (M=Hf, Ti, Y and Zr) compounds are studied using first-principles calculations by Arıkan et al.[6]. The structural, elastic, electronic and phonon properties of HfX (X = Rh, Ru and Tc) in the caesium-chloride phase have been investigated using the density functional theory within the generalized gradient approximation by İyigör et al.[7]. Wu et al.[8] studied the site substitution and ternary alloying elements M (M = Al, Si, Cu, Zn, Sn, Zr, Ta, Nb, Ti, W, V, Mo, Cr, Os, Rh, Ir, Pd and Pt) effect on the structural, mechanical, thermal and electronic properties of B_2 RuHf-based intermetallics

Label-Free Electrochemical Detection of Dibenzofuran Using MnO$_2$ Nanofibres

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Abstract—Rapid industrialization is taking a huge toll on environment. Specifically, industrial sites engaged in combustion and carbonization processes of coal-based fuels and its derivative results in the discharge of Dibenzofuran (DBF). It is considered as one of the most hazardous organic pollutants of concern by global environmental protection agencies. DBF is a Persistent, Bioaccumulate and Toxic (PBT) chemical which causes significant damage to human and surrounding environment. In this study an electrochemical sensor with the potential to be integrated with current drinking water dispensing systems to warn individuals about the presence of DBF is developed. Nanofibrous manganese dioxide (α-MnO$_2$) is employed as receptor for the detection of DBF, while the sensing performance has been probed using electrochemical impendence spectroscopy. An equivalent electrical circuit model was developed using the electrochemical impendence data in order to gain insights into the electron transfer kinetics involved. The impedance response shows a linear relationship with DBF concentration over a range from 10^{-2} - 10^6 nM. The limit of detection and sensitivity were calculated to be 1.22 nM and 0.58 kΩ/nM/mm^2 respectively. The shelf-life of the sensor was found to be around 45 days.

Index Terms—Dibenzofuran, α-MnO$_2$, Randel's circuit, Microfluidic
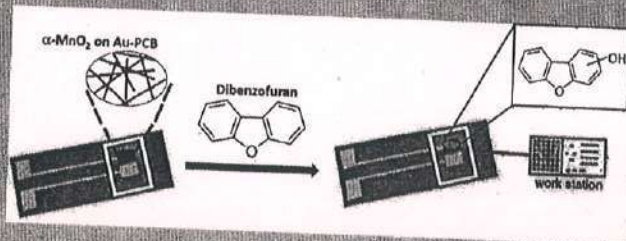
I. INTRODUCTION

GLOBAL contamination of environment by PBT chemicals including dibenzofurans, polychlorinated dibenzo-p-dioxins and biphenyl has raised the concern [1], [2]. A major source of discharge of Dibenzofuran (DBF) into the environment is the global plastic production which is increasing since the decade of 50's [3]. Other key sources include industrial

sites engaged in combustion and carbonization processes of coal-based fuels and its derivative. DBF is considered as one of the most hazardous organic pollutants of concern by global environmental protection agencies. It is a Persistent, Bioaccumulate and Toxic (PBT) chemical which causes significant damage to human and surrounding environment. DBF is also monitored in agricultural fields, and environmental soil [4]. Additionally, billions of tons of plastics enter the aquatic ecosystem [5] and oceans are severely affected by plastic contamination [6]. Fish-eating marine mammals, including seals, were found to accumulate high levels of PBTs. The immunotoxicity at low doses is reported due to such chemicals with laboratory mammals and mink. Immune system has been found to be affected in certain free-ranging seal population due to accumulation of such contaminants e.g., increased incidence of disease was observed [7]. In addition to being recalcitrant in the environment, these compounds are highly toxic and carcinogenic [8].

DBFs belong to a class of heterocyclic compounds with two benzene rings fused to a central furan ring. The structure of DBF is chemically stable due to the absence of reactive groups, and hence is degraded very slowly in the environment [8]. These PBT compounds have never been produced for a specific purpose, yet they have become ubiquitous pollutants as they are formed during incineration and as byproducts of the synthesis of haloaromatic compounds [9]. Hence, these

Ion beam modified TiO$_2$ nanotubular bio-interface for electrochemical detection of L-tyrosine towards smart bandage application

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[...] foot ulcer
[...]chemical impedance spectroscopy

ABSTRACT

One of the common complications diagnosed in Diabetes Mellitus (DM) patients is Diabetic Foot Ulcers (DFUs). It is a condition wherein the deep tissues located in the lower limb undergo inflammation and infection due to neurological abnormalities (neuropathy) and various degrees of vascular diseases (angiopathy). The concentration of L-tyrosine (Tyr) rises abruptly in DFUs, and therefore may be used as an indicator for early monitoring of the patient's condition during the onset of diabetic foot disease. Herein, we report the electrochemical enzymatic detection of Tyr using low energy ion beam modified titania nanotube (TiNT) thin films with nitrogen (N$^+$) and gold (Au$^-$) ions. Electrochemical Impedance Spectroscopy (EIS) analysis was performed to investigate the levels of Tyr using ion beam modified TiNT thin film electrodes. The modified electrodes exhibited excellent sensor performances with Au-TiNT and N-TiNT within the Tyr concentration range of 100 fM $-500\,\mu M$ with limit of detection (LoD) 1.76 nM and 1.25 nM respectively and response time ~ 1 min. The results indicate that low energy ion beam modified TiNT/enzyme bio-electrodes can potentially be employed as a highly sensitive and portable sensor for real-time detection of L-tyrosine in wound fluids for the development of a smart bandage.

Introduction

L-tyrosine (Tyr) is a non-essential amino acid present in the human [body] and plays a vital role in performing various important physiological activities. It is synthesized in the body by the hydroxylation process of L-phenylalanine [1]. It is widely known that abnormal levels of [Tyr] can lead to different ailments such as depression, hypochondria, [autis]m and visceral fat accumulation [2,3]. However, in diabetic [patien]ts, a drastic increase in the concentration of Tyr, among other [amin]o acids, has been found in the wound exudate of DFUs [4]. The [chroni]c DFUs are often associated with slow and non-healing ulcers due [to pol]ymicrobial infections, eventually leading to co-morbidity and [lowe]r limb amputations [5,6]. Surveys have reported that 15 % of the [patien]ts suffering from diabetes have DFUs during their life expectancy [and th]ese patients have a greater risk of heart attack, stroke as well as [premat]ure death [7]. Therefore, a regular wound diagnosis is crucial for [diabeti]c patients, for assessing the probability of occurrence of chronic [DFUs] in the near future.

The conventional detection methods for Tyr include Tandem Mass spectrometry [8] and high performance liquid chromatography (HPLC) [9]. The disadvantages of these techniques include the requirement of an elaborate experimental setup, skilled personnel, large sample volume and high cost. Moreover, these conventional techniques are time consuming. Therefore, there is an urgent need to develop cost effective, rapid, and efficient point-of-care (PoC) diagnostic method for early monitoring of the patient's condition especially during the onset of DFUs.

With rapid advancement in nanotechnology, various nanomaterials – especially nano-metal oxides have been widely explored for the detection of biomolecules. The unique properties related to high surface area and quantum confinement effects, leads to signal enhancement, and hence better sensing parameters [10–13]. Among the vast array of metal oxide nanostructures, titanium dioxide (TiO$_2$ or Titania) is widely reported for sensing of analytes due to numerous advantages such as biocompatibility, chemical inertness, nontoxicity, strong immobilization ability, inexpensiveness and abundant availability. Amongst

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Investigation of zirconium nanowire by elastic, thermal and ultrasonic analysis

Abstract: The elastic, thermal and ultrasonic properties of zirconium nanowire (Zr-NW) have been investigated at room temperature. The second and third order elastic constants (SOECs and TOECs) of Zr-NW have been figured out using the Lennard–Jones Potential model. SOECs have been used to find out the Young's modulus, bulk modulus, shear modulus, Poisson's ratio, Pugh's ratio, Zener anisotropic factor and ultrasonic velocities. Further these associated parameters of Zr-NW have been utilized for the evaluation of the Grüneisen parameters, thermal conductivity, thermal relaxation time, acoustic coupling constants and ultrasonic attenuation. On the basis of the above analyzed properties of Zr-NW, some characteristics features of the chosen nanowire connected with ultrasonic and thermo-physical parameters have been discussed.

Keywords: elastic constants; thermal conductivity; ultrasonic attenuation; Zirconium nanowire.

Introduction

Researchers and material scientists are always excited to discover advanced materials with exotic properties which can extrude to the old conventional materials. The

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development of nanotechnology in earlier phase gives the potential benefits to the material science. Nowadays, nanoscience has become one of the most stimulating forces to influence the interdisciplinary science and technology. The investigations in these areas begin with the understanding of material's behaviour at nanoscale. The attempts were done to control over the crucial physical properties of the materials such as conductivity, capacity, strength, ductility, reactivity etc. in different combination of the matters. This will result in the enhancement of the material's performance at ambient physical conditions. When the size or dimension of a material is continuously reduced from a large or macroscopic size to a size up to 100 nm, the properties remain the same but below 100 nm, dramatic changes in properties can occur [1]. Thus, the bulk properties of the materials become modified when their sizes are reduced to the nano range (1–100 nm). If one dimension is reduced to the nano-range, keeping other two dimensions unchanged, we obtain a structure known as a 'quantum well'. If two dimensions are reduced and one remains unchanged, the resulting structure is referred as a 'nanowire'. The single crystalline NWs are considered as the imperative division of the nanostructure materials due to its superior properties. Currently, the magnetic NWs have drawn considerable interest of researchers worldwide due to their applications in the high-density magnetic storage media, giant magnetoresistance (GMR) sensors [1, 2], bio-magnetic [3], medical devices [4], etc. Among the magnetic nanowires, Zirconium nanowires (Zr-NWs) are widely studied material for its two unusual properties. The first one is the temperature induced phase transformation and the second one is the plastic deformation by twinning. Zr-NWs are the phase changing material and exist in hexagonal close packed (HCP) phase at room temperature (300 K) [5]. Figure 1 shows the HCP structure of the Zr nanowire and its cross-sectional view. Figure 1 clearly indicates that very few Zr atoms are lying on the surface of nanowire in comparison to the volume.

In the field of non-destructive characterization, the ultrasonic non-destructive technique (NDT) has been the most extensively used for the characterization of the materials. The structural inhomogeneities, non-linear elastic properties, phase transformations, electrical properties,

Short Communications

Elastic and ultrasonic properties of cadmium oxide

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The attenuation of ultrasonic waves has been estimated in rocksalt type (B1) and CsCl type (B2) structures of CdO at room temperature along <100>, <110> and <111> directions. First of all, the higher order elastic constants have been computed using Born model with Mori and Hiki approach. Then, the second order elastic constants (SOECs) were applied to compute the mechanical constants such as shear modulus, Young's modulus, bulk modulus, tetragonal modulus, Poisson's ratio, Pugh's indicator for finding performance of CdO. Numerous physical quantities, such as ultrasonic velocity, Debye temperature, thermal conductivity, ultrasonic Gruneisen parameter and acoustic coupling constants have been determined for the chosen material. Finally, the attenuation of ultrasonic waves has been compared in B1 and B2 phases of CdO and discussed in correlation with available findings.

Keywords: Cadmium oxide, elastic constants, thermal properties, ultrasonic properties.

Introduction

Over the past few years metal oxides semiconductors have received enormous attention due to their interesting electrical and optical properties in several technologically challenging areas. One of the important semiconductor material is Cadmium Oxide (CdO). It is the transparent conductive oxides (TCOS) and are of high interest from industrial applications such as liquid crystal display (LCD), photoelectric devices, gas sensors, IR detectors, etc. It normally crystallizes into rock-salt structure (NaCl) under pressure[1-4]. Sahoo *et al.*[5] carried out Ab initio calculations on structural, elastic and dynamic stability of CdO at high pressures and concluded the transformation of CdO from B1 to B2 phase under hydrostatic pressure of ~87 GPa. Bhardwaj[6] studied the structural and thermophysical properties of cadmium oxide using the Three-Body Potential (TBP) model. Jentys *et. al.*[7] studied the structural properties of CdO and CdS clusters in zeolite *Y*. The structural properties of CdO in the rock-salt (sodium chloride), cesium chloride *etc* was studied using first-principles

total energy calculations by Moreno *et. al.*[8]. Dou *et. al.*[9] performed the experimental and theoretical investigation of the electronic structure of CdO using periodic Hartree-Fock and density functional methods. Piper *et. al.*[10] studied the electronic structure of single-crystal rocksalt CdO by soft x-ray spectroscopies and ab initio calculations.

In the present study, a computational approach has been followed for the investigation of ultrasonic attenuation in order to study the inherent properties of CdO. The Coulomb and Born-Mayer potentials model have been used to determine the elastic, mechanical and thermo-physical properties at room temperature. The van der Waals' forces of interaction have been neglected. To the best of our knowledge, no calculation has been done on the temperature dependent study of CdO using this model.

Theory

The temperature dependent elastic, mechanical and ultrasonic properties at room temperature have been

Synthesis of MWCNT/PPY nanocomposite using oxidation polymerization method and its employment in sensing such as CO$_2$ and humidity

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ABSTRACT

This paper includes the synthesis of a composite of multiwall carbon nanotube (MWCNT) and conducting polymer polypyrrol (PPY) and its characterizations along with the applications direct liquid injection chemical vapour deposition (DLICVD) and oxidation polymerization method have been used for the synthesis of MWCNT and MWCNT/PPY nanocomposite respectively. MWCNT/PPY's thin film was prepared using the technique of spin coating and characterized by scanning electron microscope (SEM), transmission electron microscope (TEM), particle size analyzer and X-ray diffractometer (XRD). Raman spectroscopy has been used to observe the vibrational and rotational spectra of MWCNT and MWCNT/PPY nanocomposite. The optical bandgap and minimum crystallite size have been calculated and found to be 3.2 eV and 8.1 nm respectively. The synthesized MWCNT/PPY has been used for CO$_2$ and humidity sensing at room temperature (300 K). The sensor response of thin-film towards CO$_2$ was found to be 7.2 at 1000 ppm and minimum response and recovery time at 250 ppm were found to be 30 s and 37 s respectively. The sensitivity of thin-film towards humidity was found to be 41.33 kΩ/%RH. The theoretical calculation was also performed in support of experimental data.

1. Introduction

Nowadays the detection of toxic gas has become an important area of research. The leakage of such gases causes many disasters so we need to design such sensors that may be used for the detection of such toxic gases. CO$_2$ is one of the toxic gases which is very hazardous for the environment. The increment in the level of carbon dioxide causes the greenhouse effect which increases the earth's temperature and causes global warming which is one of the major issues of the present scenario [9]. Regulation of climate change has become a major problem and leads to an increase of researchers on gas sensors. Mostly CO$_2$ is responsible for such changes so that it is necessary and urgent to trace and monitor CO$_2$ released from motor vehicles, factories, and other pollutant sources in the atmosphere. The sensors are required to trace the gas concentration of the accumulated CO$_2$ gas to minimize the leaked amounts. For humans, a gas mixture containing 5–20% CO$_2$ is required for safety regulations in enclosed spaces such as mines, wells, and weirs.

The researchers have developed sensors using different types of nanomaterials. R. Chapple et al. developed a CO$_2$ sensor using CuO—CuFe$_3$O$_4$ nanocomposite material but the response time of the sensor was very high i.e. 9.5 h [1]. For reducing the response time of the sensor, J Herra et al. doped Ag-BiTiO$_2$ with CuO so the response time was found to be reduced up to 15 min [2]. The researchers have used other nanomaterials like La$_{1-x}$Sr$_x$FeO$_3$, CdO, and La$_2$O$_2$CO$_3$ for reducing the response time of the sensor, these nanomaterials reduce the response time but the sensor response was also reduced which was proven as the drawback of these sensors [4–6]. Some nanomaterial like ZnO-La [7] have very low response time i.e. 90 s but all these sensors have one another major drawback that they are operated at high temperatures. Therefore, it was our priority to design such a gas sensor which might be operated at room temperature. When we replaced the metal oxide sensor with a carbon-based sensor then we found that the sensor has operated at room temperature with low response and recovery time. Modification of carbon nanomaterials like CNTs with functional groups, metal nanoparticles, oxides, and polymers will change the electronic properties of them and enhancing the selectivity and response to specific gases through the interaction of the target molecules with the functional groups or additives is
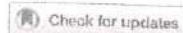
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Mechanical and thermophysical properties of high-temperature Ir_xRe_{1-x} alloys

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ABSTRACT

The Ir_xRe_{1-x} ($0.1 \leq x \leq 0.7$) alloys are hexagonal structured inclusion material used in an on-orbit communication satellite. The characteristic features of high-temperature alloys Ir_xRe_{1-x} ($0.1 \leq x \leq 0.7$) are investigated by the theoretical evaluation of thermophysical and ultrasonic properties at room temperature. Initially, higher-order elastic constants of the alloys are calculated using the simple interaction potential model approach. With the help of this other elastic moduli, elastic stiffness constants and hardness parameters are estimated at room temperature for elastic and mechanical characterization. Later on, the ultrasonic velocity and thermal relaxation time of chosen alloys are evaluated utilizing calculated values of SOECs and lattice parameters within the same physical conditions. The orientation-dependent ultrasonic velocities and thermal relaxation time have been also evaluated for the determination of anisotropic behaviour and thermophysical properties. The obtained results are analysed to explore the inherent properties of Ir_xRe_{1-x} alloys.

1. Introduction

The compelling demand of materials' sustained use at temperature greater than about 1500 °C, there are challenging tasks for material-scientists and engineers to develop high-temperature materials [1,2]. The high-temperature alloys paved the way to overcome this difficulty. Such types of alloys have very high melting point and exhibit improved resistance to oxidation at higher temperature regime [3]. These alloys are used to manufacture flight-type rockets, turbine blades and other components of jet engine. Unfortunately, the materials that have higher melting points are rapidly oxidized in the environments. Iridium (Ir) has very high melting point (2454 °C), so it is the most promising material for applications in high-temperature environments [4]. Iridium is a quite expensive element compared with other elements used in high-temperature applications. The incorporation of rhenium (Re) into iridium-containing alloys overcomes this difficulty because Re has also a higher melting point like Ir, but generally Re is less expensive than Ir. Iridium-rhenium (IrRe) alloys are very economical and used to make thruster chamber in an on-orbit communication satellite. These alloys demonstrate the excellent reliability and compatibility in a high-temperature oxidizing environment [4–10].

For any cast restoration to be successful, the fundamental aspects such as mechanical deformation and structural stability of the materials must be understood. Elastic constants of materials play a vital role in describing their structural stability and mechanical deformation under the action of external loading condition [11]. The linear elastic properties of the materials can be understood with the

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The Palaeogene record of Himalayan erosion in the Andaman Basin

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The Himalayan orogeny has been recognized as one of the most important Cenozoic events that shaped the geography, climate and ocean chemistry of our planet. The erosion in the Himalayas is believed to have played a critical role in crustal deformation and changes in the chemistry of the ocean water since the Eocene. In spite of the fact that the orogeny began after India–Asia collision at 59±1 Ma, the record of its earliest erosional history is meagre. In an attempt to fill this gap in the knowledge, we studied temporal changes in provenance of Paleogene–Neogene siliciclastic sediments of the Andaman Islands, deposited in a trench-forearc basin in the Bay of Bengal. Using Sr-isotope stratigraphy and tephrochronology we determined the timings of depositions of various lithologies. Sediment sources were identified using trace element and isotopic (Sr–Nd) fingerprinting. Results of our study suggest that the Myanmar Arc had remained a constant sediment source to the Andaman basin during 55–5 Ma, whereas the basin started receiving significant continental sands input after 35 Ma that increased with time until ∼20 Ma. Geochemical provenance of these sands suggests their derivation from Precambrian crustal sources in the Himalaya, which probably is an outcome of higher erosional rates subsequent to a rapid exhumation of the orogen in the late Eocene and efficient sediment transport through the palaeo-channels of the rivers Brahmaputra and Ganga under optimal conditions of the Indian monsoon. Such a scenario is consistent with the idea that the Himalayan sediment input is the cause for the conspicuous rise in marine $^{87}Sr/^{86}Sr$ since ∼40 Ma. Our data also suggest that since the Miocene, sediment sources in the Indo-Burman Ranges and the Myanmar arc have become the major contributors to the Andaman Basin through the Irrawaddy river system.

Keywords. Andaman Islands; provenance; tectonics; Himalaya; Sr–Nd isotopic ratios.

1. Introduction

The interaction between tectonics and climate is probably best manifested in the Cenozoic geological events in South Asia linked to the formation of the Himalayan mountain belt, which began ∼60 million years ago (Hu *et al.* 2016, 2017). It has been hypothesized that the rise of the Himalaya and the formation of the Tibetan Plateau had profound thermal and dynamic effects on the Asian climate (Molnar *et al.* 2010). The rise of the Himalaya and the surrounding mountain belts is generally attributed to multiple phases of thrusting and folding events following the closure of the

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Tracking Indian monsoon variability from changes in sediment provenance

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Terrestrial and marine sediments preserved on the Indian sub-continent and in seas/oceans around it are excellent archives for studying and reconstructing past variations in monsoonal climate. Based on the multiproxy studies on the sediment cores, a coherent relationship between the intensities of the monsoon and glacial–interglacial conditions and a strong atmospheric teleconnection between the Asian and North Atlantic climates has been suggested. Terrestrial sediment cores clearly established that the variations in the monsoonal climate and/or change in glacial extant played an important role in varying weathering/erosion in source regions and relative supply of sediments. Marine sediment studies presented a more complicated picture because their depositions were influenced by changes in sea-levels, movement of shorelines, river mouths, deltas and sea surface-circulations. A composite climate record suggested that the intensity of Indian SW monsoon has weakened and NE monsoon strengthened during glacial periods and vice-versa during the interglacial periods.

Keywords: Climate, Himalaya, Indian monsoon, sediment cores, Sr–Nd isotopes, weathering-erosion.

Introduction

THE Indian monsoon system is one of the most important weather systems on the Earth[1,2]. The monsoonal rains are looked forward to with great anticipation and have widespread socio-economic impacts on the large populations inhabiting the South and Southeast Asian countries[3]. By controlling food and agricultural production and growth of regional flora and fauna, it largely controls the life of people living in these regions. The Indian subcontinent experiences two monsoons annually, the south-west (SW) or summer monsoon and the north–east (NE) or winter monsoon (Figure 1). These monsoons bring rainfall by picking up the moisture during seasonal reversals of the wind directions along the shore of the Indian Ocean especially in the Arabian Sea and surrounding regions.

Several studies have emphasized that the monsoonal changes played an important role in the origin, evolution and dispersal of mankind not only in the present times, but also during the geological past[4–6]. However, it has been always difficult to accurately understand, evaluate and reconstruct the climate variability records for longer time scales of several thousand or million years, for which we have to rely on a variety of physical and chemical proxies available both over the lands as well as in the oceans[7]. Constant efforts have been made in past few decades to refine the available records and reconstruct the variability of the monsoon on longer time scales through analyses of various physical and chemical parameters like distribution of grain size, clay minerals, heavy minerals, mineral magnetism, phytoliths, palynology, diatoms, major and trace elements and isotope ratios (of C, O, N, Sr and Nd) in ice cores, detrital sediments, organic and inorganic matter on sedimentary archives like sediments in lakes and ocean, peat bogs, loess, and speleothems[3]. Thus, the continental and marine sediment records have proven to be consistent proxies for reconstructing millennial scale palaeoclimate variability records; despite that considerable discrepancies still exist in analytical precision and resolution.

