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 2020-2021	01-112

Polyhedron 200 (2021) 115142

Contents lists available at ScienceDirect

Polyhedron

journal homepage: www.elsevier.com/locate/poly

Non-covalent interactions governing the supramolecular assembly of copper(II) complexes with hydrazone-type ligand: Experimental and quantum chemical study

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ARTICLE INFO

Article history:
Received 16 January 2021
Accepted 26 February 2021
Available online 13 March 2021

Keywords:
Copper(II) complexes
Supramolecular structures
EPR
Antiproliferative activity
SOD activity
Magnetic studies
Hirshfeld analysis

ABSTRACT

A series of two new mono- and one binuclear μ-nitrato bridged copper(II) complexes $[Cu(L)(HL)]ClO_4$ (1), $[Cu(HL)(NO_3)(H_2O)]2NO_3{\cdot}H_2O$ (2) and $[Cu_2(L_2)(\mu\text{-}NO_3)_2]$ (3), with an unsymmetrical NNO donor Schiff base (HL) have been synthesized and characterized by elemental analysis, FTIR, CV, UV–vis and EPR spectroscopy. Their molecular structures were also determined by single crystal X-ray crystallography. In the binuclear complex 3, the Cu··· Cu distance is 3.494 Å. In 1, 2 and 3, the Cu(II) centers have distorted square pyramidal geometry (τ_5 = 0.05–0.17). Evidence of weak π···π stacking intermolecular interactions along with other non-covalent interactions (hydrogen bonding) was observed by analyzing the respective crystal structures of the complexes. Thus, these hydrogen bonds, π···π stacking interactions and other weak intermolecular interactions establish in the form of supramolecular architectures a crystalline "network" environment. The non-covalent interactions were also investigated by employing Hirshfeld Analysis. The room temperature magnetic moments of the mononuclear complexes are less than the spin only values which are indicative of small interactions. Also, significant magnetic interactions were not exhibited by binuclear copper(II) complex 3 in the variable temperature magnetic measurements. The X-band EPR spectra of all three complexes exhibit copper(II) hyperfine structures as well as zero-field splitting which are appropriate for the triplet states of dimers. In complexes 1 and 2, the presence of pseudo dipolar interactions is proposed. Quantum chemical calculations (DFT) were carried out on complexes 1–3 to explore the electronic and spectral properties of these newly synthesized complexes. These complexes show significant antiproliferative and SOD activity. The SOD activity measured in terms of k_{McCF} is in the range 4.94–12.31 $(mol\ L)^{-1}s^{-1})\times 10^4$.

1. Introduction

Supramolecular chemistry deals with weak and reversible non-covalent interactions in and between molecules and resulting multimolecular systems. These interactions include hydrogen bonding, CH···π interactions, π···π interactions and hydrophobic forces that are essential in supramolecular assembly, host–guest chemistry and molecular recognition [1]. It have been observed that the counter ions have a major role on the formation of metal complexes. Different coordination potentials, size and geometries of anions have a significant effect on the structural assembly and largely influence the prediction of the overall molecular architectures of metal complexes [2]. Synthetic molecular coordination assemblies have gained their inspiration in biological systems. The combination of supramolecular chemistry with biology allows existing biological and chemical methods for the study and modulation of biological systems. Thus, supramolecular biology provides opportunities to bridge the gap between classical synthetic molecules and biomolecules. Molecular aggregates have received significant attention owing to their

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https://doi.org/10.1016/j.poly.2021.115142
0277-5387/

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Journal of Molecular Structure 1243 (2021) 130928

Contents lists available at ScienceDirect

Journal of Molecular Structure

journal homepage: www.elsevier.com/locate/molstr

Syntheses, characterization and oxygen evolution reaction (OER) electrocatalytic properties of M(II) based bromo-salophen complexes

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ARTICLE INFO

Article history:
Received 21 March 2021
Revised 3 June 2021
Accepted 14 June 2021
Available online 18 June 2021

Keywords:
Salophen
Oxygen evolution reaction
Electrocatalyst
PXRD

ABSTRACT

Efficient oxygen evolution reaction catalyst can be prepared via controlled decomposition method, and there is still minimal mechanistic understanding of such method. Here, we introduce a 3-Bromo-salophen ligated nickel(II) and copper(II) complexes as a precursor to obtain a Ni and Cu-based oxygen evolution reaction electrocatalyst via the controlled decomposed method. In our case, the unique O,N chelation mode of the 3-Bromo-salophen ligand (bis[2-bromosalicylydene]-1,2-iminophenylenediamine) was used to synthesize M(II) complexes. By regulating the decomposition conditions, we successfully obtained varied structures. The designing of a nonprecious, highly efficient and long-lasting oxygen evolution reaction electrocatalyst for electrochemical water splitting is a current emergency for reducing energy demand in the future. In this study, we found cost-effective decomposed products of NiO and CuO which are prepared by a simple one-step chemical precipitate method at high temperature (500 °C). The chemical composition, structure and morphology of the decomposed products NiO and CuO were confirmed by PXRD, FTIR and SEM spectroscopy. The decomposed products were loaded onto a glassy carbon electrode by a drop-casting method. For the oxygen evolution reaction, the complexes as well as their decomposed products, NiO and CuO achieve an ultralow over-potential exhibit onset lower potential 1.5 V in 0.1 M KOH solution.

1. Introduction

To fulfill global energy needs and scarcity of fossil fuels, materials scientists have devoted their attention towards the development of renewable energy sources [1]. In the present scenario, renewable energy sources are of much interest to realize green energy technology [2,3]. Among all renewable energy sources, electrochemical water splitting is one of the most efficient and clean energy sources for future eco-energy technology advancement. To attain the highest efficiency of electrochemical water splitting the oxygen evolution reaction (OER) is most promising [4]. Despite different types of established OER catalysts such as valuable metal oxides (e.g., RuO_2 and IrO_2) with good catalytic performance, now there is a need to introduce new low-cost catalysts for large-scale implementation [5–Table 18]. It has been observed that Pt/Ir-based catalysts can perform well for OER, but their prospect is limited due to the high cost and instability of these catalysts [9,10]. Hence, the designing of nonprecious, highly efficient and long-lasting OER electrocatalysts is a very demanding task [11]. To complete this purpose a broad range of OER catalysts have been announced in the recent past [12-15]. Among them, there are different types of transition- metal oxides including NiO, Co_2O_3, Fe_2O_3, etc. are extensively devoted as higher-level catalysts for OER arisen from their strong chemical property and effortless preparation procedure [16–19]. In electrocatalytic water splitting, OER is a basic process because of the slow kinetics (the complex four-electron transfer process), which determines the conversion efficiency and practical application of hydrogen energy [20–22]. For improvement of the sluggish reaction kinetics, effective electrocatalysts are used that can significantly improve the kinetics of the reaction and facilitate both hydrogen evolution reaction (HER) and OER at low overpotential draws the attention in the catalysis research [23].