The available records of monsoonal patterns based on the studies of atmospheric CO_2, Asian speleothems and cores from the Arabian Sea, uniformly indicate centennial to millennial scale variations in the intensities of the Indian monsoon in tune with the changes in glacial and interglacial conditions[8–11]. These studies have demonstrated that the low latitude solar insolation, driven by precession and eccentricity of the Earth's orbit around the Sun have largely controlled these intensities of monsoon at least since the last 1 myr (refs 12–14). Several of these studies, emphasized that the NE monsoon strengthened during the glacial periods and were closely associated with the contemporaneous changes recorded in the Greenland ice cores and cold Heinrich events recognized in the North Atlantic during the last glacial cycle[14,15]. In contrast, during the interglacial periods the SW monsoon was stronger coinciding with the Dansgaard–Oescher (DO) events. Strong NE monsoon was also recognized during the cold event of Younger Dryas (YD) whereas strong SW monsoon was witnessed during the warm Bolling–Allerod (B–A) period[14,16].

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Silver linings in the dark clouds of COVID-19: Improvement of air quality over India and Delhi metropolitan area from measurements and WRF-CHIMERE model simulations

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ABSTRACT

The current study examines the impact of the COVID-19 lockdown (25th March until May 17, 2020) period in particulate matter (PM) concentrations and air pollutants (NO_x, SO_2, CO, NH_3, and O_3) at 63 stations located at Delhi, Uttar Pradesh and Haryana states within the Delhi-NCR, India. Large average reductions are recorded between the stations in each state such as PM_{10} (−46 to −59%), $PM_{2.5}$ (−49 to −55%), NO_2 (−27 to −50%), NO (−54% to −59%), CO (−4 to −44%), NH_3 (−2 to −38%), while a slight increase is observed for O_3 (+4 to +6%) during the lockdown period compared to same periods in previous years. Furthermore, PM and air pollutants are significantly reduced during lockdown compared to the respective period in previous years, while a significant increase in pollution levels is observed after the re-opening of economy. The meteorological changes were rather marginal between the examined periods in order to justify such large reductions in pollution levels, which are mostly attributed to traffic-related pollutants (NO_x, CO and road-dust PM). The WRF-CHIMERE model simulations reveal a remarkable reduction in $PM_{2.5}$, NO_2 and SO_2 levels over whole Indian subcontinent and mostly over urban areas, due to limitation in emissions from the traffic and industrial sectors. A $PM_{2.5}$ reduction of −48% was simulated in Delhi in great consistency with measurements, rendering the model as a powerful tool for simulations of lower pollution levels during lockdown period.

1. Introduction

Air pollution and human health are issues of growing concern all over the globe, especially in the highly-populated countries in Asia such as India and China (e.g. Lu et al., 2011; Cao et al., 2014; Das et al., 2018; Wang et al., 2019a). In India, due to the rapid economic growth, vast expansion of metropolitan areas, urbanization and fast-paced development of infrastructure, air pollution has been significantly increased to levels causing important premature mortality and cancer risk (Khanna et al., 2015; Izhar et al., 2016; Kumar and Mishra 2018; Pant et al., 2018; Balakrishnan et al., 2019; Guo et al., 2019). Particulate matter ($PM_{2.5}$ & PM_{10}; aerodynamic diameters less than 2.5 and 10 μm, respectively) is the most dominant air pollutant, mainly emitted from vehicular exhausts, industries and power plants, residential wood burning, agricultural biomass burning and dust outbreaks (e.g. Hopke et al., 2008; Mukherjee and Agrawal, 2018; Dumka et al., 2019a; Guo et al., 2019).

ORIGINAL PAPER

Enhanced piezoelectricity properties of reduced graphene oxide (RGO) loaded polyvinylidene fluoride (PVDF) nanocomposite films for nanogenerator application

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Abstract

Flexible and lightweight films of Polyvinylidene fluoride (PVDF) loaded with nanosheets of reduced graphene oxide (RGO) have been prepared via solution casting method. The structure of RGO nanosheets have been examined through X-ray diffraction (XRD), Transmission electron microscopy (TEM) and Raman spectroscopy technique. FTIR studies revealed that the enhancement of β-phase from 53 to 70% has been observed by adding RGO nanosheets in PVDF matrix. The frequency dependent dielectric constant and dielectric loss have been studied. Ultraviolet–visible spectra show a decrease in optical band gap with increases RGO concentration in nanocomposite films. The ferroelectric behavior of RGO loaded PVDF nanocomposite films showed remarkable improvement in remnant polarization values as compared to bare PVDF. The piezo-response of RGO loaded nanocomposite films showed significant enhancement in output voltage from 0.886 to 1.915 V. On exposure to ultraviolet–visible light, RGO loaded nanocomposite PVDF films showed about 13.8% enhancement in piezo- voltage with action of same pressure.

Keywords PVDF · Piezoelectric · β-phase · RGO · Nanocomposite

Introduction

The piezoelectric energy conversion from mechanical energy to electrical energy referred as the 'Direct piezo-electric effect' is one of the most versatile phenomenon in an energy harvesting process [1]. Therefore, Energy harvesting from irregular air flow/vibration, ultrasonic waves, and body movement has created enormous interest in the scientific community because of the easily available and environmental factors which exist enormously in our daily activity. In the past few decades, a piezoelectric material has an utmost demand in various devices and application in modern society. With their intrinsic electromechanical properties, applied strain produces an electrical signal, whereas electrical input induces mechanical deformation. Piezoelectric materials devices are components of choice in strain sensors, self-powered wireless sensors, acoustic and ultrasonic devices, precision positioning in scanning probe microscopes, fuel injection systems, active damping control, and adaptive control systems. For that designing of flexible piezoelectric nanogenerator (PNG), using electroactive polar Poly(vinyldene fluoride) (PVDF) polymer is a very attractive polymer which having dielectric, piezoelectric, ferroelectric, pyroelectric and other excellent physical properties [2].

Poly(vinyldene fluoride) PVDF $(-CH_2-CF_2-)_n$ is a semi-crystalline polymer and possesses five different crystalline phases α, β, γ, δ and ε in which α phase is non-polar whereas β, γ, δ and ε are polar phases. Although PVDF has higher piezoelectric coefficient, d_{33} than other polymers yet it is not preferred suitable for the application of energy harvesting because of low piezoresponse [3]. The non-polar α phase,

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Fabrication of nanostructured magnesium ferrite polyhedrons and their applications in heat transfer management and gas/humidity sensors

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Abstract

In this paper we report the sol–gel synthesis of $MgFe_2O_4$ nanostructures of polyhedron morphology. X-ray diffraction (XRD) patterns revealed the presence of pure phase $MgFe_2O_4$ crystalline materials whereas Energy dispersive X-ray analysis (EDX) confirmed the presence of Mg, Fe and O in the compound. Scanning electron microscopy (SEM) image shows the porous scenery on the surface of the material whereas transmission electron microscopy (TEM) image displays polyhedron morphology of the particles. Sensor films fabricated utilizing these nanostructures were tested for gas/humidity sensing with notable success as the average sensitivity of the humidity sensor was found to be ~0.0237 $M\Omega$/%RH over the entire range of humidity tested for and maximum % sensor response was found to be 27.19 corresponding to exposure of 4 vol% LPG. Minimum response and recovery times were found to be 79 and 60 s respectively for 0.5 vol% LPG. The magnesium ferrite nanoparticles were tested for heat transfer applications as ethylene glycol based nanofluid component. The result shows that the thermal conductivity of ethylene glycol nanofluid was significantly increased compared to pure ethylene glycol due to the presence of suspended $MgFe_2O_4$ nanoparticles.

1 Introduction

Nanostructured spinel ferrites (MFe_2O_4; M=Mg, Ni, Zn, Cu, Co, Ca etc.), saddled with an impressive array of electronic, magnetic, optical, electrical and catalytic properties, have been amongst the most fascinating class of materials with existing or potential applications in contemporary technological industry [1–8]. Magnesium ferrite ($MgFe_2O_4$), a soft magnetic n-type semiconducting material, in particular,

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is an important member of the spinel family that has been garnering attention in recent years due to its intriguing electronic and magnetic properties and applications towards absorption, catalysis, sensing and biomedical drug delivery purposes [9–12]. Additionally, local hyperthermia or localized heating of tumours can be better realized by $MgFe_2O_4$ when compared to other ferrite materials [13]. Furthermore, interesting superparamagnetic properties of magnesium ferrite nanoparticles generate potential for its applications in ferrofluids, magnetocaloric refrigeration, and contrast agents for magnetic resonance imaging (MRI) [14]. With the context of $MgFe_2O_4$ being utilized in catalysis, a largely surface dominated property; it is worthwhile exploring its effectiveness as sensing material [15]. In fact, there have been several reports of nanostructures based on $MgFe_2O_4$ having been investigated for sensing of hazardous gaseous substances such as methane, NH_3, H_2, LPG, ethyl alcohol, carbon monoxide, carbon dioxide etc. [16–21]. Table 1 summarizes these reported gas sensing performances utilizing magnesium ferrite nanoparticles as the sensor material. A noticeable component of these reports is the fact that most of the reported sensing studies have been conducted at high operating temperatures which requires power consumption of various degrees depending upon the operating

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Fullerene (C$_{60}$)-modulated surface evolution in CH$_3$NH$_3$PbI$_3$ and its role in controlling the performance of inverted perovskite solar cells

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Abstract

We report here the effect of fullerene (C$_{60}$) incorporation on the growth of CH$_3$NH$_3$PbI$_3$ perovskite crystals and the effect on photovoltaic performance of perovskite solar cells (PSCs) prepared in inverse geometry. Incorporation of C$_{60}$ induced the growth of larger gains and compact thin film of perovskite with reduced defects, which led to its enhanced photovoltaic performance. Apart from that, C$_{60}$ also participates in transportation and collection of photo-generated electrons. The optimum incorporation of C$_{60}$ resulted in an impressive improvement in the power conversion efficiency (PCE) of champion PSC from 9.2 to 12.8%. Moreover, the C$_{60}$-doped PSCs exhibited improved air stability compared to undoped devices. The enhanced PCE in C$_{60}$-doped PSCs is a result of enhanced optical absorption and separation of photo-generated charge and their transportation in the active layer. Since the size of C$_{60}$ molecules is of the order of nm, they easily get filled into the perovskite voids and facilitate another percolation path ways for charge carriers to transport and suppress the recombination losses via passivating the recombination centres in perovskite layers. The compact perovskite layer with larger grains led to reduced inter-granular grain boundaries with reduced defects, which restricts the fast diffusion of moisture into active layer and resulted in improved stability in device performance.

1 Introduction

Perovskite solar cells (PSCs) technology is one of the fastest growing photovoltaic technologies as they have shown very high efficiency with high cost-effectiveness [1–3]. The potential of this technology could be understood from the improvement in its power conversion efficiency (PCE) itself, which reached to a record value of ~ 25.2% just within few years [4]. Moreover, they offer low production cost, light weight and feasibility with sheet to

sheet and roll-to-roll processing on flexible substrates. However, this technology is still far from the market as its overall performance is still not high enough to sought marketplace. Some of the issues that have been observe to affect their performance significantly are the grain size of perovskites crystallites, compactness of thin films, charge carriers traps, hysteresis in the I–V characteristics and poor stability [5–7]. It is important to note that usually high efficiency PSCs are prepared in a well-controlled inert environment and from perspective of commercialization they should be prepared in air. In recent years, a large volume of research activities have been carried out regarding formation of pin hole free compact perovskite layers [8–19]. It is a well reported fact that the compact and dense perovskite films without pinholes will facilitates the better pathway and reduces the charge carrier recombination between photoactive and charge transport layers [20–22]. To improve the quality of perovskite thin films and control the crystallization rate, many researchers have used additive or solvent engineering and solvent vapour treatment methods, viz. Methanol, Ammonium chloride (NH$_4$Cl), Lithium chloride (LiCl), 1,8-diiodooctane (DIO), Water, Methylamine (CH$_3$NH$_2$), pseudohalide Lead(II) thiocyanate (Pb(SCN)$_2$) and N,N-Dimethylmethanamide

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RESEARCH ARTICLE

Birth Defects Research | WILEY

Maternal biomarkers for early prediction of the neural tube defects pregnancies

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Abstract

Background: Neural tube defects (NTD) are one of the most common congenital birth defects. The reason for the NTD cause is still not completely known, but it is believed that some genetic and environmental factors might play a role in its etiology. Among the genetic factors the polymorphism in the folate gene pathway is crucial. Numerous studies have suggested the possible role of maternal higher plasma concentration of homocysteine and low concentration of folate and cobalamin in the development of NTD but some negative studies are also published.

Aim: Aim of the present was to find out the exact relation between NTD and maternal biomarkers like folate, cobalamin and homocysteine by conducting a meta-analysis.

Method: Different electronic databases were searched for the eligible studies. Standardized mean difference (SMD) with 95% confidence interval (CI) was used to determine association between maternal markers as risk for NTD pregnancy. The p value <0.05 was considered statistically significant in all tests. All the statistical analyses were done in the Open Meta-Analyst program.

Results: The homocysteine is significantly associated with the increased risk of NTD (SMD = 0.57; 95% CI: 0.35–0.80, p = <0.001; I2 = 93.01%), s-folate showed protective role in NTD (SMD = −0.48; 95% CI: −0.77 to −0.19, p = 0.001; I2 = 95.73%), similarly cobalamin is also having protective role (SMD = −0.28; 95% CI: −0.43 to −0.13, p = <0.001; I2 = 80.40%).

Conclusion: In conclusion this study suggest that different maternal biomarkers may be used for the early prediction of the NTDs.

KEYWORDS

folate, homocysteine, maternal biomarker, meta-analysis, neural tube defects

1 | INTRODUCTION

Neural tube defects (NTD) are very common congenital birth defects (Verma, 1978). NTD is the general term for a number of malformations but the most common of them are anencephaly, encephalocele and spina bifida. The prevalence of NTD is 1 in 33 infants globally (WHO, 2012). A recent meta-analysis suggests that the prevalence of NTD in India is 4.5 per 1,000 births (Allagh et al., 2015). NTDs are caused by the failure of closure of neural tube either partially or completely. The reason for the same is still not clear but it is believed that some genetic and environmental factors might play a role in the etiology of NTD (Wilde, Petersen, & Niswander, 2014). Among the genetic factors the most important is the polymorphism in the methylenetetrahydrofolate reductase (*MTHFR*) gene. This

REVIEW ARTICLE

Catechol-O-methyltransferase gene Val158Met polymorphism and obsessive compulsive disorder susceptibility: a meta-analysis

Pradeep Kumar[1] · Vandana Rai[1]

Abstract

Obsessive–compulsive disorder (OCD) is a common psychiatric disorder that affects approximately 1–3% of the general population. It is characterized by disabling obsessions (intrusive unwanted thoughts) and/or compulsions (ritualized repetitive behaviors). Catechol-O-methyltransferase (COMT) enzyme has an important role in inactivation of dopamine and higher dopamine levels may be implicated in OCD, hence COMT gene is a suitable candidate for OCD. Several case-control studies have evaluated the role of COMT Val 158Met (rs4680;472G->A) polymorphism as a risk factor for OCD but the results remained inconclusive, hence present meta-analysis was designed to find out correct assessment. All studies that investigated the association of COMT gene Val158Met polymorphism with OCD risk, were considered in the present meta-analysis. Statistical analysis was performed with the software program MetaAnalyst. In the current meta-analysis, 14 case-control studies with 1435 OCD cases and 2753 healthy controls were included. The results indicated significant association between COMT Val158Met polymorphism and OCD risk using allele contrast, homozygote and dominant models ($OR_{A\ vs\ G} = 1.14$; 95% CI = 1.02–1.27; $p = 0.01$; $OR_{AAvs.GG} = 1.33$; 95% CI = 1.09–1.62, $p = 0.004$; $OR_{AA+AGvs.GG} = 1.14$; 95% CI = 1.0–1.32; $p = 0.04$). In subgroup analysis based on case gender, meta-analysis of male cases showed significant association using all five genetic models ($OR_{AAvsGG} = 1.99$; 95%CI = 1.42–2.59; $p = <0.001$; $OR_{AA+AGvs.GG} = 1.59$; 95% CI = 1.20–2.10; $p = 0.001$), but did not show any association between COMT Val 158Met polymorphism and OCD risk in females. In conclusion, results of present meta-analysis supports that the COMT Val158Met polymorphism is a risk factor for OCD especially for males.

Keywords COMT · OCD · Val158Met · Polymorphism · Meta-analysis

Introduction

Obsessive–compulsive disorder (OCD) is a common and debilitating neuropsychiatric disorder that affects approximately 1–3% of the global population (Rasmussen and Eisen 1992; Eisen et al. 1999; Weissman et al. 1994). OCD is characterized by repetitive, persistent, intrusive thoughts and repetitive, compulsive behaviors (Ruscio et al. 2010). Although etiology of OCD is not completely known, but it is well reported that OCD is a multifactorial disorder (Nicolini et al. 1996; Pauls 2010) and twin, case-control association, and family segregation studies suggested that OCD has strong genetic component (Nicolini et al. 1996; Pauls 2010; Black et al. 1992;

Rosario-Campos et al. 2001). Based on the evidence that dopamine (DA) antagonists are beneficial for OCD patient's treatment (McDougle et al. 2000; Ramasubbu et al. 2000; Denys et al. 2002), the COMT gene has been suggested as one of the most important candidate genes. Catechol-O-methyltransferase (COMT) is an important enzyme involved in the metabolic inactivation of the dopamine and norepinephrine catecholamines by catabolizing dopamine (DA) (Gogos et al. 1998; Yavich et al. 2007).

Several polymorphism is reported in COMT gene, which is present on chromosome 22 q11. Out of all reported polymorphisms Val158Met (G to A) polymorphism is the most studied and clinically important. Substitution of Val by Met at 158th position in COMT protein reduces its activity. COMT inactivates dopamine in prefrontal cortex region of brain and Val to Met substitution leads to higher concentration of dopamine in prefrontal cortex (Lachman et al. 1996; Lotta et al. 1995; Chen et al. 2004).

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Vitamin D receptor (VDR) gene *FokI*, *BsmI*, *ApaI*, and *TaqI* polymorphisms and osteoporosis risk: a meta-analysis

Upendra Yadav, Pradeep Kumar and Vandana Rai*

Abstract

Background: Osteoporosis is a disease of the bones in which the density of the bones decreases. The prevalence of this disease greatly varies in different populations of the world. Numerous studies have been investigated VDR gene polymorphisms as osteoporosis risk in different ethnic groups. In present meta-analysis, the aim is to find out the role of VDR gene polymorphisms (*FokI*, *BsmI*, *ApaI*, and *TaqI*) in osteoporosis risk.

Methods: Suitable case-control studies for present meta-analysis were retrieved from four electronic databases. Open Meta-Analyst program was used for statistical analyses.

Results: Studies investigated *BsmI* (65 studies; 6880 cases/8049 controls), *ApaI* (31 studies; 3763 cases/3934 controls), *FokI* (18 studies; 1895 cases/1722 controls), and *TaqI* (26 studies; 2458 cases/2895 controls) polymorphisms that were included in the present meta-analysis. A significant association was found between the dominant model of *FokI* ($OR_{Ff + Ffvs.FF}$ = 1.19, 95% CI = 1.04–1.36, p = 0.01, I^2 = 39.36%) in the overall analysis and recessive model of the Caucasian population of *TaqI* polymorphism ($OR_{TT + Ttvs.tt}$ = 1.35, 95% CI = 1.11–1.63, p = 0.002, I^2 = 50.07%) with osteoporosis. On the other hand, no such effect is found in any other genetic models and in any other gene polymorphisms of the overall analyses or sub-group analyses.

Conclusion: In conclusion, the authors found that the dominant model of *FokI* in the overall analysis and recessive model of *TaqI* in the Caucasian population are significantly associated with the development of osteoporosis.

Keywords: Osteoporosis; Vitamin D receptor, *BsmI*, *ApaI*, *FokI*, *TaqI*

Background

Bone is an active tissue that maintains itself by continuous formation and reabsorption [1]. Osteoporosis is a condition in which the density of the bone decreases due to the increased activity of the osteoclasts [2]. A great variance is observed in the prevalence of osteoporosis in different ethnic groups [3]. Age and gender are the two major contributing factors in the occurrence of osteoporosis. Worldwide, one out of three women over the age of 50 experiences osteoporotic fractures in comparison to one in five men of the same age group [4].

Genetic and environmental factors play a crucial role in the etiology of osteoporosis [5, 6]. Calcium intake and exercise are the main risk factors for osteoporosis [5]. It is very well established that along with the environmental factors, individual genetics plays a key role in the development of osteoporosis, e.g., (i) low bone density is found in the female offspring of the osteoporotic women [7], (ii) male offspring of idiopathic osteoporotic men have low bone mineral density [8], and (iii) studies of female twins have shown heritability of bone mineral density (BMD) to be 57 to 92% [9, 10].

Amongst all the genes studied in osteoporosis, the vitamin D receptor (VDR) gene polymorphism is the most important in the etiology of the disease [11, 12]. VDR gene polymorphisms have been reported to be

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Evaluation of COMT Gene rs4680 Polymorphism as a Risk Factor for Endometrial Cancer

Pradeep Kumar[1] · Garima Singh[1] · Vandana Rai[1]

Abstract Catechol-O-methyletransferase (COMT) enzyme is involved in the inactivation of catecholamine and catechol estrogens. Catechol estrogens have carcinogenic potential and DNA damaging ability. Several studies investigated COMT Val158Met polymorphism as risk factor for endometrial cancer but the results were inconclusive. Hence the objective of present study was to find out exact association between COMT gene Val158Met polymorphism and endometrial cancer by a meta-analysis. Pubmed, Google Scholar, Springer Link and Science Direct databases were searched for case–control articles which investigated COMT Val158Met polymorphism in endometrial cancer cases. All statistical analysis was performed using MetaAnalyst and Mix programs. The results of meta-analysis suggested that there were no association between COMT Val158Met polymorphism and endometrial cancer risk (allele contrast model—$OR_{A \text{ vs. } G} = 0.97$, 95% CI = 0.86–1.10, $p = 0.67$; co-dominant model—$OR_{AG \text{ vs. } GG} = 0.91$, 95% CI = 0.77–1.06, $p = 0.23$; homozygote model—$OR_{AA \text{ vs. } GG} = 1.01$, 95% CI = 0.84–1.19, $p = 0.29$; dominant model—$OR_{AA+AG \text{ vs. } GG} = 0.93$, 95% CI = 0.77–1.11, $p = 0.43$; recessive model—$OR_{AA \text{ vs. } AG+GG} = 1.02$, 95% CI = 0.89–1.20, $p = 0.62$). Publication bias was absent. Subgroup analysis based on source of controls was also performed. In conclusion, results of present meta-analysis showed no association between COMT Val158Met polymorphism and susceptibility to endometrial cancer.

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Introduction

Endometrial cancer is the fourth common cancer among women [1, 2]. Several environmental and genetic factors are reported risk factor for endometrial cancer such as hormone therapy, obesity, metabolic disorder and allelic variants/genetic polymorphisms of small effect genes etc. Estrogen biosynthesis and metabolism are closely associated with endometrial carcinogenesis. The functional gene polymorphisms regulating estrogen metabolism can influence the levels of estrogen and intermediate products, which may potentially contribute to the susceptibility to endometrial cancer [3]. Catechol-O-methyltransferase (COMT) catalyzes catechol estrogens to form methyl conjugates, a process that detoxifies the catechol estrogens and prevent them from forming depurinating adducts [4].