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https://doi.org/10.1016/j.molstruc.2021.130928
0022-2860/

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Carbon 175 (2021) 534–575

Contents lists available at ScienceDirect

Carbon

journal homepage: www.elsevier.com/locate/carbon

Review article

A comprehensive review on the prospects of multi-functional carbon nano onions as an effective, high- performance energy storage material

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ARTICLE INFO

Article history:
Received 8 October 2020
Received in revised form
21 December 2020
Accepted 27 December 2020
Available online 30 December 2020

Keywords:
Carbon nano onions
Properties
Synthesis
Patent
Energy storage
Purification
Growth mechanism
Market analysis

ABSTRACT

The present review offers readers with an update over current and novel developments of carbon nano onions (CNOs) in recent years. Here we concisely detailed out the synthesis routes, growth mechanism in different synthetic routes, purification methods, chemical, electronic, optical, electro-magnetic and tribological properties, applications in energy storage sectors especially in the field of ion batteries and supercapacitors, polymeric composites of carbon nano onion, publication, patent-research trends data (1980–2020) and a brief market analysis respectively.

Contents

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https://doi.org/10.1016/j.carbon.2020.12.083
0008-6223/

Registrar
V.B.S. Purvanchal University
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Mithilesh Yadav
07.05.2022

JOURNAL OF COORDINATION CHEMISTRY
https://doi.org/10.1080/00958972.2021.2022128

Taylor & Francis
Taylor & Francis Group

Synthesis, spectroscopic characterization, computational studies, theoretical investigation of NLO properties and antibacterial activities of mixed ligand complexes of Co(II) and Cu(II)

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ABSTRACT

The reaction of Schiff base 2-(4-(dimethylamino)benzylideneamino)phenol (DBAP) and diethylenetriamine/ethylenediamine with cobalt(II) and copper(II) metal ion in equimolar ratio afforded mixed ligand complexes $[M(DBAP)(L)Cl(H_2O)_n]$ (1–4), where M = Co(II) 1, 2; Cu(II) 3, 4; L = diethylenetriamine (1, 3); n = 0 and ethylenediamine (2, 4); n = 1. All the newly synthesized complexes were characterized by elemental analysis, spectroscopic techniques *viz.*, UV-vis, FT-IR, ESR, PXRD and mass spectrometry. The influence of chelation of cobalt(II) and copper(II) ion on nonlinear optical properties of Schiff base (DBAP) were examined with DFT study. The polarizability (α_o) and first-order hyperpolarizability (β) of ligand and their metal complexes were calculated and compared with reference molecule *p*-nitroaniline. The hyperpolarizability of Schiff base and their metal complexes show a good nonlinear optical behavior. Theoretical investigation of the complexes was performed by DFT using B3LYP level of theory on the basis set 6-31 G (d, p)/LanL2DZ. On the basis of spectroscopic data and DFT computation, a six-coordinate geometry is tentatively proposed around the metal ion. *In vitro* antibacterial activities of these complexes were also screened against *V. cholerae* and *E. coli*, and found to have good antibacterial activity.

ARTICLE HISTORY
Received 1 February 2021
Accepted 10 December 2021

KEYWORDS
Transition metal complexes; Schiff base; DFT; NLO properties; antibacterial activities

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Supplemental data for this article is available online at https://doi.org/10.1080/00958972.2021.2022128

https://doi.org/10.1080/00958972.2021.2022128

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Jaunpur

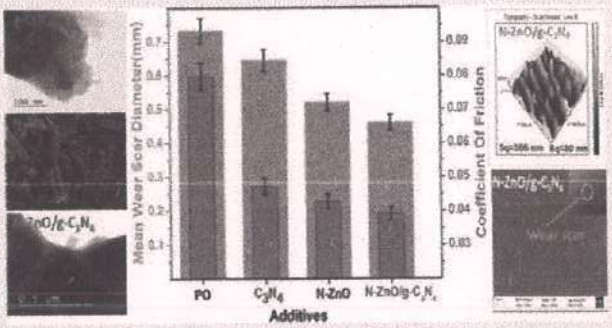
I&EC research
Industrial & Engineering Chemistry Research
pubs.acs.org/IECR
Article

Enhancement of Triboactivity of Nanolamellar Graphitic-C_3N_4 by N-Doped ZnO Nanorods

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

Cite This: https://dx.doi.org/10.1021/acs.iecr.0c03955
Read Online
ACCESS | Metrics & More | Article Recommendations | Supporting Information

ABSTRACT: The tribological activity of the synthesized nanosheets of a polymeric graphitic carbon nitride, g-C_3N_4, was upgraded by introducing hydrothermally synthesized N-doped zinc oxide nanorods. The high-resolution scanning electron microscopy, TEM, and HR-TEM studies of the hybrid (N–ZnO/g-C_3N_4) reveal that N-doped ZnO nanorods were spread over g-C_3N_4 nanosheets. The tribological activity of well-characterized nanomaterials was graded in paraffin oil (PO) at an optimized concentration, 0.20% w/v, on a four-ball tester conducting ASTM D4172 and ASTM D5183 tests. According to the observed tribological data, mean wear scar diameter, friction coefficient (COF), and seizure load, nanorods performed much better than the nanosheets. The hybrid exhibited highly advanced activity because of the synergy between noncovalently interacting nanorods and nanosheets. The SEM and AFM analyses of the wear pathway corroborated the tribological results. The energy-dispersive X-ray and X-ray photoelectron spectroscopy studies of the tribofilm confirmed the elemental composition and chemical states of all the elements, respectively. A possible mechanism of lubrication has been presented.



1. INTRODUCTION

Frictional losses in a mechanical system are of great concern. For the conservation of energy and enhancement of the active life of mechanical components, such losses have to be curtailed categorically. Employing lubricants with additional friction modifiers produces encouraging results. An extensive overview of literature proclaims that several types of nanomaterials such as nanoparticles, nanosheets, or nanocomposites have been used for the purpose owing to their fast tribo-action.[1−7] Nowadays, carbon-based materials such as graphene, fullerene, and carbon nanotubes are the center of attention in this innovative research area.[3−11] From our laboratory, too, carbon microspheres,[12,13] reduced graphene oxide, and their composites with nanoparticles, doped nanoparticles, or nanosheets have been recently documented as tribologically active materials.[14−18] A carbon nitride polymer of high thermal stability possessing graphitic structure g-C_3N_4 with weak van der Waals forces amid the 2D-nanosheets appears to be very influential in the field. Still, it has been seldom studied.[19,20] Zhu et al. have described the antiwear performance of bulk g-C_3N_4 with polyvinylidene difluoride (PVDF).[21] The nanosheets of octadecylamine grafted g-C_3N_4 have been used as antiwear and antifriction lubricant additives by Ajay Kumar and associates.[22] Synergistic friction reduction and wear-resistant properties were found by Xu and co-workers for the composite MoS_2/g-C_3N_4.[23] A nanocomposite of copper nanoparticles with g-C_3N_4 has been studied as a lubricant additive.[24] In the recent past, Wu and his associates have used CuO/g-C_3N_4 for enhancing wear resistance of polyimide composites.[25] They have also evaluated the tribological performance of phenolic coatings with varying percentages of g-C_3N_4.[26] Tribological performance of the hybrid g-C_3N_4/TiO_2 has been studied by Zhang and his group.[27] Thus, the enhanced tribological activity of functionalized g-C_3N_4 with nanoparticles or nanosheets motivated us to explore the use of zinc oxide for its functionalization because zinc oxide nanoparticles have been widely studied as a triboactive material.[17,28−30]

Zinc oxide has an open hexagonal crystal structure.[31−33] Doping with different atoms as zinc or oxygen substitutes promotes the formation of defects, which affect the structure and eventually result in improved properties.[34−39] These defects may lead to the formation of slip systems that can change the electronic structure and lower the shear strength; ultimately, tribological properties are enhanced.[38,39] The metal ions such as magnesium, copper, and aluminum are known to

Received: August 14, 2020
Revised: December 29, 2020
Accepted: December 30, 2020

Dr. DINESH K. VERMA

Journal of Molecular Liquids 289 (2019) 111171

Contents lists available at ScienceDirect

Journal of Molecular Liquids

journal homepage: www.elsevier.com/locate/molliq

Mechanism of triboactivity of Schiff bases: Experimental and molecular dynamics simulations studies

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ARTICLE INFO

Article history:
Received 26 November 2018
Received in revised form 4 June 2019
Accepted 10 June 2019
Available online 12 June 2019

Keywords:
Schiff bases
Antiwear additives
Molecular dynamics

ABSTRACT

Schiff bases derived from *o*-tolidine through its condensation with salicylaldehyde (OH-BT), naphthaldehyde (H-NT) and 2-hydroxynaphthaldehyde (OH-NT) have been synthesized and characterized by FT-IR and ^{1}H NMR spectroscopic techniques. The synthesized Schiff bases are environmentally safe from tribological aspect as these do not contain undesirable elements like sulfur, phosphorus, and halogens which are known to affect the efficiency of catalytic converters. The triboactivity of these compounds has been studied in paraffin oil (PO) using four-ball tester (FBT) at an optimized concentration of 0.25% w/v under ASTM D4172 and D5183 test conditions. The results have been compared with that of a reference additive, zinc dialkyl dithiophosphate (ZDDP), under similar conditions. Based on tribological data, mean wear scar diameter (MWD), mean wear volume (MWV), coefficient of friction (COF), load carrying ability and wear rate, the following order has emerged for tribological behavior of the investigated additives:

OH-BT>OH-NT>H-NT>ZDDP.

Morphology and composition of wear scar have been studied by Atomic Force Microscopy (AFM) and Scanning Electron Microscopy (SEM) with Energy Dispersive X-ray analysis (EDX) and relate very well with the observed tribological data. The EDX analysis of the wear scar lubricated with synthesized additives provides evidence for the presence of nitrogen and oxygen. To ascertain the active involvement of the imine group towards tribological behavior, the reaction of the most active compound OH-BT was carried out with thioglycolic acid. Reduced antiwear performance of the reaction product (OH-BTS) may be directly associated with the absence of the imine group (-CH=N-). Molecular dynamics (MD) simulations have been used to study the mechanism of adsorption of the studied Schiff bases in paraffin oil on the iron slab. The order of adsorption energies of the Schiff base additive molecules has been found to agree well with the experimentally observed data. The nature of orientation or configuration of molecules after adsorption has been presented. The findings of the MD simulations have been used to propose the mechanism for tribological behavior of the investigated Schiff base molecules and product OH-BTS obtained by cyclisation of OH-BT with thioglycolic acid. The mechanism proposed from MD simulation studies points to the combined effect of heteroatoms and planarity of the additive molecule after adsorption. Accordingly, molecules with tribological properties of a high order may be formulated.

1. Introduction

For improving the durability and efficiency of a machine, frictional wear of its mechanical components must be minimized effectively. Addition of lubricants reduces frictional energy losses. The viscosity of lubricants plays a vital role in reducing the energy losses; in fact, lower the viscosity more is energy saving [1,2]. Lubricants with low viscosity, imposing boundary or thin film lubrication regime are, therefore, usually preferred [3]. Under thin film lubrication, suitable additives may be added which further reduce friction and wear. The literature survey reveals that several organic compounds containing heteroatoms like boron, oxygen, nitrogen, halogens, sulfur, and phosphorus, etc. have been extensively used as multifunctional additives like antiwear, extreme pressure, antioxidant and corrosion inhibitor in lubricating oil [4–18]. Antiwear and friction reducing additives get physically and chemically adsorbed on the interacting surfaces through different adsorption centers like heteroatoms, phenyl rings, and double bonds, etc. Thus, in situ generated chemical film, formed through the process of adsorption prevents proximity of the contact surfaces, reducing friction and wear [19–22]. Numerous literature reports [23–25] are available where surface characterization techniques have provided adequate