COMT gene is present on chromosome 22q11.2 and is expressed in various mammalian tissues including liver, kidney, and breast [5, 6]. Several polymorphisms are reported in COMT gene, but the most widely studied and clinically important polymorphism is Val158Met polymorphism [7]. Val158Met polymorphism (rs4680) is a substitution of guanine to adenine nucleotide (G472A) in exon 4 of COMT gene, leading to substitution of valine to methionine amino acid at 158th position in protein. The homo-zygous mutant Met/Met (AA) genotype has been reported to decrease the COMT enzyme activity by 3–4 folds compared with wild-type Val/Val (GG) genotype; whereas the heterozygous Val/Met(AG) genotype has intermediate activity [8]. In the past decade, many studies have investigated the relationship between COMT

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RESEARCH PAPER

Journal of Basic Microbiology

Enhanced growth and yield of oyster mushroom by growth-promoting bacteria *Glutamicibacter arilaitensis* MRC119

Simpal Kumari | Ram Naraian ©

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Abstract

Promotion of mushroom growth by means of biological agents replacing chemicals is an emerging and highly demanded issue in the sector of mushroom cropping. The present study was aimed to search for a novel bacterium potentially able to enhance mushroom growth and yield. A total of 2165 bacterial isolates purified from different samples were scrutinized through various growth-promoting attributes. As a consequence of rigorous screening, 26 isolates found exhibiting positive traits of mushroom growth promotion. Thereafter, in response to the cocultivation (fungus and bacteria), a potent bacterial strain was isolated capable to improve significantly the mycelial growth. In cocultivation the highest radial and linear growth rate was 7.6 and 8.1 mm/day on 10th and 11th days, respectively. The fruitbody yields and biological efficiency (BE) of the inoculated sets were 28% and 58% higher than the uninoculated control sets. The bacterium was molecularly identified based on 16S ribosomal RNA sequencing and confirmed as *Glutamicibacter arilaitensis* MRC119. Therefore, the bioinoculant of the current bacterium can be potentially useful as an ecofriendly substitute stimulating the production of mushroom fruit bodies with improved BE.

KEYWORDS

bioinoculant, biological efficiency, Glutamicibacter sp., Pleurotus sp., mycelial growth rate

1 | INTRODUCTION

Biological approaches particularly the use of growth-stimulating microorganisms to improve crop growth and yield have been extensively practiced for eco- and agriculture-friendly cropping worldwide. Beneficial microbes not only promote growth but also maintain the health and development of individual plants [1]. Though, the use of chemical and biological additives has shortened the crop and enhances the yield of oyster mushrooms but only up to a certain limit [2]. Potent microbial population indeed plays a very crucial role in mycelial growth and other cultivation stages of mushrooms including fructification [3]. Various bacterial species belonging to particularly genus *Pseudomonas* may play a significant role in the artificial growing of edible mushrooms [4]. The knowledge about the role of microorganisms in the development of mushrooms is

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Abbreviations: ACC deaminase, 1-aminocyclopropane-1-carboxylic acid deaminase; BE, biological efficiency; IAA, indole acetic acid; MGPB, mushroom growth-promoting bacteria; SEM, scanning electron microscopy.

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INFLUENCE OF BACTERIA ON THE MYCELIAL GROWTH AND BIOLOGICAL EFFICIENCY OF OYSTER MUSHROOM *PLEUROTUS FLORIDA* PF05

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Abstract

Oyster mushroom *Pleurotus florida* was cultivated in poly bags employing wheat straw as substrate. The effect of bacterial culture (BC) and culture filterate (CF) of a bacterial isolate (*Glutamicibacter arilaitensis* MRC119) was investigated on the growth rate, ACC deaminase, fruitbodies and the biological efficiency of oyster mushroom. The growth rate of mycelia was faster when treated with culture filtrate and bacterial culture in comparision to untreated control. The fastest radial and lineal growth rate achieved were as 8.97 mm/d, 8.11 mm/d respectively with the treatments of CF and BC on 20th day, while control showed 4.98 mm/d. The highest ACC-deaminase (687.76 IU/g) production with CF while BC showed as 513.67 IU/g. However, the highest number of fruiting body were recorded as 41.32 and 32.23 with CF and BC treatments, which were higher than control (17.32) sets. The treatment with CF resulted highest yield of biological efficiency (256.45%) followed by 204.65% with BC and 154.87% of control. Therefore, the use of mushroom growth promoting bacterial culture and its culture is recommended for better biological efficiencies.

Keywords: Mushroom cultivation, oyster mushroom, bacteria, fruiting body and biological efficiency.

Introduction

Mushroom have big advantage of their cultivation in small spaces of a landless farmer's house and may generate appropriate income that aids in family support (Mamiro and Mamiro, 2011; Tesfay *et al.*, 2020) and the supply of proper food. Supplementing the cultivation substrates with various additives, shorten the crop period and also increases mushroom productivity (Curvetto *et al.*, 2002; Naraian *et al.*, 2009, 2010; Carrasco *et al.*, 2018). However, the excess supplementations with harsh chemicals cause loss in the quality and texture of mushrooms. Thence, there is a thrust need to search a new inoffensive biological alternative to improve the sustainable cultivation of mushroom and can enhance the fruit body yield of mushrooms.

Many microorganisms have been shown to promote the yield of *P. ostreatus* and other cultivated mushrooms, the biological properties of substrate appears very important for induction of fructification. Growth and development of mushrooms are particularly affected by bacteria pseudomonads (Grewal and Rainey, 1991). The beneficial bacterial microflora positively affect growth of fungal mycelia (Mohammad and Sabaa, 2013). Moreover, bacteria also initiate primordia formation and stimulate growth of fungi (Cho *et al.*, 2003). Young *et al.* (2012) reported bacteria such as *Pseudomonas resinovorans*, *Microbacterium*

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esteraromaticum significantly improved yield and biological efficiency of button mushroom. Many bacteria have the ability to produce ACC deaminase enzyme which has potential to degrade ACC into a-ketobutyrate and ultimately increase mushroom growth (Dong *et al.*, 2010).

Kim *et al.* (2008) revealed that *Pseudomonas* sp. P7014 enhance the growth of oyster mushroom (*Pleurotus eryngii*) in bottle culture. Besides; Cho *et al.* (2003) also found the similar result of growth promotion with culture of edible fungus *Pleurotus ostreatus* and fluorescent pseudomonads. The *Arthrobacter* sp. improves the growth plus yield of mushroom (Young *et al.*, 2012; Zhou *et al.*, 2017) and the bacterium *Arthrobacter arilaitensis* presently named as *Glutamicibacter arilaitensis* (Sutthiwong *et al.*, 2018; Cleary *et al.*, 2018). Therefore the present work was conducted to investigate the effect of a bacteria *Glutamicibacter arilaitensis* MRC119 (GenBank accession: MN626391) on the different aspects (Radial & lineal growth rate, yield and biological efficiency) of oyster mushroom *Pleurotus florida*.

Materials and Methods

Microbial strains and their maintenance

Fungal culture of oyster mushroom *Pleurotus florida* and growth promoting bacteria *Glutamicibacter arilaitensis* MRC119 were obtained from Mushroom Training &

Geogenic source of arsenic and their effect on vegetable seed germination

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Abstract: The serious health and environmental problem arises due to arsenic, across the globe. Several researcher have drawn their attention to these problems, arsenic mainly found in soil, aquifer water/drinking water through naturally. In the present study, physicochemical and arsenic content were observed in two types of soil from different agricultural sites of district Ballia, one type of agricultural sites were irrigated by BWDI and other agriculture sites were not BWNDI. Agricultural soil sites (∑N= 209) of BWDI revealed that all soil samples have arsenic content and maximum arsenic concentration (55 ppb) were observed at sites of Basdih, district Ballia, while arsenic content was not detected on the soils of other agricultural field sites (N=∑30) which were based on BWNDI. Interesting and significant observation observed on the surveys based on farmers of the chosen sites, there are no industries or activities found who are able to correlate the high concentration of arsenic in soil except bore well water. Arsenic contents were observed in the 250 bore well water samples and their concentrations were varied with bore well depth. Beyond the 100 foot depth of bore well water showed the maximum concentration of arsenic as compared with 40 foot depth. The high concentration of arsenic, as well as its more retention time, reduces seed viability of radish and carrot plants.

Keywords: Arsenic - Aquifer water - Agricultural soil - Seed viability - Radish & carrot plant

INTRODUCTION

Arsenic metal has a metalloid property exist in inorganic as well as organic form, highly mobilized in environment through soluble in water or in air through their volatile behavior in the form of arsine AsH_3, monomethylarsine (CH_3AsH_2), dimethylarsin $(CH_3)_2AsH$, and trimethylarsine $(CH_3)_3As$ (Cullen & Reimer 1989, Smedley & Kinniburgh 2002). Arsenic is wildly present in soil, rock, sediment, and metal ore in the form of sulfide or compounds of various metals (Aronson 1994). Arsenic introduced into soil/groundwater by weathering of rocks and minerals by leaching and surface runoff naturally. Man-made activities also enhance the arsenic availability in soil or water body through organic chemicals, pesticides, insecticides, mining etc. (Benbrahim & Waalkes 2008, Meharg et al. 2009). In spite of that many factors are responsible to regulate the concentration of arsenic and its transport in environment including ground water, like redox potential, adsorption/absorption, dissolution, pH and biological transformation etc. Four oxidation states (+5, +3, 0, -3) of arsenic exist under normal Eh condition in aquatic system, while predominant form of arsenic is inorganic form having As^{+5} stage and As^{+3} stage (Smedley & Kinniburgh 2002). Jain & Ali (2000) reported that As^{+3} stage is about 60 times more toxic as compared to As^{+5} stage and inorganic arsenic is about 100 times toxic than organic toxic; in general toxicity of arsenic species are arsenite > arsenate > monomethyl arsonate > dimethyl arsinate. Adriano (2001) reported that uses of arsenicals as pesticides has significantly contributed to increase the concentration of arsenic in soil; use of arsenic in 1992 was about 23,900 metric tons of which 67% was used for the production of wood preservatives (Adriano 2001). High concentration of arsenic in drinking water

Chemistry

ScienceDirect

Modelling studies for remediation of Cr (VI) from wastewater by activated *Mangifera indica* bark

Deepak Pathania [a, b] ✉, Arush Sharma [c], A.K. Srivastava [d]

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Highlights

- Activated bark prepared from *Mangifera indica* was used for the removal of Cr(VI) from aqueous solution.

- Activated bark was characterized by techniques such as FTIR, SEM, and TGA.

- The effect of different adsorption parameters was optimized. Langmuir, Freundlich, and Tempkin's isotherms were studied to investigate the adsorption capacity.

- Langmuir model was found to be best fitted with a maximum adsorption capacity of 78.96 mg/g with monolayer adsorption.

- The adsorption kinetics confirmed the pseudo-first-order model which indicates that physio-adsorption.

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Abstract

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Microwave-Induced Montmorillonite-Mediated Facile Synthesis of Enamines

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Montmorillonite clay-mediated simple and high yielding protocol for the synthesis of various enamines with secondary amines and ketones is developed under microwave condition. This protocol is very convenient to accesses the enamines from cyclic amines with various carbonyl compounds in high yield under mild reaction conditions with short reaction time.

Keywords: Microwave, Montmorillonite, Enamine.

INTRODUCTION

Enamines are synthetic equivalents of enol and enolates and synthesized by the condensation of aldehydes or ketones with 2° amines under acidic or basic condition [1]. These are important precursors in organic synthesis because they can undergoes alkylation and acylation reaction with diverse reagents with high degree of regioselectivity [2]. Enamines have also serve important synthetic building block to execute 1,4-conjugate addition and annulation reaction in the synthesis of diverse heterocyclic and bioactive natural products including anticonvulsant, anti-inflammatory and antitumor agents [3]. Enamines are used to produce 1,4-dihydropyrines, pyrroles, pyrazoles, pyridones, quinolines, dibenzodiazepines, tetrahydrobenzo-xazines, tetronic acids, azasteroids with potential biological activities [4-7]. There are a number of methods available in the literature for the synthesis of enamines. For example, condensation of 1,3-dicarbonyl compounds with amines, silica gel-mediated synthesis [8], ionic liquid-induced reactions [9], bismuth(III) trifluroacetate-catalyzed conditions [10], ultra-sonication method [11], palladium-catalyzed coupling reaction [12] and iodine catalyzed reactions [13].

Different types of clay-mediated reactions are easy to perform because they are not soluble in organic solvents. Most of the clays or solid surfaces are acidic or neutral in nature. Clays have the capability to absorb water and organic compounds inside the cavity in their structures. It is reported that clays are catalyze a diverse organic reaction including substitution, addition, elimination, hydrogenation, hydrogenolysis, dehydration, aromatization, annulation, Diels-Alder and isomerization. These methods are efficient in the synthesis of a wide range of diverse molecules of biological and medicinal interests. Montmorillonite K-10 has been proven its versatile catalytic efficiency in organic synthesis [14].

In this article, microwave-induced montmorillonite K-10 clay-mediated facile synthesis of enamines in good yield is performed. This reaction proceeds at a much faster rate than the conventional heating method. Clays work well in microwave induced processes in the absence of any solvent [15,16]. Microwave assisted reactions are extremely powerful in accelerating the rate of many chemical reactions [17]. It is not possible to know the exact temperature of the montmorillonite K-10-mediated reactions in a microwave oven. In this paper, a facile synthesis of enamines by reacting diverse ketones with secondary cyclic amines in the presence of montmorillonite K-10 under microwave irradiation is described.

Microwave-Induced Bismuth Nitrate-Catalyzed Michael Reaction of 3-Amino β-Lactams with Enones

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Microwave-induced bismuth nitrate-catalyzed reaction of 3-amino β-lactams with unsaturated ketones is performed in order to obtain substituted amino β-lactams. Amino β-lactams were obtained through the strategy of [2+2] ketene-imine cycloaddition followed by deprotection of phthalimido β-lactams with ethylene diamine.

Keywords: Microwave, Amino β-lactam, Bismuth nitrate, Catalysis, Michael reaction.

INTRODUCTION

Aza-Michael addition reaction is an important tool for the formation of C-N bond between nitrogen atom of donor and carbon atom of the acceptor molecules. This is a conjugate addition of nitrogen nucleophile to an α,β-unsaturated carbonyl compound. This is an important reaction to accesses diverse medicinally privileged molecules like antibiotics, anticancer and biomimetic molecules of oligomer of β-amino acids and peptides [1,2]. α-Amino β-lactams systems with cis-configuration are present in numerous monocyclic and bicyclic antibiotics [3]. Similar structures with antibacterial trans-configuration are also known [4]. trans α-Amino β-lactam is active against cancer cell lines in vitro [5,6], whereas cis β-lactams with anticancer activities are also reported in the literature [7]. β-Lactams are served as the key molecules for the synthesis of numerous other compounds including natural products, alkaloids, amino sugars and amino acids [8,9]. Reactions at 3-amino center of β-lactam ring is necessary to functionalize them. In this paper, a simple microwave-induced bismuth nitrate-catalyzed Michael reaction of 3-amino β-lactams with α,β-unsaturated ketone is described.

3-Amino β-lactams as donor react with electron deficient carbonyl compounds known as Michael acceptors lead to the formation of corresponding mono-aza and bis-aza-adducts under microwave irradiation (Scheme-I). Despite progress in β-lactam research [10], no paper is published which describe functionalization of 3-amino group present in β-lactam ring through a catalytic Michael reaction [11,12]. In continuation of our efforts to explore the catalytic properties of bismuth nitrate in the synthesis of numerous organic molecules of biological interests, we report here a simple and environmentally benign procedure to obtain mono and bis-aza-substituted β-lactams under microwave condition in excellent yield. In previous study, aza Michael reaction of diverse aliphatic and aromatic amines to unsaturated enones via bismuth nitrate-catalyzed reactions is reported [13].
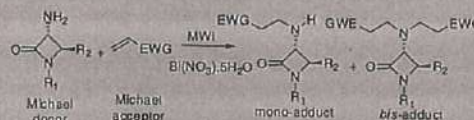
Scheme-I: Bismuth nitrate catalyzed aza-Michael mono and bi-addition under microwave condition

We extended the scope of this reaction using amino β-llactam. Our methodology of bismuth nitrate catalyzed aza-Michael reaction of enone was very simple and highly efficient.

Microwave-Induced Montmorillonite-Mediated Facile Synthesis of Enamines

Ram Naresh Yadav[1,2], Indrani Banik[3], Ashok Kumar Srivastava[1], Katherine Ramos[2] and Bimal Krishna Banik[4,*]

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Montmorillonite clay-mediated simple and high yielding protocol for the synthesis of various enamines with secondary amines and ketones is developed under microwave condition. This protocol is very convenient to accesses the enamines from cyclic amines with various carbonyl compounds in high yield under mild reaction conditions with short reaction time.

Keywords: Microwave, Montmorillonite, Enamine.

INTRODUCTION

Enamines are synthetic equivalents of enol and enolates and synthesized by the condensation of aldehydes or ketones with 2° amines under acidic or basic condition [1]. These are important precursors in organic synthesis because they can undergoes alkylation and acylation reaction with diverse reagents with high degree of regioselectivity [2]. Enamines have also serve important synthetic building block to execute 1,4-conjugate addition and annulation reaction in the synthesis of diverse heterocyclic and bioactive natural products including anti-convulsant, anti-inflammatory and antitumor agents [3]. Enamines are used to produce 1,4-dihydropyrines, pyrroles, pyrazoles, pyridones, quinolines, dibenzodiazepines, tetrahydrobenzo-xazines, tetronic acids, azasteroids with potential biological activities [4-7]. There are a number of methods available in the literature for the synthesis of enamines. For example, condensation of 1,3-dicarbonyl compounds with amines, silica gel-mediated synthesis [8], ionic liquid-induced reactions [9], bismuth(III) trifluroacetate-catalyzed conditions [10], ultra-sonication method [11], palladium-catalyzed coupling reaction [12] and iodine catalyzed reactions [13].

Different types of clay-mediated reactions are easy to perform because they are not soluble in organic solvents. Most of the clays or solid surfaces are acidic or neutral in nature. Clays have the capability to absorb water and organic compounds inside the cavity in their structures. It is reported that clays are catalyze a diverse organic reaction including substitution, addition, elimination, hydrogenation, hydrogenolysis, dehydration, aromatization, annulation, Diels-Alder and isomerization. These methods are efficient in the synthesis of a wide range of diverse molecules of biological and medicinal interests. Montmorillonite K-10 has been proven its versatile catalytic efficiency in organic synthesis [14].

In this article, microwave-induced montmorillonite K-10 clay-mediated facile synthesis of enamines in good yield is performed. This reaction proceeds at a much faster rate than the conventional heating method. Clays work well in microwave induced processes in the absence of any solvent [15,16]. Microwave assisted reactions are extremely powerful in accelerating the rate of many chemical reactions [17]. It is not possible to know the exact temperature of the montmorillonite K-10-mediated reactions in a microwave oven. In this paper, a facile synthesis of enamines by reacting diverse ketones with secondary cyclic amines in the presence of montmorillonite K-10 under microwave irradiation is described.

Page No.45

Research Article

Indium Bromide-catalyzed Unprecedented Hydrogenolysis: A Novel One-Pot Synthesis of Per-O-Acetylated β-carboxymethyl O and S-glycosides

Author(s): Ram Naresh Yadav, Amrendra K Singh and Bimal Banik*

Abstract

Numerous O (oxa)- and S (thia)-glycosyl esters and their analogous glycosyl acids have been accomplished through stereoselective glycosylation of various peracetylated bromo sugar with benzyl glycolate using InBr3 as a glycosyl promotor followed by in situ hydrogenolysis of resulting glycosyl ester. A tandem glycosylating and hydrogenolytic activity of InBr3 has been successfully investigated in a one-pot procedure. The resulting synthetically valuable and virtually unexplored class of β-CMGL (glycosyl acids) could serve as an excellent potential chiral auxiliary in the asymmetric synthesis of a wide range of enantiomerically pure medicinally prevalent β-lactams and other bioactive molecules of diverse medicinal interest.

Keywords: Glycosides, glycosylation, anomeric position, stereoselectivity, hydrogenolysis, catalysis.

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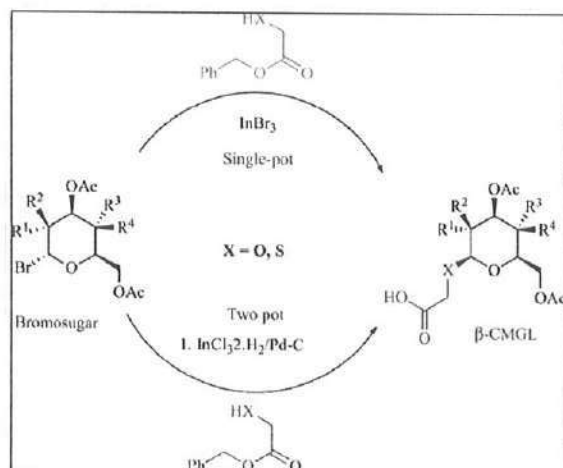
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ANTIFUNGAL ACTIVITY OF SOME ISOMERIC SPIRO PYRAZOLONES.

Amrendra Kumar Singh

Department Of Chemistry, Faculty of Engineering & Technology V.B.S. Purvanchal University, Jaunpur- India.
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Abstract: 4-Arylmethylene-2,4-dihydro-2 5-disbstituted-3H-pyrazol-3-ones (1a-f : as dipolarophile) react with benzonitrile oxide (2;as 1,3-dipole) to yield E/Z-4.5-dihydrospiro-[3-phenyl-5-substituted phenyl isoxazole-4,4' (2',4'-dihydro-5'-methyl-2'-phenyl/phenyl methyl-3'H-pyrazo-3'-ones)]

Keywords— Pyrazol, Benzonitrile, Isoxazole, Dipolarophile

I INTRODUCTION

The importance of pyrazolones chemistry lines in the fact that these have occupied a unique position in heterocyclic chemistry due to their wide applicability in various fields viz. Industry [1], medicinal therapy [2, 3] and agriculture[4]. 2,4-Dihydro-3H- pyrazol-3one derivative have physiological properties and have found application as antibacterial[5] antihypertensive [6],antinfammatory[7], anticonvulsant[8] antitumor[9] and antifungal[10] agents. These importances of pyrazolones derivative have promoted us to synthesis title compounds and our attempt in to correlate antibacterial activity and structure of the compounds.1, 3-Dipolar Cycloaddition reactions have been studied to a numerous unsaturated systems leading to five member ring heterocyclic. 1, 3, 4-Arylmethylene-2, 4- dihydro-2, 5-disubstituted -3H-pyrazole-3-ones. [(As dipolarophile) reacted with diphenylnitrilimine (as 1, 3-dipole) to yield two isomers, VIZ E and Z-4, 5-Dihydro spiro-(4-aryl-1, 3-diphenyl pyrazol-5, 4'-(2', 4'-dihydro-2', 5'-disubstituted-3'H-Pyrazole-3'-ones)].