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https://doi.org/10.1016/j.molliq.2019.111171
0167-7322/

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International Journal of Scientific Research in Science and Technology
Print ISSN: 2395-6011 | Online ISSN: 2395-602X (www.ijsrst.com)
© 2021 | IJSRST | Volume 8 - Issue 1

Mechanical and Thermophysical Properties of Mg3TH7 (T= Mn, Tc, Re) Complex Hydrides

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ABSTRACT

The Mg_3TH_7 (T= Mn, Tc, Re) compounds are hexagonal ternary complex hydrides. The characteristic features of high-temperature ternary complex hydrides are investigated by the theoretical evaluation of thermophysical and ultrasonic properties at room temperature using interaction potential model approach. From elastic constants calculations, it is noted that Mg_3MnH_7, Mg_3TcH7 and Mg_3ReH_7 brittle. With the help of second order elastic constants other elastic moduli, elastic stiffness constants and Poisson's ration are estimated at room temperature for elastic and mechanical characterization. The ultrasonic velocities and thermal relaxation time of these ternary complex hydrides are evaluated utilizing evaluated values of elastic constants 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 analyzed to explore the characteristic of complex hydrides compounds.

Keywords: Ternary Complex Hydrides, Elastic Properties, Ultrasonic Velocity, Thermal Relaxation Time

I. INTRODUCTION

Ternary complex transition hydrides have been considered to be very attractive candidates and have received significant attention as hydrogen storage materials. These compounds show a higher capacity for hydrogen storage in volume densities than compressed gaseous and liquid hydrogen [1]. In recent decades, research and development of new hydrogen storage materials opened up new possibilities for industrialists. On the other hand, the major challenges in solid state hydrogen storage are improved energy storage density, faster kinetics, and improved cycle life, using readily available elements at reasonable costs, with particular reference to fuel cells and rechargeable batteries [2, 3]. Matar et al. [4] have investigated the electronic structure and bonding of three different complex hydrides Mg3MnH7, Mg3ReH7 and Mg3TcH7 by the pseudo- potentials and computation of all electrons within the DFT. They have shown that both Mg3MnH7 and Mg3ReH7 have desorption energies within the range of MgH2 and are higher than those of covalent-like hydrogenated intermetallic compounds. The complex hydrides Mg3MnH7 and Mg3ReH7 compounds crystallize in hexagonal P63/mmc [5, 6].

In the present work, we have worked dfligently to make the relationship between thermo physical and

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International Journal of Scientific Research in Science and Technology
Print ISSN: 2395-6011 | Online ISSN: 2395-602X (www.ijsrst.com)
© 2021 | IJSRST | Volume 8 - Issue 1

Ultrasonic Wave Propagation in Hexagonal $SrMnO_3$ Compound

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ABSTRACT

In the present study, the ultrasonic attenuation due to phonon-phonon interaction has been investigated in hexagonal $SrMnO_3$ compound. Higher order elastic constants have been computed at temperature dependent following the Lenard-Jones Potentials. Second order elastic constants are used for the determination of other ultrasonic parameters. The temperature variation of the ultrasonic velocities is evaluated along different angles with unique axis of the crystal using the second order elastic constants. Temperature variation of the thermal relaxation time and Debye average velocities is also calculated along the same orientation. The temperature dependency of the ultrasonic properties is discussed in correlation with elastic, thermal and electrical properties. It has been found that the thermal conductivity and thermal relaxation times is the main contributor to the behaviour of ultrasonic attenuation as a function of temperature and the responsible cause of attenuation is phonon-phonon interaction. The mechanical properties of $SrMnO_3$ material at low temperature (50K) are better than room temperatures because at this temperature it has low ultrasonic attenuation

Keywords: Elastic constants, Ultrasonic velocity, Ultrasonic attenuation, Thermal properties

I. INTRODUCTION

Perovskite manganese oxides, commonly represented as $AMnO_3$ (A: rare-earth alkaline earth metals), have been instrumental in condensed matter physics as well as in technical applications. Perovskite $SrMnO_3$ (SMO) is a polymorphism that has complex magnetic ordering and dielectric polarization and thus attracted a lot of attention as a multiferroic material [1, 2]. An inorganic chameleon has been inorganic chameleon because of the great flexibility of the hexagonal perovskite structure. Many different compounds take it or the corresponding structure, as the mother structure is easily deformed or diffused to the relative sizes of the ions of the compounds [3]. The hexagonal $SrMnO_3$ is antiferromagnetic below at Néel temperature. Néel temperatures is reported to be 260 K by Takeda and Ohara [4]. Hexagonal polymorphisms are semiconductors. The hexagonal $SrMnO_3$ when heated in air is stoichiometric at room temperature but loses oxygen at high temperature [5].

In the present work, we have worked diligently to make the relationship between thermo physical and microstructural properties for hexagonal $SrMnO_3$ compound. $SrMnO_3$ compound will help in understanding the mechanical behaviour of this compound and it will play an important role in the illustration of industrial applications with useful physical properties under moderate operating

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journal homepage: www.keaipublishing.com/en/journals/sensors-international

Synthesis of TiO_2 nanorods using wet chemical method and their photovoltaic and humidity sensing applications

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ARTICLE INFO

Keywords:
TiO_2 nano-rod
BET
Photovoltaic cell
Humidity sensor

ABSTRACT

In this work, synthesis of TiO_2 nanorods using wet chemical method alongwith their photovoltaic and humidity sensing applications are reported. After successful synthesis of TiO_2 nanorods, the material was investigated through X-ray diffraction (XRD), Scanning electron microscopy (SEM), Energy-dispersive X-ray spectroscopy (EDS), Fourier transform infrared spectroscopy (FTIR) and UV–Vis spectroscopy. Surface morphology and topology of the synthesized nano material was analyzed by SEM showed porous and tubular structure. EDS confirmed the elemental composition. XRD revealed the rutile phase with minimum crystallite size as 78.60 nm. The optical characterization of nano material has been completed by using FTIR and UV–Vis spectroscopy to confirm the required bond formation and estimate the bandgap (5.86 eV) respectively. Brunauer–Emmett–Teller (BET) characterization exhibited the highly porous nature of the material revealing the surface area of 37.445 m^2/g together with mean pore diameter ranging from 9 to 18 nm. Further, the material was employed as photovoltaic cell and humidity sensor. The photovoltaic efficiency was obtained as ~0.3909% whereas sensitivity towards humidity as 2.93 pF/%RH and 0.42 MΩ/%RH for capacitance and impedance respectively at room temperature.

1. Introduction

Increasing the efficiency of natural energy sources and energy recycling have become important objectives for researchers and scientists worldwide. Among the several renewable energy sources such as solar, wind, hydro, geothermal etc., solar provides us with an abundant source of energy. Only 0.2% of the total solar radiation can satisfy the wordwide energy demand as of now. Thus, while the search for affordable renewable sources of energy continues at a seemingly neverending mode, the use of easily fabricable solar devices are becoming of paramount importance for the human civilization to meet their ever-growing energy demands. Photochemical reactions, an effective way to convert photons into chemical energy, have been widely studied and explored for investigating effective ways to degrade toxic organic pollutants [1], energy conversion [2], water decomposition [3], dye sensitized solar cells [4] and organic synthesis [5] etc. The solar energy is considered as a type of free energy in nature since it is freely available on the surface of the earth. Worldwide, countries should, therefore, strive to produce workable solar cells, even though these cells have low efficiency. Many attempts were made with solar cells using easily implemented inexpensive materials and producing easily scalable methods in recent years [6,7].

Titania is one of the most commonly used material having white color due to its brightness and very high refractive index, which lags behind only a few other materials. When it is deposited as a thin film, makes an excellent reflective optical coating for mystic fire topaz such as dielectric mirrors and some gems. Ultrafine TiO_2 is used in sunscreen because of its ability to block ultraviolet radiation while remaining transparent on the skin, and its photocatalytic sterilizing properties have also made it useful as an additive in building materials, in antifogging coatings and self-

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ELSEVIER Production and hosting by Elsevier

https://doi.org/10.1016/j.sintl.2021.100095
Received 21 February 2021; Received in revised form 6 April 2021; Accepted 10 April 2021
Available online 20 April 2021

PHYSICS AND CHEMISTRY OF SOLID STATE
V. 22, No. 4 (2021) pp. 687-696
Section: Physics

DOI: 10.15330/pcss.22.4.687-696

Vasyl Stefanyk Precarpathian National University

ФІЗИКА І ХІМІЯ ТВЕРДОГО ТІЛА
Т. 22, № 4 (2021) С. 687-696
Фізико-математичні науки

PACS numbers: 43.35.Cg; 62.20.Dc; 63.20.Kr

ISSN 1729-4428

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Elastic, Mechanical and Thermophysical properties of Single-Phase Quaternary ScTiZrHf High-Entropy Alloy

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Consequent to the interaction potential model, the high-order elastic constants at high entropy alloys in single-phase quaternary ScTiZrHf have been calculated at room temperature. Elastic constants of second order (SOECs) helps to determine other ultrasonic parameters. With the help of SOECs other elastic moduli, bulk modulus, shear modulus, Young's modulus, Pugh's ratio, elastic stiffness constants and Poisson's ratio are estimated at room temperature for elastic and mechanical characterization. The other ultrasonic parameters are calculated at room temperature for elastic and mechanical characterization. The temperature variation of ultrasonic velocities along the crystal's z-axis is evaluated using SOECs. The temperature variation of the average debye velocity and the thermal relaxation time (τ) are also estimated along this orientation axis. The ultrasonic properties correlated with elastic, thermal and mechanical properties which is temperature dependent is also discussed. The ultrasonic attenuation due to phonon – phonon (p-p) interactions is also calculated at different temperatures. In the study of ultrasonic attenuation such as a function of temperature, thermal conductivity appears to be main contributor and p- p interactions are the responsible reason of attenuation and found that the mechanical properties of the high entropy alloy ScTiZrHf are superior at room temperature.

Key words: high entropy alloy, ultrasonic properties, thermal conductivity, elastic properties.

Received 28 July 2021; Accepted 10 October 2021.

Introduction

High-entropy alloys (HEAs) have involved considerable attention as they have first proposed in the physical metallurgy community [1]. HEAs is distinct as an alloy involving of at least five principal elements with equivalent equilateral ratios, which could favour the construction of homogeneous solid solution stages rather than intermetallic compounds [2]. Indubitable, the presence of HEAs accelerates the development of metallurgical materials and opens a new path for the discovery of new alloys without understanding the properties [3, 4]. Several interesting properties were suggested for HEAs, acting asexcellent high strength [5, 6], high fracture toughness at low temperatures, high hardness and thermal stability [7]. The opportunity of creation of HEAs with rare-earth metal, first proposed via Zhang et al. [8], since rare earth materials have very similar atomic sizes, the same crystal structures and large or fully related solubility. This confirmed CoFeReRu alloys could form solutions as a single hexagonal solid and the equivalent hexagonal HEAs can be formed between Y, Sc, Tb, Gd, Di, Tm, Ho, Tm, Er, and Lu. Establishment of rare earth element HEAs was revealed in DyGdHoTbY by Feuerbacher et al. [9], DyGdLuTbTm and DyGdLuTbY by Takeuchi et al. [10]. High-entropy alloys have demonstrated the ability to have superior properties in many cases. A basic understanding of the mechanism of phase stability of HEAs is still a subject of active research [11]. HEAs were found own many attractive properties, like soft magnetism [12], larger hardness [13], high strength [14], excellent corrosion resistance, better thermal stability and high wear resistance etc. [15]. The certain outstanding properties of HEAs were contributed to a growing interest in research and improvement in a new exciting field [16]. Y. L. Chen and his co-workers [17] designed equimolar BeCoMgTiZn and BeCoMgTi alloys, whose component elements are all stable in

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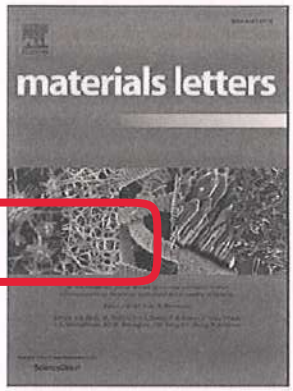