1,3-Dipolar Cycloaddition reaction of 4-arylmethylene-2,4-dihydro-5-methyl-2-phenyl/phenylmethyl-3H-pyrazol-3-ones (1a-f;as dipolarophile) with benzonitrile oxide (2; as 1,3-dipole) resulted in the formation of E/Z 4,5-dihydro spiro [3-phenyl-5-substituted phenyl isoxazole-4,4'-(2',4'-dihydro-5-methyl-2'-phenyl/phenylmethyl-3'H-pyrazole-3'-one] (scheme-1). This reaction is stereo specific as well as stereo selective and the peculiarity of the reaction commanded interest and stimulated to undertake the synthetic process. The benzonitrile oxide (2) is generated in situ by the reaction of benzhydroxamoyl chloride and triethylamine in the presence of dry chloroform at room temperature. The physical and spectral data of the compounds are presented (Table-1).

II EXPERIMENTAL

Melting points were determined on a Buchi apparatus and are uncorrected. Microanalyses were carried out on a Coleman C, H and N-analysers. IR spectra (Nujol) were recorded on Perkin-Elmer-720 and 257 spectrophotometers and PMR spectra (CDCl$_3$) on Varian A-60D and Jeol FX-90Q spectrometers using TMS as an internal standard.

4-Arylmethylene-2, 4-dihydro-2, 5-disubstituted-3H-pyrazol -3-ones [5] (1a-f) and the benzhydroxamoyl chloride [6], were prepared following the standard methods.

E/Z-4,5-dihydro spiro (3-phenyl-5-substituted phenyl isoxazol-4,4'-(2',4'-dihydro-5'-methyl-2'-phenyl/phenylmethyl-3'H-pyrazol-3'-one)(3a-f).

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Ascorbic acid-mediated reactions in organic synthesis

Ascorbic Acid-mediated Reactions in Organic Synthesis (https://www.eurekaselect.com/node/184127/article/ascorbic-acid-mediated-reactions-in-organic-synthesis)
NEWS RELEASE: 25-SEP-2020

One of the important objectives of green chemistry is the use of eco-friendly solvents and catalysts to perform chemical reactions. Catalysts such as organocatalysts, enzymes, and ionic liquids have shown very assuring results in synthesis by reducing the number of hazardous effects of chemical reactions. Among those catalysts, the activities of ascorbic acid are promising because of its extraordinary abilities.

Ascorbic acid (Vitamin C or ascorbate) is the most well-known vitamin found in different types of foods, most commonly in fruits. For many years, ascorbic acid has been used as a constituent of various dermatologic drugs and cosmetics. However, because of the lack of an enzyme called gulonolactone oxidase, humans and apes cannot synthesize ascorbic acid. Ascorbic acid was first isolated in 1928 by Hungarian biochemist Albert Szent-Györgyi and he named it as hexuronic acid. In 1932, Haworth and King independently established the molecular structure of hexuronic acid and renamed it as ascorbic acid.

Ascorbic acid is an antioxidant. Its oxidation-reduction potential and the stability of its oxidation products contribute values to the application of ascorbic acid as an antioxidant. In addition, as a water-soluble reducing agent and donor antioxidant, ascorbic acid can undergo three consecutive or active types: ascorbate (reduced form), dehydroascorbic acid (oxidized form) and ascorbate radical (intermediate oxidized form). The two-way reactions among these three forms occur very simply due to the low one-electron transfer potential. As a consequence, ascorbic acid has been accepted as a chemically unstable substnace. It is observed that ascorbic acid promptly undergoes pH-dependent autoxidation and makes hydrogen peroxide. In the presence of catalytic metals, this oxidation is accelerated. The combination of metal and ascorbic acid is a very efficient oxidizing system. This system is mainly employed for the hydroxylation of alkenes, aromatics, and other oxidation reactions. Besides, in the presence of catalytic metal ions, ascorbic acid can exert pro-oxidant effects. Ascorbic acid serves as a reducing cofactor for many enzymes.

In organic synthesis, ascorbic acid can be used as a reactant in the preparation of chiral synthons and also as a catalyst to accelerate the reaction. Several important reactions are performed with ascorbic acid: These include the oxidation of amines to carbonyl compounds, cross-coupling of disulfides with aryl iodides, ATRA of polyhalogenated compounds to alkenes, ATRP of polyhalogenated compounds to alkenes, ATRC of polychloroamides to cyclic amides, Amination of aryl halides to primary aromatic amines, oxidation of sulfides, arylation of arenes with anilines, cyclization of aryl radicals with arenes, metal-free synthesis of aryl sulfides, oxidative arylation of vinyl arenes to 2-aryl acetophenes, photoreductive

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RESEARCH ARTICLE

An Expeditious Route for the Synthesis of Oxazepine Triazolo-β-Lactams through Intramolecular Metal-Free [3 + 2] Azide–Alkyne Cycloaddition

Ram N. Yadav (https://orcid.org/0000-0001-6094-3447) [A] [B], Sunena Chandra [B], Armando Paniagua [B], Md. Firoj Hossain [C] and Bimal Krishna Banik (https://orcid.org/0000-0002-7873-9062) [B] [D] [E]

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Abstract

A copper-free intramolecular azide–alkyne cycloaddition reaction of 4-hydroxymethyl-β-lactam with sodium azide has been described. The present approach involves the incorporation of an alkyne moiety through O-alkynylation of 3-hydroxy β-lactam with various propargylic halides. The generality of the method has been demonstrated by treating the corresponding tosylates or mesylates of the hydroxymethyl functionality of a variety of β-lactam-tethered terminal and internal alkynes with sodium azide in a one-pot three-step reaction to furnish novel oxazepane-β-lactam fused triazole scaffolds of diverse interest in good yield.

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VSC-HVDC BASED LOAD FREQUENCY CONTROL OF MULTI-AREA INTERCONNECTED POWER SYSTEM UNDER VARYING LOAD

Piyush Kumar Yadav, Rajnish Bhasker and Satyam Kumar Upadhyay

Electrical Engineering Department, VBS Purvanchal University, Jaunpur, India

ABSTRACT

This paper deals with the effect of VSC-HVDC link on two area load frequency control having thermal-thermal power system interconnection under varying load as well as step change in load. The latest technology power electronic based HVDC transmission line having numerous advantage in order to improve the frequency control and enhancing the stability in the transmission network. The VSC based HVDC transmission mainly consists of two converter stations connected by a DC cable. The performance is evaluated by using MATLAB/Simulink.

Key words: Load frequency control(LFC), Automatic frequency control, VSC-HVDC, Automatic generation control (AGC), area control error

Cite this Article: Piyush Kumar Yadav, Rajnish Bhasker and Satyam Kumar Upadhyay, VSC-HVDC Based Load Frequency Control of Multi-Area Interconnected Power System Under Varying Load, *International Journal of Advanced Research in Engineering and Technology,* 11(10), 2020, pp. 423-434.
http://www.iaeme.com/IJARET/issues.asp?JType=IJARET&VType=11&IType=10

1. INTRODUCTION

The conventional A.C transmission system imposed systems impose kind of limitation to transfer the power in the deregulated power system, especially in the case of transmission between unsynchronized AC systems[1-3]. The AC transmission systems have various limitations such as the ferranti effect in the long transmission lines based on HVAC cables, the problem of reactive power due to HVAC cables, the problem of reactive power due to the HVAC cable charging is very important[15]. In addition, the length of these cables limits the ability of active power transmission, which decreased as the length of the line increases. On the other hand, the HVDC transmission system has many advantages that can provide solutions to existing problems in A.C systems thus increased the stability of the system. VSC-HVDC systems provide better grid connection solution for weak grids and unsynchronized AC systems. The VSC of HVDC can work in both directions, it provides efficient voltage control with a better power flow controllability[5-6]. The requirements in the frequency

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PERFORMANCE EVALUATION OF ENERGY MANAGEMENT SYSTEM FOR DOMESTIC PURPOSE USING SUPER- CAPACITOR WITH DC-DC CONVERTER

Piyush Kumar Yadav, Dr. Rajnish Bhasker and Satyam Kumar Upadhyay
Dept. of Electrical Engineering, VBS Purvanchal University, Jaunpur U.P, India.

ABSTRACT

In this paper, a selected combined topology and a new control scheme are proposed to control the power sharing between batteries and super-capacitors with over DC voltage charging protection by using resistor parallel to the main DC link. This paper deals about the energy storing behavior of super capacitor and as we know super capacitor is a best energy storage element which is more helpful for running of electrical vehicle even more effectively.

In the modern era power electronics devices more helpful for driven of electrical devices. DC-DC converters are used to running the system more efficiently. Our mainly focus in this paper only on super capacitor instead of battery. We can evaluate the overall performance of energy management system by using MATLAB/Simulink software.

Keywords: Super-capacitor, DC-DC converter , UPS, Energy storage system , PV array.

Cite this Article: Piyush Kumar Yadav, Rajnish Bhasker and Satyam Kumar Upadhyay, Performance Evaluation of Energy Management System for Domestic Purpose using Super- Capacitor with DC-DC Converter, *International Journal of Advanced Research in Engineering and Technology,* 11(10), 2020, pp. 1178-1192.
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1. INTRODUCTION

Now a days as we know Energy Storage Systems (ESS) are needed by the traditional electrical generation industry, which have almost zero storage capability[3-4]. After generation of power Traditional electricity transmission and distribution systems transport the electrical energy from large power plants to consumers in a unidirectional channel [1-2]. Due to this, electricity must be consumed by matching precisely the generation with demand, but the electricity demand fluctuates heavily and consequently power plants must be overloaded which implies an inefficient and expensive electrical system[4-6]. We know that the Energy production could be

PERFORMANCE EVALUATION OF GRID TIED INVERTER TO MEET THE SURPLUS DEMAND OF LOAD

Piyush kumar yadav, Dr. Rajnish bhasker, Satyam kumar Upadhyay,Vishwas kumar, Anurag Pal and Saurabh Kumar Rao

Electrical engineering departement, VBS purvanchal university, jaunpur, India.

ABSTRACT

This paper deals with The complexity of the power grid, in conjunction with the ever increasing demand for electricity, creates the need for efficient analysis and control of the power system. The evolution of the legacy system towards the new smart grid intensifies this need due to the large number of sensors and actuators that must be monitored and controlled, the new types of distributed energy sources that need to be integrated and the new types of loads that must be supported. In this context, modelling and simulation is an invaluable tool for system behaviour analysis, energy consumption estimation and future state prediction. In this paper, dynamic modelling and simulation of a single stage grid connected inverter have been carried out in this work.

Keywords: Modulation Index, Phase degree (degree), Voltage from grid, Current from grid, Voltage from inverter, current from inverter.

1. INTRODUCTION

Electricity is a crucial facet of any country's prosperity. The utility electricity sector in India has one National Grid with an installed capacity of 350.162 GW as on 28 February 2019.Renewable power plants constituted 15.3% of total installed capacity[1-2]. During the fiscal year 2017-18, the gross electricity generated by utilities in India was 1,303.49 TWh and the total electricity generation (utilities and non utilities) in the country was 1,486.5 TWh.The gross electricity consumption was 1,149 kWh per capita in the year 2017-18[3-4]. India is the world's third largest producer and third largest consumer of electricity. Electric energy consumption in agriculture was recorded highest (17.89%) in 2015-16 among all countries. The per capita

INFLUENCE OF FACTS DEVICES ON ELECTRICAL TRANSMISSION SYSTEM

Satyam Kumar Upadhyay, Piyush Kumar Yadav, Dr. Rajnish Bhasker and Saurabh V Kumar

Electrical Engineering Department, VBS Purvanchal University, Jaunpur, India

ABSTRACT

This report contains the study of Flexible AC Transmission System (FACTS) equipment operation in transmission systems. In the present scenario the demand for electrical energy has increased manifold. This has led to the facing of power transmission limitation crisis by energy transmission systems. The limitations occur due to maintaining a balance between supplying the allowed level of voltage and maintaining stability of the system. Due to the power crisis the FACTS devices play a crucial role in the present scenario. In energy transmission systems FACTS are effective equipments on power control. They help facilitating the improvement in power transmission capability while minimising the transmission losses and impact on the environment. They also aid in the improvement of power quality while maintaining the stability of the system.The principal operating modes and applications of FACTS equipment in transmission and distribution system such as Static Var Compensator (SVC), Static Synchronous Compensator (STATCOM), Thyristor controlled series capacitor (TCSC), Static Synchronous Series Compensator (SSSC) and Unified Power Flow Controller (UPFC) is discussed in this report. The characteristics of FC-TCR and UPFC were studied and their models were simulated in Matlab using simulink. In Fixed capacitor Thyristor Controlled Reactor the regulation of power flow was done by changing the firing angle of the thyristor. The compensation obtained was better than that of a normal transmission line. In case of Unified Power Flow Controller the injected voltage and the injected current were the control parameters. The power flow can be regulated by changing the magnitude or phase of the injected voltage while for the injected current the value of the injected current and the shunt resistance are varied for regulating power flow

Keywords: SSS controller, Data acquisition system, Power computation circuit, Firing pulse generator, pulse voltage source convertor.

Cite this Article: Satyam Kumar Upadhyay, Piyush Kumar Yadav, Rajnish Bhasker and Saurabh V Kumar, Influence of Facts Devices on Electrical Transmission System, *International Journal of Advanced Research in Engineering and Technology*, 11(11), 2020, pp. 1248-1270.
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INFLUENCE OF POLE PLACEMENT TECHNIQUE AND OPTIMAL CONTROL TECHNIQUE FOR ISOLATED MULTI-AREA LOAD FREQUENCY CONTROL IN POWER SYSTEM

Piyush Kumar Yadav, Dr. Rajnish Bhasker, Saurabh V Kumar,
Satyam Kumar Upadhyay and Vinod Kumar Yadav
Electrical Engineering Department, VBS Purvanchal University,
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ABSTRACT

This research paper presents and deals with centralized and decentralized control technique for multi-area Load Frequency Control in a Power System by evaluating the performance of the methods in a single area and two area power system. A list of modern control techniques are adopted to implement a reliable stabilizing controller. A serious attempt has been undertaken aiming at investigating the load frequency control problem in a power system consisting of two power generation unit and multiple variable load units. The robustness and reliability of the various control schemes is examined through simulations

Key words: LFC, AGC, ACE, Lyapunov Stability Analysis, Optimal Control Technique, Prime mover model, Load frequency control.

1. INTRODUCTION

For large scale power systems which consists of inter-connected control areas, load frequency then it is important to keep the frequency and inter area tie power near to the scheduled values [1]. The input mechanical power is used to control the frequency of the generators and the change in the frequency and tie-line power are sensed, which is a measure of the change in rotor angle [4]. A well Designed power system should be able to provide the acceptable levels of power quality by keeping the frequency and voltage magnitude within tolerable limits [3].

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Study Related To Modelling Of Multi-Area Load Frequency Control in an Electrical Power Systems

Piyush Kumar Yadav[1], Saurabh V Kumar[2], Dr.Rajnish Bhasker[3], Satyam Kumar Upadhyay[4], Vinod Kumar Yadav[5]

(Departement Of Electrical Engineering Vbs Purvanchal University Jaunpur)

ABSTRACT : This paper deals with the real operations of actual power system operations where step change in load as well as random change in load take place take place. The generation side having limited ability to changing load due to practical aspect, this will create unbalance between the real as well as determined generation volume of electrical power system. Due to this there is a frequency variation, which cause the unbalance between the real frequency as well as the frequency at synchronism , this will affectmain operation related toexpensive equipments like power electronics devices by producing unwanted harmonics. We have to use different types of harmonics elimination method to reduces the harmonics.

Keywords : LFC, AGC, ACE, MODELLING.

1. INTRODUNCTION (LOAD FREQUENCY CONTROL IN MULTI-AREA SYSTEMS)

As we know in the case of a single load loading frequency the production power of the machine takes place by turbine and is provided with a compatible generator connected to different transmission lines [2]. The sum of the basic frequency of the voltage and the form of the current in the output of the corresponding generator.is determined entirely by the output of the energy flow in the power system [4]. It is also disturbed by a change in energy demand by users i.e., it is seen as an electrical disturbance when, for example, when the load on the bus power system suddenly increases, the shaft movement under the generator will occur, and the generator frequency decreases [4]. The control system responds quickly so that the load and command variation opens the steam acceptance valve properly so that there is an increase in the output of the bulk power supply causing the load increase, and bring the shaft speed which is why the generator often returns to its original value [8] .Let us consider a fig tree illustrated with a simple drawing of a simple control system. The description of the drawing is as follows:

As we know when Steam enters the turbine with a pipe (driver valve) that is slightly choked with a smoke inlet valve. whenever the electric current operates under the fixed position of the opening valve is determined by a device called the speed changer (in the upper left corner of Fig. 1), it adjusts the position of the steam valve with two strong rods ABC and CDE [3] as shown in the fig tree. The reference value of turbine power in a constant state operation is called the power of the turbine and is indicated by Pref.

A Review on Diagnosis of Error and Fault Detection By Using Electric Drive and Artifical Intillegence in Smart Machine Learning Techniques of Power System

Piyush Kumar Yadav[1], Saurabh V Kumar[2], Dr.Rajnish Bhasker[3], Anchal Sahu[4]
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ABSTRACT : Monitoring an electric vehicle can detect malfunctions in the vehicle's operation capable of causing unforeseen failures and financial losses. This study explores a variety of error detection methods and diagnostic methods for induction motors and presents them. First, an anomaly process or external detection is used to enlarge the file accuracy of detecting broken rotor bars. It is shown how the proposed method can significantly improve network reliability through a single-phase separation process. After that, Miscellaneous findings based on ensemble are used to compare different approaches in combination learning to find broken rotor bars. Finally, a deep neural network is developed to exclude key features that will be used as network input parameters. A deep auto encoder was used to build a high-end model to make predictions of a broken rotor barriers and transmission errors from induction motors with high accuracy.

Keywords: AI, FAULT DETECTION, ED, MACHINE LEARNING.

1.INTRODUNCTION: Electric motors play an important role in our daily lives. Therefore, it is very important that they fail unexpectedly [39]. The three main types of electric motors used in the industry are DC motors, synchronous motors, and induction motors. The most popular type of electrical equipment is a poly phase induction motor. The poly phase AC power source applied to the zigzag stator is required for induction motors. This voltage generates the magnetic field revolves around the stator at the speed of sync. Magnetic flow produced by currents formed in the rotating rotor meets the production stator flux. As these motors are made of sudden inactivity for a variety of reasons; it is a very important issue to see such errors to prevent unexpected failures. Various diagnostic and diagnostic methods for induction motors are described in this article the idea. Induction motors (IMs) are considered to be the devices to convert electrical energy from the moment they convert electricity into electrical energy [44] Honestly, it's easy structure, construction, and cost-effectiveness are the main reasons for many applications of IM in the industry [48]. Three possible types of errors affecting IM performance are included electrical, mechanical, and

Distributed GenerationPlanning A Review

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Abstract: A combination of public policy, incentives and economics is driving a rapid growth of distributed generation in the electric power system. The majority of states/provinces now have renewable portfolio standards, with many requiring that over 20 percent of electricity sales be generated by renewable energy sources within the next five to fifteen years. The majority of these requirements will be addressed by adding significant amounts of wind energy and growing amounts of solar energy to the bulk power system.

Wind and solar power plants exhibit greater variability and uncertainty because of the nature of their −fuel‖ sources. Optimization is one of the tools that can be used to address concerns and costs around this variability and uncertainty. This report discusses operational and market system impacts, provides background on what can be realistically expected from distributed generation power-output forecasting, and proposes recommendations to deploy forecasting systems into operational use.

Distribution generation also includes more than wind resources: both established types, like run-of-river hydro and emerging varieties, such as wave energy. While the majority of attention in this report is on wind and solar generation, most varieties of Distribution generation share similar characteristics (though to a different extent) since the variability is largely driven by weather or other non-anthropogenic phenomena. Similar forecasting and integration approaches are also likely to apply to these Distribution generation resources as well. In fact, because load is also influenced by the weather, demand and generation forecasting may eventually come.

Keywords : DGs, RES,PV modules, DFIG, CHP, PEM, SOFCs, MCFCs, DR, LV, HV,MV, SG,GA, LTC, SVR.

NTRODUCTION

a. Overview

The distributed generation uses smaller-sized generators than dose the typical central station plant[1].They are distributed throughout the power system closer to the loads.The normal distribution system delivers electric energy through wires from a single source of power to a mulitiple of loads[2]. Thus, several power quality issues arise when there are multiple sources.Will Distributed Generation improve the quality or will it degrade the service end users have come to expect.

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Behaviour of ionic liquid adsorbed on the surface of nano silica particles and in confined system of silica matrices

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Keywords:
Ionic liquid
Confinement
Adsorption
Interactions
Porous materials

ABSTRACT

This paper presents studies on behaviour of a solid ionic liquid (IL): 1-butyl-2,3-dimethylimidazolium hexafluorophosphate [BMMIM][PF6] based ionogels obtained by two different techniques, first by physical confinement of IL into nano porous silica matrix and second by adsorption of IL on the outer surface of nano silica particles. The properties of samples have been investigated using various experimental techniques like N2-sorption measurements, TEM, DSC, TGA, and FTIR. It has been observed that the properties of IL have been affected more in confined geometry of silica pores as compared to the adsorption on the surface of nano silica particles. Loading of IL initially increases size and volume of pores while decrease the surface area by ~ 25 %. However, further increase in loading of IL does not produce significant change. This might be explained on basis of π-π stacking of imidazolium ring and an additional π-π stacking association between imidazolium cations. The Fourier transform infrared (FTIR) results show that stronger interaction of IL with the silica pore wall surface in confined matrix while weaker interaction due to the interfacial interaction of nano silica particles with the ions of the IL in surface adsorbed IL. The interactions and method of confinement of IL have been found to be the key parameters that determine the properties of confined and adsorbed IL.

1. Introduction

The optimization of the properties of materials in different synthesis conditions is interesting because it is decisive for their better performance as well as has importance from the application point of view. The study of the properties of materials has become more interesting in case of newly discovered material, "ionic liquids (ILs)", defined as a salt having low melting temperature generally less than 100 °C [1-5]. ILs possess many interesting properties such as low vapour pressure, high ionic conductivity, good electrochemical window, high chemical and thermal stability, excellent solvent characteristics etc.[4,5]. These remarkable properties of ILs make them very interesting material for application in many industrial processes [6-8]. But, ILs in bulk are not very useful for device applications because of many limitations associated with their liquidus nature like leakage, packaging and portability problem etc.[9]. Therefore, concept of immobilization of ILs on solid support comes into role. The resulting ILs immobilized materials are termed as ionogels which open a new direction for using ILs in protective ways. Generally, the ILs have been immobilized either by

physical confinement/immobilization method and or by chemical bonding (covalent) between cation or anion of IL and surface groups [10,12] of support. Recently, various studies have been reported on immobilization of ILs in different solid substrate using aqueous and non-aqueous sol-gel processes [3,13]. It has been found that properties of immobilized IL viz. phase transition temperature [14], thermal stability [15], vibrational properties [16], dynamics [3,17], structure [18] etc. are changed. Interactions between IL molecules and pore wall surfaces [19] or solid support surfaces [20-21] play interesting role in the alteration of properties of IL. The binding or linkage of the molecules on the surface is also useful for the modification of the molecules for their desired application. Surface interactions are decisive for modifications in properties of IL either into the pores or on surfaces. So, it is interesting to understand the properties of ILs in both type of confinement. Studies in these directions will definitely help to improve the understanding and differentiate between properties of IL in the three and one dimensional confinement. Thus, by getting the reasons of similar or opposite behaviour of IL in confinement or on the surface, one can optimize the properties of materials. Physically confined or surface

CSR AND ITS INTIMATION TO STAKEHOLDERS VIA SOCIAL MEDIA

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ABSTRACT

Institutions are quickly developing their usage of net based totally existence in company publicity, and several corporations are currently going right into a virtual change with companions to impart their monetary, social and natural consequences on society. However, the usage of internet based totally absolutely existence as a form of scattering in imparting agency social responsibility nonetheless remains a below-explored check out scenario. Coming from those contemplations, the incentive within the returned of the paper is to break down how companies are utilising net primarily based existence stages to expose the agency social obligation rehearses with a view to attract companions in convincing and on-going digital discoursed, contrasting how Socially responsible and no longer Socially responsible companies make use of on line life ranges to impart their company social duty sports activities and intercessions. This study focuses upon investigating that to what extent Indian companies have incorporated interactive approach in their CSR related communication strategy by the use of social media networking sites. For this, an analysis was done on a sample of two companies operating in India; one is ITC Limited and second, Nestle India Limited. The selection of these companies was done as convenient sampling. The unit of analysis is these two companies and the unit of sampling are the messages posted on the profiles of these two companies on social media websites- Twitter and Face-book. The messages were selected on simple random sampling basis.

Keywords : Corporate Social Responsibility, Corporate Communication, Corporate Disclosure, Social Media, ITC Limited, Nestle India

Introduction :

Corporate Social Responsibility is now integral part of corporate strategy of the management in any company in the world. At the same time, communicating CSR activities through various media of communication to the stakeholders – both internal and external, has become more important for the successful engagement of stakeholders with the company. CSR reporting or communication to external stakeholders always has been the risk matter for the companies for divulging their financial status of CSR activities, especially countries like India where CSR act., 2013 by Indian Parliament came into existence and companies have to spend minimum 2 percent of their annual profit mandatorily. So, companies always opted the official websites (digital media), annual report publishing on websites and Newspaper media or some news agencies in the form of Public Relations News materials and have been inhibitive for the communication of their CSR activities in all kinds of media like Television, Radio, Print and Digital and social media for the fear of being asked many questions by various stakeholders including media.

In the interest of stakeholders and shareholders, a company should adopt the right corporate social responsibility approach (CSR approach) and in this approach all kinds of stakeholders including communities, government organizations, local bodies, media all should be included in decision making process of the company (Francisco, et.al, May, 2016). For this approach, companies have to communicate with the

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The Progression of Global Remote Learning and hence Educational Sustainability in Post COVID world

(An Empirical Evidence from India)

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Abstract

Purpose: COVID-19 has affected massively to the education and learning system in India. While it has generated many hurdles, it has also resulted in numerous possibilities. The education sector in India has improved significantly as a result of COVID-19. It has advanced, considering the many obstacles and opportunities it has posed. the objective of this research is to highlight the usefulness of remote learning in the pre and post covid era, its impact on transformative learning and interdisciplinary/ transdisciplinary education module and enlighten the educational need of students and teachers for remote learning and hence education sustainability.

Design/methodology/approach: This study is qualitative as well as empirical in nature. Primary as well as secondary data has been used for the analysis. Primary data is collected through a structured questionnaire.

Findings: Good thing that is observed through this survey that teachers and students from all over the country are very optimistic about this remote way of learning or digital shift in education, teacher and students both believe that the remote learning surge in India has brought a lot of privileges for them and explored their learning possibilities.

Research limitations/implications: Since Remote learning brought an educational transformation all over the world, this study is limited to India where there are only 460 respondents this study could be more exploratory and instead of it this research can be carried out in other countries too.

Implications: This study will be helpful for various education practiser, education ministries, and various policymakers, to have a birds-eye view of the inclination of teachers and students in India towards the new way of learning that is remote learning and to overcome the challenges arise due to it. This study can also farm a base for researchers to do further research.

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ORIGINAL ARTICLE

Application of machine learning time series analysis for prediction COVID-19 pandemic

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Abstract

Purpose Coronavirus disease is an irresistible infection caused by the respiratory disease coronavirus 2 (SARS-CoV-2). It was first found in Wuhan, China, in December 2019, and has since spread universally, causing a constant pandemic. On June 3, 2020, 6.37 million cases were found in 188 countries and regions. During pandemic prevention, this can minimize the impact of the disease on individuals and groups. A study was carried out on coronavirus to observe the number of cases, deaths, and recovery cases worldwide within a specific time period of 5 months. Based on this data, this research paper will predict the future spread of this infectious disease in human society.

Methods In our study, the dataset was taken from WHO "Data WHO Coronavirus Covid-19 cases and deaths-WHO-COVID-19-global-data". This dataset contains information about the observation date, provenance/state, country/region, and latest updates. In this article, we implemented several forecasting techniques: naive method, simple average, moving average, single exponential smoothing, Holt linear trend method, Holt-Winters method and ARIMA, for comparison, and how these methods improve the Root mean square error score.

Results The naive method is best suited as described over all other methods. In the ARIMA model, utilizing grid search, we recognized a lot of boundaries that delivered the best-fit model for our time series data. By continuing the model, future predictions of death cases indicate that the number of deaths will increased by more than 600,000 by January 2021.

Conclusion This survey will support the government and experts in making arrangements for what is about to happen. Based on the findings of instantaneous model, these models can be adjusted to guide long time.

Keywords COVID-19 · SARS-CoV-2 · WHO · Forecasting techniques · ARIMA

Introduction

So far, coronavirus, which has killed millions of people throughout, is constantly taking people under its arrest. Washing hands, covering your face, isolating hygiene, and staying away from the community may be a way to prevent this communicable disease, but it is not enough (Nussbaumer-Streit et al. 2020). As per the World Health Organization (WHO), there are neither immunizations nor explicit antiviral medicines for COVID-19 (Q&A on corona viruses (COVID-19). World Health Organization

(WHO) 2020). As like Middle East respiratory syndrome (MERS) and severe acute respiratory syndrome (SARS), coronaviruses are an enormous group of infections which may cause ailment in creatures or people. In people, a few coronaviruses are known to cause respiratory contaminations going from the basic virus to increasingly extreme infections. The most as of late found coronavirus causes coronavirus infection, COVID-19. The basic symptoms for COVID-19 include fever, exhaustion, shortness of breath, and loss of smell and taste. Further there will be progress in severe respiratory disease (ARDS), multiple organ failure, septic syncope, and blood clots. The starting of side effects is usually about 5 days, but it may be increase from 2 to 14 days (Symptoms of coronavirus. U.S. Centers for Disease Control and Prevention (CDC) 2020; Hopkins and Kumar 2020; Velavan and Meyer 2020). COVID-19 spreads principally when individuals are in close contact, and one individual breathes in little droplets created by a contaminated individual sniffling, talking, or singing. Airborne

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ORIGINAL RESEARCH

Sequential Feature Selection and Machine Learning Algorithm-Based Patient's Death Events Prediction and Diagnosis in Heart Disease

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Abstract

Due to the accessibility of data with multiple features, many feature determination techniques available in written form. These features promote data with extremely high measurement values. The feature determination strategy provides us with a way to reduce calculation time, improve prediction execution, and have a better understanding of data in machine learning, as well as a way to recognize applications. As pointed out by related works that have been reviewed, in general, existing works only focus on amplifying classification accuracy. For real-world applications, the selected subset of features must be continuous instead. In this research, proposes a sequential feature selection algorithm for detecting death events in heart disease patients during treatment to select the most important features. Several machine learning algorithms (LDA, RF, GBC, DT, SVM, and KNN) are used. In addition, the accuracy obtained by this method (SFS) is compared with the accuracy of the classifier. The confusion matrix, ROC curve, precision, recall rate, and f1-score are also calculated to verify the results obtained by the SFS algorithm. The experimental results show that for Random Forest Classifier_FS, the SFS method reaches 86.67% accuracy.

Keywords Heart disease · SFS · RF · SVM · KNN · Confusion matrix · ROC · Precision · Recall

Introduction

Cardiovascular failure is a complex clinical disorder, not a disease [1]. It is difficult to distinguish coronary heart disease based on some common risk factors, such as diabetes, high blood pressure, elevated cholesterol, abnormal heart rhythm, and difficulty breathing, such as increased jugular vein weight, pulmonary cracks, and borderline edema caused by underlying diseases [2]. The characteristics of coronary artery disease are complex, so the disease must be treated with caution from now on. Not doing so may affect the heart or cause accidental death. Cardiovascular failure is a real disease associated with high morbidity and mortality

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[3]. According to statistics from the Society of Cardiology, 26 million adults worldwide suffer from heart failure, and recently 3.6 million people are analyzed each year. 17–45% of patients with heart failure die within the year, and the rest die within 5 years. Management costs determined to have cardiovascular failure account for approximately 1–2% of all healthcare consumption, most of which are related to intermittent clinical confirmation [4]. Expected coronary artery disease depends on performance, especially beating rate, gender, age and many other factors.

Although great progress has been made in understanding the complex pathophysiology of cardiovascular failure, the amount and unpredictability of information and data to be broken down and monitored transforms accurate and effective conclusions of cardiovascular failure and evaluation of useful options into very Effective testing [5]. These elements, plus the beneficial results of early detection of cardiovascular failure, are an explanation for the massive use of AI programs to investigate, foresee and characterize clinical information. Machine learning strategy is a kind of data mining program, these programs have stimulated the enthusiasm of exploring information. The precise sequence of disease stages or etiology or subtypes allows medication and intercession to be communicated in an effective

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Calculating Diagnose Odd Ratio for Thyroid Patients using Different Data Mining Classifiers and Ensemble Techniques

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ABSTRACT

Thyroid hormones disorder is very common among people now-a-days. Various data mining techniques are used to identify thyroid problems. Machine learning provides help in multiple ways by different algorithms which are analyzed dataset and also generate different patterns. In this research paper we use three classifiers "Generalized Linear Model, Neural Network and Boosted Tree". Two ensemble techniques Stacking and Random Forest are used to combine the results of three data mining classifiers. Each classifier provides different patterns of measuring the performance with thyroid dataset. The ensemble model behaves as a major classifier in which Random Forest is give more accuracy. All the experiment performed on three features of thyroid dataset Triiodothyronine (T3), Thyroxin (T4) and Thyroid Stimulating Hormone (TSH) different values. In this paper, we have proposed a new technique to find the pattern using Diagnose Odd Ratio (DOR) to find the patients that needs further treatment or not. Diagnose Odd Ratio (DOR) provides a value if this value is high then patient needs treatment and if its value is low patient does not need further treatment. Finally thyroid dataset has been analyzed and the Positive Likelihood Ratio (LR+), Negative Likelihood Ratio (LR-) and Diagnostic Odd Ratio (DOR) with the help of Sensitivity and Specificity are measure.

Key words: Generalized Linear Model, Neural Network, Boosted Tree, Random Forest and Ensemble Methods.

1. INTRODUCTION

The diagnosis of thyroid disease fully depends on hormones. Generally doctors use medical history in diagnosis but it is not sufficient because without physical exam and medical hormonal test does not diagnose clearly. In any case if pituitary gland not properly works means T3, T4 and TSH functions are not properly work. Thyroid function inter relate with every function in human body. If human body function not properly work then some symptoms overcome in human body as like fatigue, weight gain, mood issue, irregular period, muscle pain cold hand, dry and cracking skin neck swelling etc. Generally thyroid problems are two types' hypothyroidism, and hyperthyroidism. These two different problems have different own symptoms in human body. By the help of Iodine easily maintain thyroid gland hormones because thyroid gland converts Iodine in thyroxin (T4) and triiodothyroxine (T3). Many thyroid cells are in the human body. These cells absorb Iodine and amino acid tyrosine for creation T3 and t4, t3 and T4 control metabolism of the body. T3, T4 control and manage oxygen and calories and create it into energy. So it is very clear energy cell directed by thyroid hormones and they make continuous flow of metabolism. The pituitary gland manages by another gland known as process TSH releasing hormone (TRH). It is very important in human that T3 and T4 levels must be always in balancing order. If T3 and T4 levels are low then it is required to improve the production of thyroid hormones so pituitary gland releases more TSH. If T3 and T4 levels are high then no need to improve high thyroid hormone production so pituitary gland release low TSH .In this research paper tries to find the combination of T3, T4 and TSH for good health [1].

2. RELATED WORK

Cohen, Jasonet al., discussed about urinary tract infection. They observed and measure a urine culture without antibiotics. They analyzed all the dataset and presented uncomplication of urinary tract infection by attributes represented symptoms uti and also presented highly therapy in women for urinary tract infection [2].
Alexander, Kennedy et al., discussed about thyroid nodules with indeterminate cytology. After all the experiment they find in term of machine learning sensitivity (0.9), specificity (0.52) and positive predictive value (0.37) and negative predictive value (0.94) and find the highest value of odd diagnosis ratio was (9.89) [3].
Borowczyk, Martyna et al., discussed about thyroid. They observed the attribute of thyroid cancer follicular for thyroid diagnosis. After all the observation they measured sensitivity, specificity, accuracy and also measured Gene expression [4].
Harrell, Bimston et al., discussed about thyroid cytology. After all the observation they find sensitivity (0.91), specificity (0.25) and positive predictive value (0.70) and negative predictive value (0.60) and finally find the highest log likelihood ratio values (3.36) [5].

ORIGINAL RESEARCH

Applications of Machine Learning Techniques to Predict Diagnostic Breast Cancer

Vikas Chaurasia[1] · Saurabh Pal[1]

Abstract

This article compares six machine learning (ML) algorithms: Classification and Regression Tree (CART), Support Vector Machine (SVM), Naïve Bayes (NB), K-Nearest Neighbors (KNN), Linear Regression (LR) and Multilayer Perceptron (MLP) on the Wisconsin Diagnostic Breast Cancer (WDBC) dataset by estimating their classification test accuracy, standardized data accuracy and runtime analysis. The main objective of this study is to improve the accuracy of prediction using a new statistical method of feature selection. The data set has 32 features, which are reduced using statistical techniques (mode), and the same measurements as above are applied for comparative studies. In the reduced attribute data subset (12 features), we applied 6 integrated models AdaBoost (AB), Gradient Boosting Classifier (GBC), Random Forest (RF), Extra Tree (ET) Bagging and Extra Gradient Boost (XGB), to minimize the probability of misclassification based on any single induced model. We also apply the stacking classifier (Voting Classifier) to basic learners: Logistic Regression (LR), Decision Tree (DT), Support-vector clustering (SVC), K-Nearest Neighbors (KNN), Random Forest (RF) and Naïve Bays (NB) to find out the accuracy obtained by voting classifier (Meta level). To implement the ML algorithm, the data set is divided in the following manner: 80% is used in the training phase and 20% is used in the test phase. To adjust the classifier, manually assigned hyper-parameters are used. At different stages of classification, all ML algorithms perform best, with test accuracy exceeding 90% especially when it is applied to a data subset.

Keywords Classification · Linear regression · Machine learning · Multilayer perceptron · k-Nearest neighbors · Support vector machine · Ensemble · Stack

Introduction

The abnormal growth of human cells is widely known as a cancer that attacks healthy cells. Abnormal growth of breast cells will invade cells around the breast more quickly and spread to other parts of the body. Breast cancer occurs when a malignant tumor (mass of tissue) occurs in the breast. Two types of breast cancer are: non-cancerous or benign and cancerous or malignant [1].

In machine learning, many researchers start their work from here to discover the severity of breast cancer, that is, whether the tumor is cancerous or non-cancerous. To find answers to these questions, two things are important: what is the role of the machine, and how does the machine learning combine medical data to predict the severity of the disease. Machine learning is the way to make data decisions with minimal human intervention. It is part of AI (artificial intelligence), which can learn from data, make decisions, discover patterns and build analytical models through data analysis. Clinical or medical data is part of information related to human health, which is based on routine patient care or clinical trial plans. It includes patient electronic health records based on patient health information. AI can obtain information from health-related data, process the data, and provide clear output to end users. This process is done through machine learning [2]. The algorithm used by this technique recognizes the data pattern and gives its own logic. The main goal of the algorithm used by AI is to find

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ORIGINAL RESEARCH

COVID-19 Pandemic: ARIMA and Regression Model-Based Worldwide Death Cases Predictions

Vikas Chaurasia[1] · Saurabh Pal[1]

Abstract

COVID-19 has now taken a frightening form. As the days pass, it is becoming more and more widespread and now it has become an epidemic. The death rate, which was earlier in the hundreds, changed to thousands and then progressed to millions. If the same situation persists over time, the day is not far when the humanity of all the countries on the globe will be endangered and we yearn for breath. From January 2020 till now, many scientists, researchers and doctors have been trying to solve this complex problem so that proper arrangements can be made by the governments in the hospitals and the death rate can be reduced. The presented research article shows the estimated mortality rate by the ARIMA model and the regression model. This dataset has been collected precisely from DataHub-Novel Coronavirus 2019-Dataset from 22nd January to 29th June 2020. To show the current mortality rate of the entire subject, the correlation coefficients of attributes (MAE, MSE, RMSE and MAPE) were used, where the average absolute percentage error validated the model by 99.09%. The ARIMA model is used to generate auto_arima SARIMAX results, auto_arima residual plots, ARIMA model results, and corresponding prediction plots on the training dataset. These data indicate a continuous decline in death cases. By applying a regression model, the coefficients generated by the regression model are estimated, and the actual death cases and expected death cases are compared and analyzed. It is found that the predicted mortality rate has decreased after May 2, 2020. It will help the government and doctors prepare for the forthcoming plans. Based on short-period predictions, these methods can be used to forecast the mortality rate for a long period.

Keywords COVID-19 · Epidemic · Humanity · Breath · ARIMA model · Regression model · RMSE

Introduction

As indicated by the World Health Organization, the COVID-19 virus is a communicable disease that spreads from one person to another. Personal contact and small droplets in the breath of infected person can cause the virus to spread to others and cause severe acute respiratory syndrome [1]. In 2020 of January, WHO initially informed the humanity regarding pneumonia for obscure reasons, and the world came to know that this disease spread from person to person

[2]. The incidence of this mysterious disease started from a city called Wuhan of China [3]. The status report of WHO says that till date from January 15, 2020 to July 1, 2020: 507,435 people have lost their lives worldwide and this number is continuously increasing [4]. The group of RNA viruses are called coronavirus [5]. In humans, it causes respiratory tract infections. It has SARS, MERS and COVID-19 deadly varieties. There are no immunizations or antiviral medications to protect from corona infection in people yet. Common symptoms include high fever, tiredness, cough, shortness of breath, and loss of taste and smell, and complications include pneumonia and acute breathing infection [6]. The confirmation of the first death case from Asia to Europe was as follows: initial confirmed casualty in Wuhan, China on 9th of January, 2020, initial confirmed death in Philippines outside China on February 1, 2020, and on February 14, 2020 the first confirmed death in the European country France [7]. The ratio of death rate is 5.4% till 16 June 2020

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Machine Learning Algorithms and Ensemble Technique to Improve Prediction of Students Performance

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ABSTRACT

Measuring Student's performance is necessary for the mordent society. Applications of Machine learning algorithms increased the growth in various fields like disease prediction, student's performance prediction, and crop productions prediction and in various other fields. The main aim of this study is to improve the prediction of students' performance using various machine learning algorithms and ensemble technique to get better accuracy over individual machine learning algorithms. We have used the student's dataset, which consists of 1000 instances and 22 attributes for evaluating the performance of students. In this paper we have applied four machine learning algorithms Decision Tree (DT), Naïve Bayesian (NB), K-Nearest Neighbors (KNN) and Extra Tree (ET) and then we have developed a model to combine the results of each individual base learner using Bagging and Boosting ensemble methods. The results obtained using bagging and boosting ensemble techniques were compared to select the best model.

The results of all machine learning algorithms and ensemble techniques are tested with various factors like accuracy, sensitivity, specificity and f1-score. After comparison of results we find that bagging is the best method which gives the better result as compared to bagging ensemble techniques. The developed model can be applied on the admission seeking students to identify the perdition of their performance in the selected course, which can be beneficial for both the students and Institution.

Key words: Educational Data Mining, Machine Learning; K-Nearest Neighbor Classifier, Extra Tree Classifier, Ensemble Technique.

1. INTRODUCTION

Academic performance evaluation is a type of clustering problem where clusters are their grades like first division, second division, third division and fail, which measures the intelligence level of students. The Intelligence level bases groupings are essential for selecting the deserving students and to provide them good education so that they achieve their aim of life. As cost of electronics equipments prices are reduced the application of IT equipments are increased in the educational institutions for collecting huge amounts of data about their students. At present days generally affiliating Universities collect registration data using registration for and examination data using examination form and also Universities provide e-mark sheet, certificate, migration to students, but most time these data remains unused because Universities does not further analyzed these data. Data mining techniques can help to develop machine learning model with the help of these data. The application of data mining techniques on these data is Educational Data Mining (EDM). EDM includes study of new tools and development of new models and applying new algorithms on a huge amount of data to find useful unknown patterns and, thus, help to understand students' behavior and learning capabilities. Therefore, educational data mining provides discovering of new applications for solving problems which are related to educational fields.

Now a day's higher education institutions are utilizing ITC (Information Technology and Communication) resources, as Management Information Systems, which are providing high volumes of data [1]. Perfect machine learning techniques can be used in analyzing educational data. In this paper, we use machine learning classifiers to develop a new model for prediction of academic performance of students.

The objective of the study is to find the factors taken admission in courses which affect low academic performance in Bachelor of Computer Applications (BCA) for students at the United College of Management, Prayagraj, UP. The developed model can be effectively work for BCA department to take right decisions and for monitor and support students which need special attention to enhance the performance of students and quality of Institute.

The rest paper is prepared as follows. The next Section 2, describe the previous work done on EDM field using machine learning algorithms. In Section 3 we discus about the dataset used, the machine learning algorithms applied, ensemble

Research Article

Prediction of Heart Disease Using Feature Selection and Random Forest Ensemble Method

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ABSTRACT

The heart is very soft and sensitive part of body by which brain handles blood related system in body. The heart disease that greatly affects in body as like: pulmonary artery, atalata, enzaina and birth defects included. Heart disease is mainly related to contraction or blocked blood vessels in the heart. The symptoms of heart disease depend on the type of disease. Heart disease occurs not only in adults but also in children. The infection affecting the tissues is known as percarditis. In this, the tissues closest to the heart are affected. Infections affecting the lining of the heart muscle are known as myocardium .The study of medical datasets is made very intuitive by machine learning algorithms. The machine learning algorithms provide techniques to identify dataset attributes and the relationship between them.

In this research work, we used heart disease related information from UCI repository. The dataset contained 1025 Instances with 14 attributes, sick and nonstick patients in target variable. In this paper, we proposed and analyzed classification accuracy, precision and sensitivity by four tree based classification algorithms: M5P, random Tree and Reduced Error Pruning with Random forest ensemble method. All the prediction based algorithms have applied after the features selection of heart patient's dataset. In this paper, we used three features based algorithms: Pearson Correlation, Recursive Features Elimination and Lasso Regularization. The data table analyzed by different feature selection methods for better prediction. All the analysis is done by three experimental setup; First experiment applied Pearson Correlation on M5P, random Tree, Reduced Error Pruning and Random forest ensemble method. In the second experiment we used Recursive Features Elimination and applied on above four tree based algorithms. In the third experiment we used Lasso Regularization and applied on as above tree based algorithms. After all the performance we analyzed and calculated classification accuracy, precision and sensitivity.

With the results, we finally concluded that feature selection methods Pearson correlation and Lasso Regularization with random forest ensemble method provide better results 99% accuracy. We analyzed and find the random forest ensemble method predicted better result compare to other algorithms in the previous year's works.

Keywords: Data mining Tree based Algorithms, Random Forest Ensemble Method, Features Relevant Method, Features Elimination Method Lasso Regularization Method and Heart Disease.