Large area semitransparent inverted organic solar cells with enhanced operational stability using TiO_2 electron transport layer for building integrated photovoltaic devices

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PII: S0167-577X(20)31432-4
DOI: https://doi.org/10.1016/j.matlet.2020.128725
Reference: MLBLUE 128725

To appear in: *Materials Letters*

Received Date: 18 August 2020
Accepted Date: 20 September 2020

Please cite this article as: D.K. Chaudhary, P.K. Dhawan, S.P. Patel, H.P. Bhasker, Large area semitransparent inverted organic solar cells with enhanced operational stability using TiO_2 electron transport layer for building integrated photovoltaic devices, *Materials Letters* (2020), doi: https://doi.org/10.1016/j.matlet.2020.128725

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Enhancement of thermal conductivity and ultrasonic properties by incorporating CdS nanoparticles to PVA nanofluids

https://doi.org/10.1515/zna-2020-0334
Received December 5, 2020; accepted April 14, 2021; published online May 6, 2021

Abstract: In the present work, semiconducting cadmium sulfide (CdS) nanoparticles have been synthesized by co-precipitation method. X-ray diffraction (XRD), UV–visible (UV/Vis) absorption spectroscopy, and high-resolution transmission electron microscopy (HRTEM) have been used for the characterization of the synthesized nanoparticles. Two-step technique has been used to formulate stable polyvinyl alcohol (PVA)-based CdS nanofluids at room temperature. Thermal conductivities of nanofluids at different temperatures have been measured using Hot Disc Thermal Constants Analyzer. Significant enhancement in thermal conductivity is noted at very low nanoparticle loading. Ultrasonic velocity and ultrasonic attenuation in the prepared nanofluids have been investigated using ultrasonic interferometer and Acoustic Particle Sizer (APS-100), respectively. APS-100 has been also used for the analysis of particle size distribution (PSD) of CdS nanoparticles in the prepared nanofluids. The PSD result of APS-100 is in good agreement with that of HRTEM. The characteristic behavior of CdS nanofluid is illustrated on the basis of its ultrasonic and thermal properties. The thermal conductivity enhancement increases with the temperature and reaches up to 61.6% for 1.0 wt% particle loadings at 80 °C. Our analysis shows that CdS nanofluids have potential application for effective heat transfer management in various cooling industries.

Keywords: CdS nanoparticles; nanofluids; thermal conductivity; ultrasonic attenuation spectroscopy; ultrasonic velocity.

1 Introduction

Nanofluid is a simple and emerging product of nanotechnology. Nanofluids (NFs) are made by suspension of nanoparticles (NPs) in conventional base fluids such as water, oils, ethylene glycol, polyvinyl alcohol (PVA), etc. Since the pioneering work done by Choi in 1995, nanofluids have seen enormous growth in nanotechnology [1]. Nanofluids exhibit heat transfer properties superior to that of the conventional fluid due to the large surface to volume ratio of the suspended nanoparticles [2]. Nowadays, nanofluids have attracted great interest in the industrial field because of their broad applications such as heat exchangers, cooling of microchips, drug delivery, heat transfer augmentation in solar collectors, solar power generation, and enhanced oil recovery [3, 4].

There are many works reported in the literature about enhancement of thermal conductivity of NFs. In the last few years, many works have been done on the enhancement of thermal conductivity of the various NFs at different concentrations and temperatures by a number of researchers [5–8]. Masuda et al. [5] reported the effect of particle volume fraction in the enhancement of thermal conductivity in Al_2O_3, SiO_2, and TiO_2 nanoparticles–water-based NFs. At room temperature, they reported 32.4% thermal conductivity enhancement (TCE) for Al_2O_3/water nanofluid at 4.3 vol% concentration of NPs. This was the first experimental study regarding the thermal conductivity of NFs. Lee et al. [6] reported on the TCE of nanofluids by dispersing Al_2O_3 and CuO NPs in the matrix of water and ethylene glycol at room temperature. They observed 20% TCE for [illegible] glycol nanofluid at 4.0 vol%. Wang et al. [7] reported a similar kind of study in water-based nanofluid by dispersion of Al_2O_3 and CuO NPs and reported a 30%

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https://doi.org/10.1515/zna-2020-0334

International Journal of Thermophysics (2021) 42:60
https://doi.org/10.1007/s10765-021-02809-w

Study of Ultrasonic and Thermal Properties for Heat Transfer Enhancement in Fe_2O_3 Nanoparticles-Ethylene Glycol Nanofluids

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Received: 5 December 2020 / Accepted: 1 February 2021

Abstract
In present work, semiconducting iron (III) oxide (Fe_2O_3) nanoparticles have been synthesized by sol–gel method. X-ray diffraction (XRD), UV–Visible (UV–Vis) absorption spectroscopy and transmission electron microscopy (TEM) have been used for the characterization of the synthesized nanoparticles. Two-step technique was used to formulate stable ethylene glycol (EG) based Fe_2O_3 nanofluids at room temperature. Thermal conductivity of nanofluids has been measured using hot disc thermal constants analyzer. Significant enhancement in the thermal conductivity is noted at very low nanoparticle loading (up to 1 wt%). Ultrasonic velocity and ultrasonic attenuation in the prepared nanofluids were investigated using an ultrasonic interferometer and acoustic particle sizer (APS-100), respectively. APS-100 was also used for the analysis of particle size distribution (PSD) of Fe_2O_3 nanoparticles in the prepared nanofluids. The PSD result of APS-100 has been found in good agreement with that of TEM. The characteristics behaviour of Fe_2O_3 nanofluid has been illustrated based on its ultrasonic and thermal properties. Our investigations advocate that Fe_2O_3 nanofluids have potential application for effective heat transfer management in various cooling industries.