INTRODUCTION

Research is going on, in large research institutions to ensure factors related to heart disease. In some institutions, smoking, age, high/low blood pressure, obesity, diabetes and lack of exercise have been included as main factors for diseases. According to the instructions of the researchers, it is considered helpful to identify the disease related to heart disease. Heart disease is also revealed due to blockage in the blood vessels, which later expresses the possibility of heart attack, chest pain or stroke. Valve and heart muscles are mainly affected in heart disease. The level of mortality among the world population by heart disease is quite large.

Cardiovascular data are available in very large quantities in healthcare. Due to the large amount of data, it becomes very difficult to study it in general. But with the help of data mining, large collections are easily converted into information. Which shows how the condition of heart disease has been in children and adults in the past years and its study also helps in estimating how to reduce the mortality caused by cardiovascular diseases in the future. Machine learning algorithms can improve the treatment of a person suffering from the disease by comparing its factors.

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Application of Machine Learning Algorithms to Predict Students Performance

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Abstract

Student's performance is a major problem for the society. Rapid growth of technologies and the application of differentmachine learning methodsin present years, the development of good models increase the progress of student's performance progress have become more and more accurate. Therefore, development of machine learning techniques, which can effectivelypredict student's performance, is of vastimportance.In this research paper, we apply five different data mining techniques Passive Aggressive Classifier (PAC), Support Vector Machine (SVM), Linear Discriminant Analysis (LDA), Radius Neighbour Classifier (RNC) and Extra Tree (ET) and then compare the results of five machine learning algorithms to choose the best performing algorithm. We use educational data toanalysis differentmachine learning techniques to evaluate the performance of student.

The results obtained by different machine learning algorithms are discussed in this paper and we get the highest accuracy in the case of Support Vector Machine (SVM).Various metrics are also evaluated to verify the results of accuracy like sensitivity, specificity and precision. These results can be applied on the new coming students to check whether they perform well or not and by knowing the non-performing students, higher educational institutions can pay attaint ion for improving student's performance.

Keywords: Educational Data Mining; Support Vector Machines, Radius Neighbor Classifier, Linear Discriminant Analysis, Passive Aggressive Classifier.

1. Introduction

The quality of an academic institution is depend on the performance of student and dropout rate between the enrolled students in a course and finally completed the course. The dropout rate is high because students do not know whether the course in which they are going to take admission is suitable for their study or not. In India parents forced the student to take admission in Engineering or professional courses without knowing their interest and this is the main reason of the dropout and low performance.

Educational Data Mining (EDM) is an area focusing to use technologies and data mining techniques in the teaching environment. EDM relates to the machine learning for identifying hidden patterns within huge academic data, to develop data mining and statistical methods, research and implementation, which would provide fruitful results

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RESEARCH ARTICLE

Prediction of thyroid disease using decision tree ensemble method

Dhyan Chandra Yadav[1] · Saurabh Pal[1]

Abstract

Thyroid disease is spreading very rapidly among women after the age of 30 years. Therefore, it is necessary to examine the thyroid dataset for predicting the disease at early stage so that precautions can be taken to protect the dangerous condition of thyroid cancer. A decision tree is used to extract hidden patterns from the stored datasets. The objective of this research paper is to examine the thyroid disease dataset using decision tree, random forest, and classification and regression tree (CART), and after obtaining the results of these classifiers, we enhanced the results using the bagging ensemble technique. The proposed experiment was done on 3710 instances and 29 features of thyroid patients. The overall prediction depends on target variable whch is divided in sick and negative class. The accuracy of the prediction was calculated on the basis of different num-fold and seed values. Different classification algorithms are analyzed using thyroid dataset. The results obtained by individual classification algorithms like decision tree, random forest tree, and extra tree give an accuracy of 98%, 99%, and 93%, respectively. Then, we developed a bagging ensemble method combining the three basic tree classifiers and apply again on the same dataset, which gives a better accuracy of 100% in the case of seed value 35 and num-fold value 10. This proposed ensemble method can be used for better prediction of thyroid disease.

Keywords Decision tree · Random forest · Extra tree and boosted tree ensemble model · Triiodothyronine · Thyroxin and thyroid stimulating hormone

1 Introduction

Hormones play a vital role in blood flow for maintaining metabolism in human, and high hormones and low hormones both are equally dangerous. Thyroid hormones are produced by thyroid gland to maintain blood stream for the regulation of metabolism; three types of hormones produced by the thyroid gland are triiodothyronine (T3), thyroxin(T4), and thyroid-stimulating hormone (TSH). If the thyroid gland produces more hormones, then, it will be hyperthyroidism, and if the thyroid gland produces less hormones, then, it will be hypothyroidism. Thyroid disease has various symptoms, like fatigue, weakness, intolerance to cold, muscle aches and crams, constipation, weight gain, or difficulty of losing weight, in initial stage; therefore, it is necessary to recognize thyroid disease in the initial stage (Ozyilmaz and Yildirim 2002).

Tahani et.al used adaptive clustering ensemble model and combine multiple clustering models for prediction of thyroid disease. Adaptive clustering method computed and transformed initial clusters into binary representation to predict final clusters using K-means algorithm (Alqurashi and Wang 2019).

Ahmad et.al discussed feature selection techniques and achieved different testing phase of clustering one, two, three, and four for each class and 12 fuzzy rules to calculate the maximum absolute difference, linguistic hedge, and total serum thyroxin. They achieved classification accuracy of 98.60% (Azar et al. 2012).

Xiyu et.al analyzed traditional tissue P systems to generate new class of tissue system. They used thyroid disease analysis, tissue P system, membranes structure, and clustering algorithm for the prediction of thyroid disease using classification algorithms (Liu and Xue 2012).

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ORIGINAL ARTICLE

Skin disease prediction using ensemble methods and a new hybrid feature selection technique

Anurag Kumar Verma[1] · Saurabh Pal[1] · B. B. Tiwari[2]

Abstract

Now-a-days Skin disease is very common worldwide problem. We have preset this study for the prediction of skin disease. Based on data from UCI data set, there are 34 attributes which plays a vital role in the skin disease diagnosis but all are not important. In this paper we have analyzed only those important attributes which give best accuracy in prediction of skin disease. To select important attributes, we have applied a new hybrid approach using three feature extraction techniques Chi Square, Information Gain and Principle Component Analysis (PCA) and then combining them to select the best possible data subset of skin disease data set. Six base learners Gaussian Naïve Bayesian (NB), K-Nearest Neighbour (KNN), Decision Tree (DT), Support Vector Machine (SVM), Random Forest (RF) and Multilayer Perceptron (MLP) are used to evaluate the prediction performance of base learners. Boosting, Bagging and Stacking ensemble techniques are applied on base learners to enhance the results of the proposed model. In this paper, a new proposed method of hybrid feature selection technique is used for evaluating the performance of base learners and we find that reduced data subset performed is higher as compared to whole data set. The metrics are necessary to evaluate the model and calculated to illustrate the performance of prediction. Hybrid feature selection technique along with base learners are then applied on Bagging, Boosting and Staking ensemble techniques to enhance the results. These results are compared with individual base learners. The result obtained in this research paper is higher than previous studies.

1 Introduction

Erythemato-squamous disease is also called the skin disease. Skin disease can be classified in six classes C1: psoriasis, C2: seborrheic dermatitis, C3: lichen planus, C4: pityriasis rosea, C5: chronic dermatitis, C6: pityriasis rubra [1]. Skin disease diagnosis is difficult, because six classes possess identical clinical properties with very small changes. Basically Biopsy is used for treatment of these skin diseases.

In past decade many expert systems were developed for providing fruitful decisions in various fields, as data related to medical field is widely available freely on internet. Therefore, a great improvement in the clinical area for predicting the various diseases using machine learning algorithms and deep learning on data sets from the previous patient's history. The development of expert systems using data mining in the field of medical decision support system is beneficial for patients which were do not bear high cost medical tests. Expert systems now provide assistance to doctors for helping in diagnose better [2].

Many research paper published on skin diseases with the help of decision tree [3–8]. They conducted different experiments focusing on six major skin diseases classes as its research subjects. They uses decision tree, Random Forest, Chi-square Automatic Interaction Detector (CHAID) and Extra tree of data mining classification methods to construct the best predictive model in dermatology. They used data set from UCI machine learning repository for calculating the accuracy of prediction model.

Some papers have studied the skin image and predict the accuracy of skin disease [9–11]. The application of deep convolution neural network (CNN) changes the quality of computer-aided supporting systems. A computer-aided diag-

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Discovery of Hidden Pattern in Thyroid Disease by Machine Learning Algorithms

Dhyan Chandra Yadav[1], Saurabh Pal[2]

[1]Research Fellow, Dept. of MCA, [2]Associate Professor, Head Dept. of MCA, VBSPU Jaunpur, U.P.

Abstract

Background: Decision tree provides help in making decision for very complex and large dataset. Decision tree techniques are used for gathering knowledge. Classification tree algorithms predict the experimental values of women thyroid dataset. The objective of this research paper observation is to determine hyperthyroidism, hypothyroidism and euthyroidism participation in hormones can be good predictor of the final result of laboratories and to examination whether the propose ensemble approach can be similar accuracy to other single classification algorithm.

Results: In the proposed experiment real data from 499 thyroid patients were used classifications algorithms in predicting whether thyroid detected or not detected on the basis of T3, T4 and TSH experimental values. The results show that the expectation of maximization classification tree algorithms in those of the best classification algorithm especially when using only a group of selected attributes. Finally we predict batch size, tree confidential factor, min number of observation, num folds, seed, accuracy and time build model with different classes of thyroid sickness.

Conclusion: Different classification algorithms are analyzed using thyroid dataset. The results obtained by individual classification algorithms like J48, Random Tree and Hoeffding gives accuracy 99.12%, 97.59% and 92.37 respectively. Then we developed a new ensemble method and apply again on the same dataset, which gives a better accuracy of 99.2% and sensitivity of 99.36%. This new proposed ensemble method can be used for better classification of thyroid patients.

Keywords: J48, Random Tree, Hoeffding, Prediction, T3, T4, TSH, hypothyroidism, hyperthyroidism, euthyroidism and ensemble model.

Introduction

Hormones play major role in blood stream to maintain metabolism in human. The production of high hormones and low hormones both are dangerous. The general objective of thyroid gland is to produce thyroid hormones. The main objective of thyroid gland is to maintain bloodstream through the regulation of metabolism. If thyroid gland produces more hormones then it will be hyperthyroidism and if thyroid gland produces less hormones then it will be hypothyroidism[1].

The three hormones tri-iodothyronine (T3), L-thyroxin and TSH regulate the metabolic functions of human body. These hormones utilize proteins and manage fats in human body. In pituitary gland thyrotrophic stimulating is released if require more hormones. The pituitary gland control and manage production of hormones in the blood stream [2].

Thyroid disease is a different thing about all other diagnosis system. It's visibility and treatments are different. Thyroid hormone has many symptoms in initial to final stage. It is generally arises from disorder life style and foods after it increasing and decreasing hormones production finally make health system [3].

The paper analysis is organized on batch size, confidential factor, num decimal places, num folds, seed and accuracy of a model in decision making through J48, Hoeffding and Random Tree. The discuss about all dataset of thyroid in multiple way of classification tree algorithm and finally measure the evaluation accuracy increases with time built model training set.

Prediction of Skin Disease with Three Different Feature Selection Techniques Using Stacking Ensemble Method

Anurag Kumar Verma[1] ⓘ · Saurabh Pal[2] ⓘ

Abstract

Skin disease is the most common problem between people. Due to pollution and deployment of ozone layer, harmful UV rays of sun burn the skin and develop various types of skin diseases. Nowadays, machine learning and deep learning algorithms are generally used for diagnosis for various kinds of diseases. In this study, we have applied three feature extraction techniques univariate feature selection, feature importance, and correlation matrix with heat map to find the optimum data subset of erythemato-squamous disease. Four classification techniques Gaussian Naïve Bayesian (NB), decision tree (DT), support vector machine (SVM), and random forest are used for measuring the performance of model. Stacking ensemble technique is then applied to enhance the prediction performance of the model. The proposed method used for measuring the performance of the model. It is finding that the optimal subset of the erythemato-squamous disease is performed well in the case of correlation and heat map feature selection techniques. The mean value, slandered deviation, root mean square error, kappa statistical error, and area under receiver operating characteristics and accuracy are calculated for demonstrating the effectiveness of the proposed model. The feature selection techniques applied with staking ensemble technique gives the better result as compared to individual machine learning techniques. The obtained results show that the performance of proposed model is higher than previous results obtained by researchers.

Keywords Erythemato-squamous disease · SVM · Stacking · RMSE · KSE

Introduction

The skin of human body is the major organ, with a total 20 square feet covered area. The skin protects us from heat and cold and helps regulate body temperature. The disease related to skin

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ORIGINAL RESEARCH

Thyroid prediction using ensemble data mining techniques

Dhyan Chandra Yadav[1] · **Saurabh Pal[2]**

Abstract Data mining algorithms provide easy way to solve problem in medical data analysis. Data mining supports in complex data analysis to identify each issue in dataset. Now-a-days every person suffers for a good heath. The life style of every person is very fast so it is very difficult to maintain his health. Every person cannot easily maintain the hormone system in the body. Nowadays hormone disturbance are major issue in ladies. The major issues behind thyroids are hormonal disturbance. Initially we do not care the symptom of thyroids. If we have some knowledge about thyroid symptom then prior of major problem we protect his life. The symptoms of thyroid are very similar so we easily can not eliminate for identification. Data mining provide major help in thyroid dataset with different algorithms for classification, clustering, association etc. We use different types of machine learning meta classifier algorithms for thyroid dataset classification. In this analysis we analyze thyroid large and complex dataset by data mining meta classifier algorithm: Boosting, Bagging, Stacking and Voting with new ensemble model and con comparing classification accuracy, sensitivity and specificity. We easily classify thyroid dataset in different class level. Thyroid is a very common disease found in the human body, which is related to human diet and daily living with the help of classification algorithms, they can be avoided by studying various types of functions in thyroid, with the help of classification, after the disease consisting of experienced doctor walking expert system can be developed.

Keywords Data mining meta classifier algorithms · Boosting · Bagging · Stacking · Voting algorithms

1 Introduction

Nowadays many problems arise in ladies as like thyroid gland cancer, hypothyroidism and hyperthyroidism etc. It is very necessary for every person to know about every symptom of thyroid as like: Fatigue (tired), Cold Intolerance, Skin dry, Weight gain, Face Swelling, Menstrual Cycles, and Hair Fall etc. Just as the population is growing very fast, so in today's environment, human being is rapidly suffering from disease. In this situation, having a good health has become a matter of great challenge for the human, but in the field of medicine with the rapid growth, new technologies have been developed, through which the precise diagnosis of disease can be easily done by the technique of machine learning by the medical field. The medical data set to help in the thyroid disease. The medical datasheet of diseases helps in controlling the body's metabolism of the hormones produced by the thyroid gland, but in some cases when the hormone generated from the thyroid gland is correct and the metabolism of the body can lead to various types of disorders, which can lead to the form of fatal disease. Generally some women suffers hormonal disturbance and sickness which are arises by these hormonal disturbance. If a lady suffers by face swelling but she does not know any idea about this situation so generally she avoid it but actually it is a symptom of hormonal disturbance. If a lady suffers from cold intolerance and she

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Decision Tree Ensemble Techniques To Predict Thyroid Disease

Dhyan Chandra Yadav , Saurabh Pal

Abstract: Decision tree provides help in making decision for very complex and large dataset. Decision tree techniques are used for gathering knowledge. Classification tree algorithms predict the experimental values of women thyroid dataset. The objective of this research paper observation is to determine hyperthyroidism, hypothyroidism and euthyroidism participation in hormones can be good predictor of the final result of laboratories and to examination whether the propose ensemble approach can be similar accuracy to other single classification algorithm. In the proposed experiment real data from 499 thyroid patients were used classifications algorithms in predicting whether thyroid detected or not detected on the basis of T3, T4 and TSH experimental values. The results show that the expectation of maximization classification tree algorithms in those of the best classification algorithm especially when using only a group of selected attributes. Finally we predict batch size, tree confidential factor, min number of observation, num folds, seed, accuracy and time build model with different classes of thyroid sickness. Different classification algorithms are analyzed using thyroid dataset. The results obtained by individual classification algorithms like J48, Random Tree and Hoeffding gives accuracy 99.12%, 97.59% and 92.37 respectively. Then we developed a new ensemble method and apply again on the same dataset, which gives a better accuracy of 99.2% and sensitivity of 99.36%. This new proposed ensemble method can be used for better classification of thyroid patients.

Keywords : J48, Random Tree, Hoeffding, Prediction, T3, T4, TSH, hypothyroidism, hyperthyroidism, euthyroidism and ensemble model

I. INTRODUCTION

Hormones play major role in blood stream to maintain metabolism in human. The production of high hormones and low hormones both are dangerous. The general objective of thyroid gland is to produce thyroid hormones. The main objective of thyroid gland is to maintain bloodstream through the regulation of metabolism. If thyroid gland produces more hormones then it will be hyperthyroidism and if thyroid gland produces less hormones then it will be hypothyroidism [1].

The three hormones tri-iodothyronine (T3), L-thyroxin and TSH regulate the metabolic functions of human body. These hormones utilize proteins and manage fats in human body. In pituitary gland thyrotrophic stimulating is released if require more hormones. The pituitary gland control and manage production of hormones in the blood stream [2].

Thyroid disease is a different thing about all other

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diagnosis system. It's visibility and treatments are different. Thyroid hormone has many symptoms in initial to final stage. It is generally arises from disorder life style and foods after it increasing and decreasing hormones production finally make health system [3].

The paper analysis is organized on batch size, confidential factor, num decimal places, num folds, seed and accuracy of a model in decision making through J48, Hoeffding and Random Tree. The discuss about all dataset of thyroid in multiple way of classification tree algorithm and finally measure the evaluation accuracy increases with time built model training set. Classification decision tree provide many types help in identification of thyroid disease. It provides better help in dataset classification as a tree model in which attributes represents root ,nodes and leaf nodes. Analyst easily analysis all the functions of related dataset [4].

By the help of proposed three algorithms easily classify hyperthyroidism, hypothyroidism and euthyroidism. We easily indentify as a tree path and finally reach on decision node to leaf nodes. Present paper discuss to all the symptoms of thyroid patients and declare types of problem. It is very difficult to identify hyperthyroidism and hypothyroidism problems in another way [5].

II. RELATED WORK

Ahmad et.al discussed about thyroid endocrine gland in blood issue and function of the body. They discussed by feature selection, Fuzzy rule, maximal absolute difference Linguistic Hedge and total serum thyroxin. They provided classification accuracy 98.604% and achieved different testing phase of clustering one, two, three and four clusters for each class and 12 fuzzy rules. The generated 88.372%, 90.6977%, 91.6744%, and 97.6744% cluster size during training phase [6].

Tahani et.al discussed about clustering ensemble model and how combines multiple clustering models. They analyzed adaptive clustering ensemble model. Adaptive algorithm measured and transformed initial clusters into binary representation aggregation to produce final clusters. They used co- association, k-means, similarity measurement, machine learning and data mining [7].

Xiyu et.al discussed about new class of tissue system .They analyzed traditional tissue P systems to new class of tissue system. They used thyroid disease analysis, tissue P system, membranes structure and clustering algorithm. They analyzed thyroid disease for classification [8].

Amrollahi et.al discussed about effect on thyroid gland of human bodies. They analyzed how thyroid function managed and balanced the metabolism. They used expert systems Bio-chemistry. They used fuzzy rules to system provided help in non expert who are suspicions

Phyto-Pharmacological Appraisal of Herbal Crude Drugs

Vinay kumar[1]*, Saurabh Pal[2], BB Tiwari[3]

*Abstract_* Plants are the very precious part of our earth. Earth is called a green planet because of the presence of plants. Many plants are used to cure many of the diseases. The medicines made by plants are also safer and don't cause any side effects. However certain plants contain toxic compounds which cause serious side effects to man and animals. Hence a proper evaluation about the plants is necessary to identify the appropriate medicinal diseases for every disease. Consequently in our paper, we present a proper description of certain herbal plants such as Acacia Nilotica, Cinchona, Cinnamon, Ginger, Mustard and Turmeric. Moreover we exhibit detailed information about the features and use of each part of the plant along with the image, which provides a unique significance to our paper.

*Keywords_* Acacia Nilotica, Cinchona, Cinnamon, Ginger, Mustard and Turmeric.

1. INTRODUCTION

In spite of great advances of modern scientific medicine, traditional medicine is still the primary form of treating diseases of majority of people in developing countries including India; even among those to whom western medicine is available, the number of people using one form or another of complementary of alternative medicine is rapidly increasing worldwide. Increasing knowledge of metabolic process and the effect of plants on human physiology has enlarged the range of application of medicinal plants.

The nature has provided an absolute resource of remedies to cure the several ailments of mankind and is best friend of pharmacy. The herbal drugs are most effective in action without any side effects. The drugs obtained from plant source constitute a major part of therapeutics in the traditional systems of medicine. The shortcomings of the drugs available today, propel the discovery of new pharmaco-therapeutic agents in medicinal plants [1, 2]. The potentialities of herbal medicines are most essential to intensify the pharmacological study of herbal crude drugs that find place in folklore and also to promote the use of herbal medicine.

Phyto-pharmacology is the study and practice of eradicating plant pathology. Plants are utilized extensively as raw drugs for many formulations in traditional systems of medicine. To check the genuineness of the raw drugs and to detect adulteration of these materials, an authentic pharmacognostic study is needed for each raw drug. Usually, the drugs are collected by traditional practitioners who have inherited Ayurvedic or other herbal practices. Their identification is mostly based on the morphological features or other traditionally known characteristics. In such cases, there is a chance of selecting incorrect raw drugs/adulterants. Our country has a long tradition of using herbal products for healthcare. There is an increasing awareness of the significance of ethnic and traditional knowledge in the development of therapeutics. In the current scenario of globalization, information technology and knowledge system on traditional medicine have significant importance [3, 4, 5, 6].

Mankind has been continuously using the medicinal plants in one or the other way in the treatment of various ailments. In India, the sacred Vedas dating back between 3500 B.C and 800 B.C give many references of ethno-medicinal plants. One of the outermost works in traditional herbal medicine is "Vrikshayurveda", compiled even before the beginning of Christian era and formed the basis of medicinal studies in ancient India. The Rig Veda, dating between 3500 B.C. to 1800 B.C. seems to be the earliest record available on medicinal plants. Herbs seem to be very important component of medicine in other cultures too; Greek, African and Chinese medicines to mention a few. Nearly 80% of the world population depends upon traditional system of health care. Allopathic drugs have brought a revolution throughout the world, but the plant base medicines have its own status. The recent surveys had revealed that, 50% of the top prescription drugs in the USA are based on natural products and the raw materials are locked up in the tropical world–interiors of Africa, Asia and Latin America.

According to the report, it is apparent that the significance of plant based medicines has been increasing all over the world. Nearly 50% of medicines in the market are made of natural basic materials. Interestingly, the market demands for medicinal herbs are likely to remain high because many of the active ingredients in medicinal plants cannot yet be prepared synthetically [7]. The universal role of plants in the treatment of disease is exemplified by their employment in all major systems of medicine irrespective of the underlying philosophical premise. As example, we have western medicine with origins in Mesopotemia and Egypt, the Unani (Islamic) and Ayurvedic (Hindu) systems centred in western Asia and the Indian subcontinent and those of the Orient (China, Japan, Tibet, etc.). How and when such medicinal plants were first used is, in many cases, lost in pre-history, indeed animals, other than man; appear to have their own materiamedica.

Following the oral transmission of medical information came with the use of writing (example the Egyptian Papyrus Ebers c. 1600 BC), baked clay tablets (some 660 conie form tablets c. 650 BC form Ashurbanipal's library at Nineveh, now in the British Museum, refer to drugs well known today), parchment and manuscript herbals, printed herbals (invention of printing 1440 AD), pharmacopoeias and other works of reference (first London pharmacopoeia, 1618, first British pharmacopoeia 1864), and most recently electronic storage of data. Similar records exists for Chinese medicinal plants (text from the 4th century BC), ayurvedic medicine (Ayurveda 2500-600 BC), and Unani medicine

Prediction of Skin Disease Using Ensemble Data Mining Techniques and Feature Selection Method—a Comparative Study

Anurag Kumar Verma[1] · Saurabh Pal[1] (ID) · Surjeet Kumar[1]

Abstract

Nowadays, skin disease is a major problem among peoples worldwide. Different machine learning techniques are applied to predict the various classes of skin disease. In this research paper, we have applied six different machine learning algorithm to categorize different classes of skin disease using three ensemble techniques and then a feature selection method to compare the results obtained from different machine learning techniques. In the proposed study, we present a new method, which applies six different data mining classification techniques and then developed an ensemble approach using bagging, AdaBoost, and gradient boosting classifiers techniques to predict the different classes of skin disease. Further, the feature importance method is used to select important 15 features which play a major role in prediction. A subset of the original dataset is obtained after selecting only 15 features to compare the results of used six machine learning techniques and ensemble approach as on the whole dataset. The ensemble method used on skin disease dataset is compared with the new subset of the original dataset obtained from feature selection method. The outcome shows that the dermatological prediction accuracy of the test dataset is increased compared with an individual classifier and a better accuracy is obtained as compared with subset obtained from feature selection method. The ensemble method and feature selection used on dermatology datasets give better performance as compared with individual classifier algorithms. Ensemble method gives more accurate and effective skin disease prediction.

Keywords Skin disease · Dermatology · Extra tree classifier · Radius neighbors classifier · Passive aggressive classifier

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Research Article

Green Nanotechnology Approaches for Synthesis of Nanoparticles and Their Characterization Techniques: A Review

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ABSTRACT

Nanotechnology is an interdisciplinary field of science and we can see its importance's in engineering, pharmaceutical, medical, food, cosmetics, environment etc. The tools of nanotechnology can be used to reduce the size of materials in nano size and this size range shown a profound quality of materials. The present review focus on biomaterial utilized for synthesis of nanoparticles (NPs). These biomaterials can obtain from biological sources like bacteria, fungi, yeast, algae and plant. Although other techniques of synthesizing NPs are physical and chemical methods are available but these uses costlier instrumentation, harmful chemicals. A lot of energy is needed to run these instruments and at last they incorporate chemicals and heat in the environment. Biomaterials are easily available and do not use any harmful chemicals or costlier instrumentation. It can easily formulate NPs by its reducing and stabilizing activity. Thus green nanotechnology is an ecofriendly technique and having much of importances.

Keywords: Nanotechnology, Green synthesis, Biomaterial, Top-down approach, Bottom-up approach

INTRODUCTION

Today nanotechnology provides a big space in field of research and facilitates to design the nanoparticles in the range of 1-100 nanometer dimensions [1]. This size range open the new doors of possibilities in the engineering, medical, pharmaceutical and many more branches of science to serve the humanity. In the field of medical improve the quality of devices and diagnosing the disease in their early stage while in pharmaceuticals in designing of drug targeting carrier, improve bioavailability of therapeutic regimens, new marker agent and numerous metals therapeutic activity. Indian therapeutic system well known as Ayurveda has used bhasmas of metals as like silver, gold etc. make nanosized, which enhance their qualities. The metals at their nanosized range exhibit unique physical, chemical and biological properties in compare to their bulk form [2].

The different methods of nanoparticle synthesis are physical, chemical and biological. Physical methods include laser ablation, laser pyrolysis, high energy ball milling, physical vapor deposition, inert gas condensation, flash spray pyrolysis. The disadvantage of physical method of nanoparticle synthesis are eliminating much of thermal energy in environment, acquired a lot of space, slow rate of nanoparticle formulation, utilizing a lot of run of energy, and much of time need to achieve thermal stability. The chemical method includes chemical reduction, micro emulsion, colloidal method, sonochemical method, electro-chemical, solvothermal decomposition. Major disadvantages of chemical methods are using harsh chemical entity like sodium borohydrate, sodium citrate as reductants and the synthesized nanoparticles are usually contaminated with ions of these reducing agent and byproducts [3]. Beside of these, chemicals have much of toxic effects and cause numbers of environmental issues. The biological method of nanoparticle formation is termed green nanotechnology and today find much of attention globally because of its eco-friendly techniques produce environmental safe formulation, highly effective, low cost and reproducible method which enhance the stability, and no need of high temperature, pressure, pH etc at the time of synthesis.

All of these three physical, chemical, and biological methods following the two basic approaches are either the top down or bottom-up. Top-down is a destructive method in which bulk material is bruised to form nano size particle, while bottom- up approach follow from atomic level to build up nano size particles.

ORIGINAL ARTICLE

INTERNATIONAL JOURNAL OF RESEARCH IN PHARMACEUTICAL SCIENCES

Evaluation of the analgesic activity of ethanolic extract of *Populus deltoides* leaves in mice

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ABSTRACT

The ethanolic leaves extract of *Populus deltoides* was tested for the presence of various phytoconstituents and designed to evaluate the analgesic activity in mice. The peripheral analgesic activity of ethanolic leaves extract of *P.deltoides* (250 and 500 mg/kg) was studied by using acetic acid stimulated writhing test and central analgesic activity of *P.deltoides* was studied by using hotplate process. The ethanolic leaves extract of *P.deltoides* professed the existence of a variety of chemical constituents like alkaloids, saponins, flavonoids, terpenes and steroids. Leaves extract of *P.deltoides* appreciably decreased the writhing actions in acetic acid-induced writhing test in mice and amplified the respond time in hotplate test. These results suggest that the extract may have NSAIDs like activity through the peripheral mechanism and central analgesic activities via opioid receptors. From our study, we endowed that leaves extract of *P.deltoides* has feasible to analgesic activity. This study reveals that it can be used in the management of pain and provide a scientific basis for its traditional use.

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INTRODUCTION

Pain is the most frequent cause for consulting physician worldwide. It is one of the significant symptoms in various health situations, and can eloquently intrude an individual's transcendence of life and general practices. Psychological factors like community prompting, hypnotic suggestion, enthusiasm, or perturbation can succinctly slacken pain's amplitude or disaffection. Pain experiences may include acute and chronic. Chronic pain is decadence status and patient receiving palliative care. It is not solely physiological but further comprises spiritual, sentimental and social amplitude (Marskey and Bugduk, 2012). Various processes can evoke pain. They include nociception, peripheral sensitization, phenotypic switches, central sensitization, ectopic excitability and structural rearrangement is the mechanism that causes nociceptive pain and comprises the processes of transduction, conduction, transmission and perception (Woolf, 2004). Transduction is an alteration of a noxious stimulus including chemical, mechanical or thermal into electrical impulses in the peripheral terminals of nociceptor of free afferent nerve fibres. Conduction is the second phase of nociception, and the action potentials from the peripheral process conducted along axons to the central process of nociceptors in the central nervous system (Mannion *et al.*, 1999) transmission is the synaptic transfer from presynaptic terminals to the postsynaptic terminals of neurotransmitter receptor (Urch, 2007) and modulation of input is an adaptive process from one neuron to another and involve excitatory of inhibitory mechanism (Kirkpatrick *et al.*, 2015). Perception of pain is dependent on neural processing in the spinal cord

Page No.78

ORIGINAL ARTICLE

INTERNATIONAL JOURNAL OF RESEARCH IN PHARMACEUTICAL SCIENCES

Evaluation of the analgesic activity of ethanolic extract of *Populus deltoides* leaves in mice

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ABSTRACT

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INTRODUCTION

Pain is the most frequent cause for consulting physician worldwide. It is one of the significant symptoms in various health situations, and can eloquently intrude an individual's transcendence of life and general practices. Psychological factors like community prompting, hypnotic suggestion, enthusiasm, or perturbation can succinctly slacken pain's amplitude or disaffection. Pain experiences may include acute and chronic. Chronic pain is decadence status and patient receiving palliative care. It is not solely physiological but further comprises spiritual, sentimental and social amplitude (Marskey and Bugduk, 2012). Various processes can evoke pain. They include nociception, peripheral sensitization, phenotypic switches, central sensitization, ectopic excitability and structural rearrangement is the mechanism that causes nociceptive pain and comprises the processes of transduction, conduction, transmission and perception (Woolf, 2004). Transduction is an alteration of a noxious stimulus including chemical, mechanical or thermal into electrical impulses in the peripheral terminals of nociceptor of free afferent nerve fibres. Conduction is the second phase of nociception, and the action potentials from the peripheral process conducted along axons to the central process of nociceptors in the central nervous system (Mannion *et al.*, 1999) transmission is the synaptic transfer from presynaptic terminals to the postsynaptic terminals of neurotransmitter receptor (Urch, 2007) and modulation of input is an adaptive process from one neuron to another and involve excitatory of inhibitory mechanism (Kirkpatrick *et al.*, 2015). Perception of pain is dependent on neural processing in the spinal cord

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REVIEW ARTICLE

Techniques of Mucilage and Gum Modification and their Effect on Hydrophilicity and Drug Release

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Abstract: *Aim*: The manuscript aims to describe the techniques of modification of gums and mucilages and their effect on hydrophilicity and drug release.

Discussion: The interest is increased in the fields of polymers which are obtained from natural origin and used in the preparation of pharmaceuticals. Mucilage and gum are natural materials widely used in the preparation of novel dosage and conventional dosage forms. They are used in the pharmaceutical industry for various purposes like suspending, emulsifying, bio-adhesive, binding, matrix-forming, extended release and controlled release agent. Gum and mucilage are biodegradable, less toxic, cheap and easily available. Moreover, mucilage and gum can be changed to acquire tailored materials for the delivery of drugs and allow them to compete with commercially available synthetic products. These polysaccharides have unique swellability in an aqueous medium that can exert a retardant effect on drug release or act as a super disintegrant, depending on the concentration utilized in the preparation. Drug release mechanism from hydrophilic matrices consisting of gums and mucilages is based on solvent penetration-induced polymer relaxation, diffusion of entrapped drug followed by degradation or erosion of the matrix.

Conclusion: The present manuscript highlights the advantages, modifications of gum and mucilage, their effects on hydrophilicity and drug release as well as aspects of the natural gums which can be assumed to be bifunctional excipient because of their concentration-dependent effect on drug release and their high degree of swellability.

Keywords: Polysaccharides, gums and mucilages, hydrophilicity, modified gums, polysaccharide modification, drug release.

1. INTRODUCTION

Nature has offered a large variety of materials directly or indirectly to enhance and maintain the health of all living things. Biodegradable polymeric materials are generally natural gums. Various studies have been conducted using gums and mucilage in the field of food technology and pharmaceuticals. Usually, excipients have been used as inert vehicles in formulation of drugs which provide required weight, consistency to the active ingredient, but in recent dosage forms of pharmaceuticals, excipients used as a multi-functional agent like modifying drug release, enhancing the stability, active ingredient bioavailability, enhancing patient acceptability and ensuing ease of manufacturing. A huge number of pharmaceutical excipients dependent on plants are available in the market today. Several researchers have investigated plant-based products as a pharmaceutical excipients. It can generate a large range of materials based on

their molecular weight and different properties. Research became a vast area related to natural polymers used in the drug delivery system. Modified natural gums meet drug delivery systems requirements and thus compete with the synthetic excipient available in the market. In plants, gums are naturally occurring components, which are cheap and plentiful. Natural gums consist of multiple units of monosaccharide which are linked with each other to create large molecules. Gums are obtained by making an incision to the plant or owing to an adverse condition such as drought and cell wall breakdown (gummosis, extracellular formation). The gums are also obtained from the seeds endosperm. Few examples of gums are acacia, guar gum, tragacanth, *etc.* Composition of gums is heterogeneous in nature. Simple monosaccharide units like galactose, arabinose, mannose, glucose, uronic acid, and xylose are obtained during hydrolysis [1]. Polymers have been widely used in the formulation of solid, semi-solid and liquid dosage forms and used in the design of drug delivery systems for modified release. For this purpose, both natural and synthetic polymers have been extensively studied, but the utilization of natural polymers for pharmaceutical applications is appealing because they are inexpensive, readily accessible, non-toxic, capable of

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A BREAKTHROUGH TO CONTROL THE CORONAVIRUS DISEASE: OVERVIEW

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Conflicts of Interest: Nil
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ABSTRACT

Coronavirus disease 2019 is also known as COVID-19, which is a kind of viral pneumonia which is caused by severe acute respiratory syndrome coronavirus 2, also called as SARS-CoV-2. Coronavirus disease 2019 (COVID-19) was first identified amid an outbreak of respiratory illness cases in Wuhan City, Hubei Province, China. It was initially reported to the WHO on December 31, 2019. On January 30, 2020, the WHO declared the COVID-19 outbreak a global health emergency. On March 11, 2020, the WHO declared COVID-19 a global pandemic, its first such designation since declaring H1N1 influenza a pandemic in 2009. It is transmitted by inhalation or contact with infected droplets. The incubation period ranges from 2-14 days. As reported by worldometer.info dated on 6th June on 10:00AM, 2020, total no of active cases was 6859597, out of which no of deaths was 398244 in the world. Where as reported by government of India dated on 6th June on 10:00AM, 2020, total no of active cases 115942, out of which no of deaths was 6642.

Keywords: Breakthrough of Corona virus, COVID-19, Pathophysiology, Wuhan.

INTRODUCTION

Coronaviruses are a large family of viruses which may cause illness in animals or humans. In humans, several coronaviruses are known to cause respiratory infections ranging from the common cold to more severe diseases such as Middle East Respiratory Syndrome (MERS) and Severe Acute Respiratory Syndrome (SARS). The most recently discovered coronavirus causes coronavirus disease COVID-19.

COVID-19 is the infectious disease caused by the most recently discovered coronavirus. This new virus and disease were unknown before the outbreak began in Wuhan, China, in December 2019. COVID-19 is now a pandemic affecting many countries globally. Illness caused by SARS-CoV-2 was termed COVID-19 by the WHO, the acronym derived from "coronavirus disease 2019 [1]. As reported by worldometer.info dated on 6th June on 10:00AM, 2020, total no of active cases was 6859597, out of which no of deaths was 398244 in the world [2]. Whereas reported by government of India dated on 6th June on 10:00AM, 2020, total no of active cases 115942, out of which no of deaths was 6642 [3].

History

The first cases were seen in Wuhan, China, in late December 2019 before spreading globally. The first mention in the medical press about the emerging infection was in the British Medical Journal (BMJ) on 8 January 2020 in a news article, which reported "outbreak of pneumonia of unknown cause in Wuhan, China, has prompted authorities in neighboring Hong Kong, Macau, and Taiwan to step up border surveillance, amid fears that it could signal the emergence of a new and serious threat to public health". On 9 January 2020, the World Health Organization confirmed that

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Impact of COVID-19 Communication on Rural Population: A Case Study

Dr. Manoj Mishra[*]

Abstract

Media has disseminated all the relevant information like the places infected and mitigation measures about the deadly coronavirus which has rapidly infected the human population across the globe. Corona warriors of the media are present throughout the nation. The present study found that elderly people (>50 year) of Buksha Block were almost unaware of the impact of the disaster brought about by COVID-19 as compared to the younger (<50 year) people. A proper source of information is required for the rural people to induce awareness among them and to communicate the strategies to fight the COVID-19 pandemic. In rural areas most people do not have the electronic gadgets and financial ability. That is why they are not using Aarogya Setu app or proper sanitizers and masks during this crucial situation, nor are they aware that physical distancing has become an important weapon to fight the COVID-19 pandemic.

Introduction

COVID-19 has reached the whole world. It emerged from Wuhan in China (Phelan et al., 2020, Wu et al., 2020). Although, its exact origin and ability to spread among human beings are still not very clear, the large number of cases reported worldwide shows the human to human transmission of the disease. According to the WHO, the symptoms of COVID-19 appear to be relatively mild as compared with SARS-CoV (Severe Acute Respiratory Syndrome Coronavirus) and MERS-CoV (Middle East Respiratory Syndrome Coronavirus).

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Flexibility in service operations: review, synthesis and research agenda

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Abstract

Purpose – The purpose of this paper is to present a systematic review of flexibility, to identify the gaps in theory and to propose a future research agenda.

Design/methodology/approach – This paper combines a systematic review and thematic analysis of scholarly articles of flexibility. The articles are analyzed to explicate the dynamics of flexibility in service operations. Thematic analysis was done using NVIVO 10.0 to identify key approaches, trends and future research agenda.

Findings – The review reveals ten different themes that highlight the future research avenues and points out that an integrative framework to assess the field of flexibility, particularly in developing countries, is largely missing in the literature. The study also provides a set of research questions to enhance its explanatory power.

Research limitations/implications – Articles that explicitly mention "flexibility" were only included, however, there may be several unexploited areas regarding the influence of different variables on flexibility. The study is based on the inductive analysis of 650 published articles on flexibility retrieved from the electronic database. The framework proposed in the study is conceptual and requires empirical testing in future research.

Originality/value – The study synthesizes the flexibility literature and contributes to a set of ten distinct themes that extricate the dynamics of flexibility. The study provides a comprehensive review of the relevant articles and identifies the theoretical gaps in the research area of service operations flexibility that can be used by academia and industry for promoting flexibility.

Keywords Uncertainty, Service operations, Flexibility, Themes, Literature review

Paper type Research paper

1. Introduction

Scholars and practitioners have extensively examined how service operations are faced with a high degree of uncertainty and argue that flexibility is essential in multiple fronts for customer value creation (Skålén *et al.*, 2015; Brozovic *et al.*, 2016). Flexibility refers to "an organization's ability to provide a rapid response mechanism to the uncertainties while simultaneously being adaptive to changes in the environment" (Dreyer *et al.*, 2012). Many authors have pointed out flexibility as adjustments in service capacity and to deliver customized service rapidly (Saurez *et al.*, 1996; Aranda, 2003). From an assessment point of view, the concepts of flexibility constitute an open system and need an exploration across the value chain. Considerable attention in the field of service operations flexibility has been received in the last two decades (Verdu-Jover *et al.*, 2004; Toni and Tonchia, 2005; Aryee and Potter, 2010). Recent studies have not only emphasized the relevancy of flexibility but also argue that it is vital for sustainability and improved performance (Lucianetti *et al.*, 2018). Therefore, to make the phenomena more visible and organize knowledge for the improved understanding of the field, an assessment of flexibility is required.

There is an increasing corpus of flexibility articles in several study context and levels of analysis. The literature of flexibility has seen impressive growth and crosses disciplinary

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Stream Function Solution of the Brinkman Equation in Parabolic Cylindrical Coordinates

Deepak Kumar Maurya[1,2] · Satya Deo[1]

Abstract

The present work concerns the general stream function solution of the Brinkman equation in parabolic cylindrical coordinates, arising in the study of fluid flow through porous medium. Analytical stream function solutions of this equation are available in the coordinates (Cartesian, cylindrical polar, spherical polar and prolate spheroidal coordinates). Stream function solution of the Stokes equation in parabolic cylindrical coordinates is also investigated analytically. The parabolic cylinder functions are a class of functions which are the solution of Weber differential equation. A transformation of parabolic cylinder function into the Whittaker function is used. Method of inverse operator is applied to obtain particular integral in solving the Stokes equation. Explicit expressions of velocity components and vorticity are also reported.

Introduction

The study of viscous fluid flow through porous media is of interest to a wide range of researchers due to its numerous applications in many fields such as bio-mechanics, physical sciences, chemical engineering, etc.. Due to vast applications, several conceptual models have been developed for describing fluid flow through porous media [11]. Henry Darcy (1856), stated that the seepage velocity of fluid flow through porous medium is proportional to the

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Some recursion formulas for q-Lauricella series

Ashish Verma[1] · Vivek Sahai[2]

Abstract

We obtain certain recursion formulas for fourteen three variable q-Lauricella series. It is derived that these recursion relations can be expressed in terms of q-derivatives of the respective q-Lauricella series.

Keywords Recursion formula · q-Lauricella series · q-Derivative

Mathematics Subject Classification 33D15 · 33D70

1 Introduction

The recursion formulas for multivariable hypergeometric functions have received considerable attention. Opps, Saad and Srivastava [7] and Wang [17], have presented recursion relations of two variable Appell functions. The authors have carried out a study of recursion formulas of multivariable hypergeometric functions including Lauricella functions, three Srivastava's triple hypergeometric functions and four k-variable Lauricella functions [10] and Exton's triple hypergeometric functions [11]. The recursion formulas for the general triple hypergeometric function [16] were obtained in [12]. In [13], recursion formulas for general Kampé de Fériet series and Srivastava and Daoust multivariable hypergeometric function [15] were presented.

Some Saigo type fractional integral inequalities and their q-analogues and q-series identities were derived in [2–4]. Also various application of special functions and q-series were given in [1,8]. Recently, recursion formulas satisfied by basic (or q-) hypergeometric series were studied [14]. In particular, recursion formulas for generalized basic hypergeometric series $_r\phi_s$, q-Appell series and the general double q-hypergeometric series were obtained. In the present paper, we find the recursion formulas for three variable q-Lauricella series. We

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Recursion formulas for Srivastava's general triple q-hypergeometric series

Ashish Verma[1] · Sarasvati Yadav[2]

Abstract

We obtain recursion formulas for the Srivastava's general triple q-hypergeometric series. It is derived that these recursion relations can be represented in terms of q-derivatives of respective Srivastava's general triple q-hypergeometric series. The peculiar outcome for three Srivastava's triple q-hypergeometric series $H_{A,q}$, $H_{B,q}$ and $H_{C,q}$ are also drawn from the recursion formulas for the Srivastava's general triple q-hypergeometric series.

Keywords Recursion formulas · Srivastava's general triple q-hypergeometric series · Srivastava's triple q-hypergeometric series

Mathematics Subject Classification 33D15 · 33D70

1 Introduction

In the recent years a lot of attention has been put on the recursion formulas for multivariable hypergeometric functions. The first attempt was made by Opps et al. [4] who gave the recursion formula for the Appell function F_2 and its application to radiation field problem. Further, Wang [16] enhanced the study of recursion formulas of all Appell functions. This work was further extended by Sahai and Verma, including fourteen three variable Lauricella functions, three Srivastava's triple hypergeometric functions, four k-variable Lauricella functions [6] and Exton's triple hypergeometric functions [7]. The generalized and unified results of [6], for three variable hypergeometric function were obtained in the recursion formulas for the general triple hypergeometric function [8]. In [9], recursion formulas for general Kampé de Fériet series and Srivastava and Daoust multivariable hypergeometric functions [11,14] are derived.

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Examples of Simple Wavelet Sets for Matrix Dilation in $\mathbb{R}^2$

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Abstract

In this article, we tried to construct some examples supporting the results mentioned on a simple wavelet set for matrix dilation with the help of results introduced by K.D. Merrill on her article with some modification and we have also seen the difference between the simple wavelet sets for the matrix dilation in $\mathbb{R}^2$ constructed by K.D. Merrill and us.