Keywords Fe_2O_3 nanoparticles · Nanofluids · Thermal conductivity · Ultrasonic attenuation spectroscopy · Ultrasonic velocity

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Published online: 02 March 2021

MAPAN-Journal of Metrology Society of India
https://doi.org/10.1007/s12647-020-00412-2

ORIGINAL PAPER

Elastic, Mechanical and Ultrasonic Properties of Nanostructured IIIrd Group Phosphides

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Received: 29 March 2020 / Accepted: 09 November 2020

Abstract: Despite the large number of III–V semiconductor studies reported every year at bulk level, the III–V material characterization at nanoscale is still required to evaluate their potential industrial applications in nanoscale electronic devices, optoelectronic devices, chemical, biosensors, etc. In this work, the non-destructive evaluation-based ultrasonic theoretical approach for the material characterization of nanostructured IIIrd group phosphides, namely indium phosphide (InP), aluminum phosphide (AlP), gallium phosphide (GaP), and boron phosphide (BP) with wurtzite crystal phase, has been reported. The second- and third-order elastic constants (SOECs and TOECs) for IIIrd group phosphides have estimated using the Lennard–Jones potential. The mechanical properties and the ultrasonic investigation of the IIIrd group phosphides materials, e.g., ultrasonic velocities, Grüneisen parameters, acoustic coupling constants, and ultrasonic attenuation, have been performed using the estimated values of SOECs and TOECs. The present investigation indicates that the ultrasonic attenuation of IIIrd group phosphides is influenced by the wave velocities and the chosen material's thermal conductivity. The other thermophysical parameters like the crystal energy density, the specific heat per unit volume, thermal conductivity, and the Debye temperature of these materials have also been reported at room temperature (300 K). The results indicate that BP is the most robust material and has superior elastic, mechanical, and thermal characteristics.

Keywords: Phosphides; Elastic constants; Mechanical properties; Thermal properties; Ultrasonic properties

1. Introduction

The recent development in the fundamental research of III and V group compound semiconductors has shown the scientific community's attraction due to their fundamental characteristics and technological developments, useful for various applications at bulk level and at the nanoscale [1–4]. The important physical properties of the III–V group semiconductors, e.g., high bulk modulus, wide band gap, low densities, high corrosion resistance, and high thermal conductivity, make them appropriate for high-temperature applications and electronic devices [5–9]. The group IIIrd phosphides are common anion semiconductors, which generally grown in zinc blende (ZB) phase at bulk scale. However, in these materials' zinc blende phase does not hold when the dimensions are reduced at the nanoscale with a high degree of control over the crystal phases. The III–V group material can be grown at the nanoscale in the wurtzite crystal (WZ) form rather than ZB form [10, 11]. At ambient conditions, the direct band gap existed in InP, while the indirect band gap was obtained for the other chosen material of IIIrd group phosphide compounds, namely GaP, AlP, and BP.

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Published online: 17 December 2020

Requires Authentication · Published by Oldenbourg Wissenschaftsverlag March 18, 2021

Capacitive micromachined ultrasonic transducers: Transmission evaluation with different membrane materials and dimensions

Semiconductor material utilization for CMUT for transduction and reception

Kapazitive mikrobearbeitete Ultraschall-Wandler: Transmissionsbewertung mit verschiedenen Membranmaterialien und Abmessungen

Halbleitermaterialnutzung für CMUT für Transduktion und Empfang

Sudhanshu Tripathi, *Rekha Agarwal*, *Rashmi Vashisth* and *Devraj Singh*

https://doi.org/10.1515/teme-2020-0073

Abstract

Capacitive micromachined ultrasonic transducers (CMUTs) are dominant in generating and receiving acoustic signals. CMUT transmission efficiency solely depends upon the membrane material utilized. This work presents the structural examination of receiving and transmitting characteristics of CMUT with divergent membrane materials, namely Silicon (Si), Silicon Nitride (Si_3N_4), Indium Phosphide (InP), Zinc Oxide (ZnO), and Polysilicon (Poly-Si). The analysis includes the membrane deflection, pull-in voltage, output pressure, resonant frequency and capacitance modification with variable DC voltage. It has been found that InP gives the pull-in voltage comparable to Si in the receiving mode and have more transduction efficiency in transmitting mode. Effect of dimensions of CMUT on pull-in voltage and resonant frequency are also discussed. The major contribution lies in the analytical and estimation study of CMUT for appropriate membrane material selection meant for transmission and reception in the field of pressure sensing application.

Zusammenfassung

Kapazitive mikrobearbeitete Ultraschallwandler (CMUTs) sind dominant bei der Erzeugung und dem Empfang von akustischen Signalen. Die Übertragungseffizienz von CMUTs hängt ausschließlich vom verwendeten Membranmaterial ab. Diese Arbeit stellt die strukturelle Untersuchung der Empfangs- und Sendeeigenschaften von CMUT mit unterschiedlichen Membranmaterialien vor, nämlich Silizium (Si), Siliziumnitrid (Si_3N_4), Indiumphosphid (InP), Zinkoxid (ZnO) und Polysilizium (Poly-Si). Die Analyse umfasst die Membranauslenkung, die Einzugsspannung, den Ausgangsdruck, die Resonanzfrequenz und die Kapazitätsänderung mit variabler Gleichspannung. Es wurde festgestellt, dass InP im Empfangsmodus eine mit Si vergleichbare Pull-in-Spannung liefert und im Sendemodus eine höhere Transduktionsleistung aufweist. Der Einfluss der Abmessungen des CMUT auf die Anzugsspannung und die Resonanzfrequenz wird ebenfalls diskutiert. Der Hauptbeitrag liegt in der analytischen und abschätzenden Studie von CMUT für die geeignete Auswahl des Membranmaterials, das für die Übertragung und den Empfang im Bereich der Drucksensoranwendung gedacht ist.

Keywords: CMUT; air transduction; pull-in voltage; membrane materials; InP; ZnO

Schlagwörter: CMUT; Luftransduktion; Anzugsspannung; Membranmaterialien; InP; ZnO

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https://doi.org/10.1515/teme-2020-0073

Materials Today Communications 27 (2021) 102189

Contents lists available at ScienceDirect

Materials Today Communications

journal homepage: www.elsevier.com/locate/mtcomm

Elastic, mechanical, thermo-physical, and ultrasonic investigation in platinum carbide

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ARTICLE INFO

Keywords:
PtC
Elastic constants
Mechanical properties
Thermo-physical
Ultrasonic properties

ABSTRACT

A comprehensive study of elastic, mechanical, thermophysical and ultrasonic properties of novel platinum carbide (PtC) have been reported. The elastic constants, mechanical properties e.g. bulk modulus, shear modulus, Young's modulus etc., direction dependent thermal and ultrasonic properties of PtC in rock-salt (RS-type) and wurtzite (WZ-type) structures are determined. Thermal properties e.g. thermal relaxation time, lattice thermal conductivity, specific heat per unit volume, crystal energy density, acoustic coupling constants, and ultrasonic attenuation were determined along different directions. In order to access the microstructural information and nature of material the direction dependent ultrasonic properties of PtC were correlated with other thermo-physical properties. The elastic, mechanical, thermophysical and ultrasonic properties of wurtzite crystal structure have been reported for first time. All results reveal that PtC would favour wurtzite crystal phase. The compound is stiffer in wurtzite phase. The obtained results may be further explored for research and industrial applications.