Subject Classification: 42C40.
Keywords: Wavelet sets, Wavelets, Translations, Dilation.

1. Introduction.

A set $W \subset \mathbb{R}^2$ is called a wavelet set for a wavelet $\psi \in L^2(\mathbb{R}^2)$, if the Fourier transform of ψ is a characteristic function on set W i.e. , $\hat{\psi} = \chi_W$, where $\psi \in L^2(\mathbb{R}^2)$ is an orthonormal wavelet means $\{\psi_{j,k} \equiv \sqrt[2]{|detA|^j}\psi(A^j. - k), j \in \mathbb{Z}, k \in \mathbb{Z}^2\}$ form an orthonormal basis for $L^2(\mathbb{R}^2)$. And a Simple Wavelet set is defined as a wavelet set $W \subset \mathbb{R}^2$ for an 2-square expansive integer dilation matrix, if wavelet set W can be scripted as finite union of convex bounded polygons. K.D. Merrill has given a partial answer of questions in her article in 2012 that of which expansive integer matrix dilations in $\mathbb{R}^2$ have a wavelet set which can be scripted as the union of convex bounded polygons up to finite no.. And, she gave a new result which supports the conjectures of the matrices that can be written as a scalar matrix by using suitable positive powers of the matrices and having the determinants greater or equal to 2.

The latest examples of two-dimensional wavelet sets for dilation by 2 were constructed by Zakharov [4], Soardi and Wieland [5], and Dai and others. [6]. Most of the recent researchers believed that these geometric structures were unavoidable. In [7], Benedetto and Sumetkijanakan have described for 2 dilation wavelet set in $\mathbb{R}^n, n \geq 2$, can not be the union of n or least convex sets and stated that it could not be the finite union of convex sets. The question has since been raised to exactly

Some results on the Srivastava's triple hypergeometric matrix functions

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February 18, 2020

Abstract

Inspired by the recent work by Abd-Elmageed *et al.*, who establish recursion formulas satisfied by the first Appell matrix function, namely F_1 and Sahai *et al.* have presented various recursion formulas for the Gauss hypergeometric matrix function and all four Appell matrix functions. In this paper, we obtain recursion formulas and infinte summation formulas for Srivastava's triple hypergeometric matrix functions H_A, H_B and H_C.

Keywords: Matrix functional calculus, recursion formulas, Srivastava's triple hypergeometric matrix functions

AMS Subject Classification: 15A15; 33C65; 33C70

1 Introduction

The theory of matrix special functions has attracted considerable attention in the last two decades. Special matrix functions appear in the literature related to Statistics [3], Lie theory [6] and in connection with the matrix version of Laguerre, Hermite and Legendre differential equations and the corresponding polynomial families [9, 10, 11]. Recently, Abd-Elmageed *et al.* [1] have obtained recursion formulas satisfied by the first Appell matrix function, namely F_1. Further Sahai and Verma [19] established recursion formulas for the Gauss hypergeometric matrix function and all four Appell matrix functions. Inspired

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Enhanced ATM Security with OTP Based Authentication

Prashant Kumar Yadav, Akhtar Husain, Surjeet Kumar

Abstract

This research article is proposed to enhance the security of traditional ATM machine. We are introducing a new technique that enhances the overall mechanism, security, and comfort of the ATM transactions. Biometric information such as face recognition or finger print detection and OTP (One-TimePassword) may be used for enhancing the security of ATM transactions as well as user's private information. Biometric authentication technique helpsa machine (biometrically enhanced) to recognize an individual user independently and uniquely. So we can introduce the face or thumb impression as a security key. This new security key can totally avoid bank fraudsdue to compromised security of ATM and bank account related information. On the other hand, one time password (OTP) will help the user as they need not to remember the password or security pin of ATM.

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Constraint length inflation in fixed high rate convolutional codes and their impact on performance of O-IDMA

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Article Info	ABSTRACT
	To cope up with the higher data rate existing in modern communication systems multiple access technologies has been investigated OIDMA (Optical Interleave Division Multiple Access Technology) is one of the prominent technology use to fulfill this demand. Convolutional codes used in OIDMA systems enhance the performances and reduces the bit error rate of the system. In the present paper, the convolutional codes with increasing number of memory elements are used, the constraint length which depends on number of memory elements are increased with a systematic manner and their combined effect on response of OIDMA system has been observed. Tree interleavers in taken into account for analysis purpose and BER with increasing number of users is plotted in graphical and tabular manner.

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1. INTRODUCTION

The multiple access schemes are frequently used in wireless & mobile communication to meet out the larger traffic intensity. Traffic intensity, measured in erlang is a tool to identify and count total quantity of users in a particular territory [1-2]. As traffic intensity is increasing multiple access interference (MAI) problem, inter-symbol interference (ISI) problem multiuser detection, near far problems are arising in existing multiple access technique like CDMA, TDMA, FDMA, DS-CDMA etc. [3-4]. To cope up heavy traffic intensity of users, solution is to use IDMA technology which drastically removers the all problems mentioned earlier in multiple access techniques.

The performance of CDMA-UWB signal is examined by using Gaussian pulses shape at optical source [5]. The performance of Multi Carrier Code Division Multiple Access (MC-CDMA) modulation using MERRY algorithm and provides the better performance as compaererd to OFDM system [6]. They described the BER performance in F-OFDM system using the BCH code over a multipath fading channel and fulfilled the requirement of 5G [7]. The authors also described the PAPR performance of F-OFDMA system using the Arithmetic coding and Huffman coding [8]. They evaluate the BER performance of OFDM systems using various channels (Fading, Rayleigh, Rician and AWGN) [9].
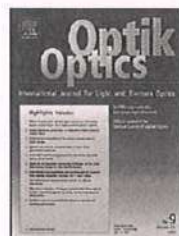
When optical technology is incorporated in IDMA it is more effective known as OIDMA. As we know that optical technology possesses advantages in terms of enormous potential bandwidth, low loss, less interference, low cross talk, minimum bit error rate which makes it preferable for longer distance transmission. IDMA is special form of CDMA where extension of bandwidth is done by same PNS code to all users while user's separation is achieved by specific interleavers for each user [10-12]. By using single

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Impact of Code Rate and Constraint Length Variation on Qualitative Performance of OIDMA System with Random Inter-Leaver

Ajay Kumar Maurya, Ravi Prakash, S.K. Sriwas, Pramod Kumar, R.K. Singh

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Sasakian Hypersurfaces in a Hermitian Manifold

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Abstract: The object of present paper is to study the properties of Sasakian hypersurfaces in a Hermitian manifold.
Keywords: Sasakian manifold, Hypersurfaces, Hermitian manifold.
2010 AMS Classification Number: 53C15, 53C25.

1. Introduction

The almost contact metric structures are closely connected to the almost Hermitian structures. For instance, if $\left(N, \{\varphi, \xi, \eta, g\}\right)$ is an almost contact metric manifold, then an almost Hermitian structure is induced on $N \times \mathbb{R}^1$. If this almost Hermitian structure is integrable, then the input almost contact metric structure is called normal. As it is known, a normal contact metric structure is called Sasakian[1]. On the other hand, we can characterize the Sasakian structure by the following condition:

$$(\nabla_X \varphi)(Y) = (X, Y)\xi - \eta(Y)X, \quad X, Y \in TM,$$

As it is well known, the Sasakian structures have many remarkable properties and play a fundamental role in contact geometry. In the present paper, almost contact metric hypersurfaces in Hermitian manifolds are considered.

Perceived work–life balance and organizational talent management: mediating role of employer branding

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Abstract

Purpose – This paper aims to examine the effect of perceived work–life balance on the perceived level of employer branding attraction value and organizational talent management. Accordingly, the structural model is developed that delineates the interactions among these and explores the mediating effect of employer branding attraction value between the relationship of work–life balance and organizational talent management.

Design/methodology/approach – This study is based on survey results and review of literature in terms of their implications for the proposed framework. Data have been collected by convenience incidental sampling from middle-level executives working in different information and technology (IT) companies. The model and posited hypotheses were tested through structural equation modeling analysis.

Findings – Perceived work–life balance was found to be positive and significantly predicted the employer branding attraction value and organizational talent management. The study also showed that there exists a significant and positive correlation between employer branding attraction value and perceived organizational talent management. Further, employer branding attraction value found to be a mediating construct between the relationship of work–life balance and organizational talent management.

Research limitations/implications – The present study will add insight into the human resource practitioners to design cost-effective and prolonged popular practices in order to meet the employees work and personal expectations under the organizational association. The research investigated issue within focused IT sector employees to understand and solve the issues generated with changing factors in an organizational environment such as increasing women participation, duel earning couple, and maintaining the difference between various categories of employees at the practice level.

Social implications – The study has value at both the scholarly and practice level. At a scholarly level, the research investigated an important contemporary issue at both level individual as well as organizational level. In practice if organization implements people friendly work-life balance policies, then this will be surely be helpful in organizational productivity in form of talent management and employer branding and further this will improve the personal and professional performance of most elementary component of developing society

Research Progress of Artificial Psychology and Artificial Intelligence in India

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Abstract- Artificial Psychology is a discipline that uses information science to achieve a more comprehensive coverage of human psychological activity with artificial machine like: computer and algorithmic models. In the field of information science, researchers have regarded the imitation of human brain, human intelligence, and human behavior as important research directions and contents. A review of automation science and technology shows that more people use brain science, psychology, neuroscience or cybernetics and theory of controlled source in studying algorithms

Artificial Intelligence refers to the ability of machines to perform cognitive tasks like thinking, perceiving, learning, problem solving and decision making. Initially conceived as a technology that could mimic human intelligence, AI has evolved in ways that far exceed its original conception.

Index Terms- Artificial Intelligence, Artificial Psychology, Deep Learning, Machine Learning.

I. INTRODUCTION

After decades of research, today AI has topped the heights of achievements in technology.

With incredible advances made in data collection, processing and computation power, intelligent systems can now be deployed to take over a variety of tasks, enable connectivity and enhance productivity. As AI's capabilities have dramatically expanded, so have its utility in a growing number of fields.

The truly transformative nature of the technology, yet the nascent stage of its adoption worldwide, provides India with an opportunity to define its own brand of AI leadership. #AI for All - the brand proposed for India implies inclusive technology leadership, where the full potential of AI is realized in pursuance of the country's unique needs and aspirations. The strategy should strive to leverage AI for economic growth, social development and inclusive growth, and finally as a Garage for emerging and developing economies.

Adoption of AI across the value chain viz. startups, private sector, PSUs and government entities, will truly unlock the potential by creating a virtuous cycle of supply and demand. The barriers to AI development and deployment can effectively be addressed by adopting the marketplace model – one that enables market discovery of not only the price but also of different approaches that are best suited to achieve the desired results. A three-pronged, formal marketplace could be created focusing on data collection and aggregation, data annotation and deployable models.

The content of artificial intelligence research focuses on how to express, acquire, and use knowledge. Artificial intelligence, however, is only the preliminary stage in the field of personification research because human psychological activities include feeling, perception, memory, thinking, emotion, will, character, and creation. Among these activities, only feeling, perception, memory, and thinking are encompassed by artificial intelligence; thus, its scope is limited. Therefore, to study artificial psychology and artificial emotion and develop cutting-edge technology and industrial applications in these fields, artificial intelligence research (research results and research methods) must be used as theoretical basis; new theories and methods in psychology, brain science, neuroscience, information science, computer science, and automation science should be integrated; and psychological activities, particularly emotion, will, character, and creation, should be simulated .

Two CLOSELY RELATED ASPECTS of Artificial Intelligence that have received comparatively little attention in the recent literature are research methodology and the analysis of computational techniques that span multiple application areas. We believe both issues to be increasingly significant, as Artificial Intelligence matures into a science and spins off major application efforts. It is imperative to analyze the repertoire of AI methods with respect to past experience, utility in new domains, extensibility, and functional equivalence with other techniques, if N is to become more effective in building upon prior results rather than continually reinventing the proverbial wheel. Similarly, awareness of research methodology issues can help plan future research by learning from past successes and failures. We view the study of research methodology to be similar to the analysis of operational AI techniques, but at a meta-level; that is, research methodology analyzes the techniques and methods used by the researchers themselves, rather than their programs, to resolve issues of selecting interesting and tractable problems to investigate, and of deciding how to proceed with their investigations. A public articulation of methodological issues that typically remain implicit in the literature may provide some helpful orientation for new researchers and broaden the perspective of many AI practitioners.

AI assistants are set to transform the way humans and machines interact:
Convenient and time saving

From physical to digital: what drives generation Z for mobile commerce adoption?

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Abstract

Purpose – This study aims to identify factors affecting generation Z as the early adopters of mobile commerce (m-commerce). The research seeks to explore their behavioral intention to adopt m-commerce in India with consideration of gender differences while providing empirical validation for the theory of planned behavior (TPB).

Design/methodology/approach – In this study, a modified TPB model has been used to explain generation Z's intention to adopt m-commerce. The proposed model was tested using a survey method with a sample of 245 students from a private university in Northern India. Subgroup analysis was performed to find gender differences in the process of adopting m-commerce.

Findings – All three independent constructs have a positive influence on the behavioral intention of generation Z to adopt m-commerce. Further, the male subgroup has a lower beta value for attitude and higher beta value for subjective norm in comparison to the female subgroup. For perceived behavioral control, no significant difference in beta value across gender could be established.

Practical implications – A better understanding of generation Z behavioral intentions will be of great use to telecom companies, marketers and electronic commerce companies to formulate strategies to expedite the use of m-commerce. As gender plays an important role in attitude and subjective norms, companies are advised to target their communication tactics in accordance to gender.

Originality/value – To the best of the authors' knowledge, this study is one of the first to test TPB and generation Z association in the context of m-commerce adoption in India. Data regarding the difference between the two genders has also shed light on the uniqueness of the context.

Keywords Subjective norm, Theory of planned behavior, M-commerce, Perceived behavioral control, Buying intention, Generation Z, Attitude

Paper type Research paper

1. Introduction

The growing popularity of mobile devices and the proliferation of mobile technologies has led to the emergence of mobile commerce (m-commerce) as a new business phenomenon (Zheng et al., 2019). m-commerce refers to the business activities conducted through internet-enabled mobile devices (Ko et al., 2009). Compared to electronic commerce, m-commerce offers a unique set of advantages such as instantaneity, ubiquity, localization, personalization and identification (Wang et al., 2015). Mobile technology is a new, fast-growing marketing communication tool that has evolved, and in India, it is supposed to surpass electronic commerce (Nielson report, 2013). This shift from "e" to "m" happened quickly (Business World, 2014). As envisaged by the Government of India (GoI) in their "Digital India" 2019 vision document, the aim is to achieve a leadership position for India in the field of information technology (IT). According to Deb and Agrawal (2017), until every Indian adopts digital channels to access a wider range of financial and non-financial services, the GoI's initiatives for "Digital India" cannot be realized.

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PARADIGM SHIFTING FROM CLASSROOM EDUCATION TO ONLINE CLASSES DURING COVID-19 PANDEMIC

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ABSTRACT

Corona virus disease (COVID-19) is an infectious disease caused by newly discovered corona virus. It is slowing down the world economy. Each and every sector whether working or non-working has been totally affected by it. Educational issues have grown up to a very large extent due to the pandemic. Educational issues are one of major issues among those topics which need to be taken into consideration now days. Internet has changed the things that how we communicate nowadays, Online teaching during this pandemic Covid-19 has proved to be another perk of technology. Teachers are efficiently taking online classes but the questions arise the consideration and challenges that students and teachers are facing. Study is to throw light on some of the major concerns regarding it.

KEYWORDS: Paradigm shift, education, online teaching, technology.

INTRODUCTION

Online teaching is major technological evolution from traditional classroom teaching. "Paradigm shift", word as identified by American physicist Thomas Kuhn, is a fundamental change in the basic concept and experimental practices of scientific discipline. (Kuhn,1962). During the pandemic online education has become a big platform for students and teachers to make study possible to very much extent. In the last two decades, online education has been considered to be highly important in the field of higher education (Allen& Araman,2014). In a developed country like America, making online learning an integral part of higher education due to many courses being made online (Li& Irby,2008; Luyt,2013; Lyons,2004). In this time of epidemic, UGC has given the guidelines of online education, it is mandatory that it is due to technology that teachers and students are able to do the work of teaching studies smoothly in this period. Online education has a great flexibility in terms of the its diversity. there are huge classes of online courses available for students where age, community, gender, timing and any other type of discrimination does not matter. Online education also helps the full time employed students. online learning programme contributes not only the preference for an online course format but also to their success in any academic setting (Richardson et all 1999).

Relation Between Spirituality and Well Being Among Adolescents

Smriti Srivastava   *Dr. janhvi Srivastava***

Abstract : This paper is a study of adolescents, well being and spirituality. 100 participant , included in this study which comprised of 47 males and 53 females. The questionnaires included, The Daily Spiritual Experience Scale (DSES) is a 16-item self-report (Underwood,L.G.2006) measure designed to asses ordinary experiences of connection with the transcendent in the daily life. The Personal Well Being Index (PWI) was developed by the International Well Being group (2006). In spirituality, the mean of female are greater than male but S.D. of male is greater than female . In well being, the mean and S.D. of female is greater than male . Result of the study revealed that there is positive correlation between spirituality and well being among adolescents.

INTRODUCTION

Spirituality : Spirituality is the broad concept of a belief in something beyond the self. It may involve religious traditions centering on the belief in a higher power, but it can also involve a holistic belief in an individual connection to others and to the world as a whole.

Spirituality offers a worldview that suggests there is more to life than just what people experience on a sensory and physical level. Instead, it suggests that there is something greater that connects all beings to each other and to the universe itself. It also proposes that there is ongoing existence after death and strives to answer questions about the meaning of life, how people are connected to each other, truths about the universe, and other mysteries of human existence.

Spirituality means different things to different people. For some, it's primarily about a belief in God and active participation in organized religion. For others, it's about non-religious experiences that help them get in touch with their spiritual selves through quiet reflection, time in nature, private prayer, yoga, or meditation.

Many people identify as spiritual but not religious : With a few exceptions, the percentage of adults who identify as religious in many industrialized countries is declining, while remaining generally high in less developed nations. Even as religious affiliation decreases, though, a sense of spiritual identification could remain steady or even increase.

Spiritual and well-being plays an important role in mental, emotional and physical health. Spiritual and well being is associated with a specific religion but does not have to be. Spirituality provide an opportunity to detach from circumstances and observe life with clarity and integrity. Spirituality can either be positive or negative. Spiritual and well-being is a state in which the positive aspects of spirituality differs from one person to the other. Through proper spiritual and well-being, people are empowered and realize their issues, stressors, and challenges, and these are not defined by these circumstances. This realization paves a pathway to greater peace, freedom of self-expression, increased manageability over the healing process and higher self-esteem.

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Reviewing the Status of Open Defecation Free India

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ABSTRACT

"Open defecation free" is a phrase first used in community-led total sanitation (CLTS) programs. ODF has now entered use in other contexts. The original meaning of Open defecation free stated that all community members are using sanitation facilities (such as toilets) instead of going to the open for defecation. This definition was improved and more criteria were added in some countries that have adopted the CLTS approach in their programs to stop the practice of open defecation. The Indian Ministry of Drinking and Sanitation has in mid-2015 defined Open defecation free as "the termination of fecal-oral transmission, defined by no visible feces found in the environment or village and every household as well as public/community institutions using safe technology option for disposal of feces". "Safe technology option" means a toilet that contains feces so that there is no contamination of surface soil, groundwater, or surface water; flies or animals do not come in contact with the open feces; no one handles excreta; there is no smell and there are no visible feces around in the environment which is a part of the Swachh Bharat Abhiyan (Clean India Campaign). In this paper, we will review the current status or one can say peek into the present-day situation of the Open defecation free program based on the data provided by various national agencies.

Keywords: Rural India, Open defecation, Women Safety, Women Health.

I. INTRODUCTION

Open defecation is the human practice of defecating outside ("in the open") rather than into a toilet. People may choose fields, bushes, forests, ditches, streets, canals, or other open space for defecation. They do so either because they do not have a toilet readily accessible or due to traditional cultural practices. The practice is common where sanitation infrastructure and services are not available. Even if toilets are available, behavior change efforts may still be needed to promote the use of toilets. "Open defecation free" (ODF) is a term used to describe communities that have shifted to using toilets instead of open defecation. This can happen, for example, after community-led total sanitation programs have been implemented.

Open defecation can pollute the environment and cause health problems. High levels of open defecation are linked to high child mortality, poor nutrition, poverty, and large disparities between rich and poor.

As of 2019, estimated 673 million people practices open defecation, down from about 892 million people (12 percent of the global population) in 2016. In that year, 76 percent (678 million) of the people practicing open defecation in the world lived in just seven countries.

Defecating in the open is a very ancient practice. In ancient times, there were more open spaces and less population pressure on land. It was believed that defecating in the open causes little harm when done in areas with low population, forests, or camping type situations. With development and urbanization, open defecating started becoming a challenge and thereby an important public health issue, and an issue of human dignity. With the increase in population in smaller areas, such as cities and towns, more attention was given to hygiene and health. As a result, there was an increase in global attention towards reducing the practice of open defecation.

Open defecation perpetuates the vicious cycle of disease and poverty and is widely regarded as an affront to personal dignity. The countries where open defecation is most widely practiced have the highest numbers of deaths of children under the age of five, as well as high levels of malnutrition, high levels of poverty, and large disparities between the rich and poor.

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सूचना का अधिकारः मीडिया का अचूक हथियार

डा. सुनील कुमार
असिस्टेंट प्रोफेसर, जनसंचार विभाग, वीर बहादुर सिंह पूर्वांचल विश्वविद्यालय, जौनपुर

स्वतंत्र भारत में लोगों को मिले मौलिक अधिकार के बाद सूचना का अधिकार सबसे बड़ा अधिकार है। इसके लागू होने के बाद सामाजिक संगठनों के तो ऐसे मालूम होता है कि अच्छे दिन आ गए हैं। खासतौर से यह लग रहा है कि मीडिया को अचूक हथियार मिल गया है। हालांकि इसे समाचार का स्रोत तो नहीं मान रहे हैं मगर खोजी पत्रकारिता करने वाले रिपोर्टरों के लिए यह बहुत ही संजीदा हथियार है। आज सामाजिक संगठन हो या कोई एक्टिविस्ट भ्रष्टाचार को उजागर करने के लिए इसका जमकर उपयोग कर रहा है। इस मामले में पत्रकार भी पीछे नहीं हैं, वह सूचना एकत्र करने और उसे प्रमाणित बनाने में भी इस अधिनियम का भरपूर इस्तेमाल कर रहे हैं। राजनीतिक लोग तो अपने प्रतिद्वंदी को नीचा दिखाने के लिए इसका जमकर इस्तेमाल कर रहे हैं। बाद में मोदी सरकार ने सूचना के अधिकार बिल में संशोधन करके नया विधेयक 2019 में पेश कर दिया। इस विधेयक का कांग्रेस समेत तमाम विपक्षी दलों ने जमकर विरोध किया। विपक्षी दलों का कहना था कि इससे विधेयक के उद्देश्य की मूल आत्मा मर गई है। साथ ही इसकी पारदर्शिता पर भी चोट की गई है। यह भी आरोप लगाया गया कि अब सरकार की मर्जी पर है कि वह सूचना दे या नहीं। कहने का अभिप्राय यह कि इस कानून को भोथरा बना दिया गया है।

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