1. Introduction

In last three decades, intensive experimental and theoretical researches have been done on group IV and V transition metal carbides (TMCs) [1–3]. TMCs are the potential candidate for research due to their widespread technological applications in cutting tool and hard coating due to their durability, hardness and great strength [4]. TMCs have also shown interesting superconducting, optoelectronic, semiconducting, and thermal properties [4,5]. Platinum carbide is one of the noble metal carbide belongs to refractory compound very popular among researchers in the last decade [6,7]. Dahliah *et al.* [7] have investigated the structural stabilities of PtC compound in seven different crystallographic phases using full-potential linearized augmented plane wave method based on density function theory. They have reported temperature and pressure dependent variation of thermodynamic properties of PtC and observed that PtC shows metallic behaviour in all phases under study. The enormous mechanical, thermal properties, high thermal conductivity, superior mechanical properties and great hardness are the basic reasons for growing interest in PtCs [8–10]. Recently the structural and mechanical properties of noble metal carbides in different phases have been reported using generalised gradient approximation scheme (GGA) in literature [11]. The rock-salt (RS) structure synthesis reported using X-ray diffraction (XRD) pattern under high temperature and high pressure with large value of bulk modulus [12]. However, it has been reported in literature that the stable structure of PtC is obtained in zinc blende (ZB) structure within low temperature regime [13]. Ab intio study [14] reveals the investigation of electronic and structural properties of low index surfaces i.e. <100>, <110> and <111> surfaces of ZB PtC. Rabah et al. [15] reported the ground state properties of PtC in the, rock-salt (RS), zinc-blende (B3), wurtzite (WZ), nickel-arsenide (B8) and lead (II) oxide (B10) structures using the full-potential linearized muffin-tin orbital method (FP-LMTO) within the local density approximation (LDA) to density-functional theory (DFT) and compared with available experimental and theoretical data. They have also reported that possibility of phase transition from RS-structure to ZB-structure is possible once the pressure reduces to ambient condition. They have predicted that RS-structure is unstable at zero pressure while ZB-structure is stable at ground state. The studies on the ground states,

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https://doi.org/10.1016/j.mtcomm.2021.102189
Received 18 September 2020; Received in revised form 31 January 2021; Accepted 18 February 2021
Available online 21 February 2021
2352-4928/

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https://doi.org/10.1016/j.mtcomm.2021.10218

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Pressure dependent ultrasonic properties of hcp hafnium metal

https://doi.org/10.1515/zna-2021-0013
Received January 19, 2021; accepted March 22, 2021; published online April 26, 2021

Abstract: The elastic and ultrasonic properties have been evaluated at room temperature between the pressure 0.6 and 10.4 GPa for hexagonal closed packed (hcp) hafnium (Hf) metal. The Lennard-Jones potential model has been used to compute the second and third order elastic constants for Hf. The elastic constants have been utilized to calculate the mechanical constants such as Young's modulus, bulk modulus, shear modulus, Poisson's ratio, and Zener anisotropy factor for finding the stability and durability of hcp hafnium metal within the chosen pressure range. The second order elastic constants were also used to compute the ultrasonic velocities along unique axis at different angles for the given pressure range. Further thermophysical properties such as specific heat per unit volume and energy density have been estimated at different pressures. Additionally, ultrasonic Grüneisen parameters and acoustic coupling constants have been found out at room temperature. Finally, the ultrasonic attenuation due to phonon–phonon interaction and thermoelastic mechanisms has been investigated for the chosen hafnium metal. The obtained results have been discussed in correlation with available findings for similar types of hcp metals.

Keywords: elastic properties; hafnium; thermal properties; ultrasonic attenuation.

1 Introduction

Hafnium (Hf), with atomic number 72, is a group IV B element in the periodic table. At ambient conditions, hafnium, similar to its homologous Ti and Zr, shows a hexagonal closed packed (hcp) structure (α-phase) as shown in Figure 1 created using *Vesta* 3 [1]. Its narrowed band makes Hf a useful material for electronics and semiconductor devices and its high neutron absorption cross-section makes Hf and its isotopes suitable for control rods in nuclear reactors [2]. The excellent hardness and corrosion-resistance properties of Hf and its alloys [3] allow its use in harsh environments like pressurized water reactors [3–5] and liquid rocket thruster nozzles [6]. For example, nozzle of Apollo Lunar Modules' main engine 'C103' consists of 89% niobium, 10% hafnium and 1% titanium [6]. The hafnium oxide-based compounds like hafnium oxynitride are high dielectric constant materials which make them perfect for gate insulators in generation of integrated circuits [7].

At high temperature, around 2030 K, Hf undergoes a phase transformation from hcp (α-phase) to a body centred cubic (bcc) structure (β-phase), similar to Zr and Ti, though the transition temperatures in the case of Zr and Ti are around 1155 and 1135 K, i.e. lower by factor of ~2 in comparison to Hf [8]. At ambient temperature, under elevated pressure, the hcp structure transforms to hexagonal (ω-phase, three atoms per unit cell) structure. Hf along with Zr and Ti follows the $\alpha \rightarrow \omega \rightarrow \beta$ transition sequence with pressure [9]. Xia et al. [10] reported the transition pressures of $\alpha \rightarrow \omega$ and $\omega \rightarrow \beta$ to be 38 ± 8 and 72 ± 1 GPa, respectively.

The reports of varying transition pressures for Hf corresponding to $\alpha \rightarrow \omega$ within the range of 10.6–50 GPa and $\omega \rightarrow \beta$ within the range of 30.7–78 GPa were found in literature, which could be attributed to employing different methods and techniques [10–16].

Qi et al. [17] measured the ultrasonic velocities of the α-phase of hafnium up to 10.4 GPa at room temperature. Further, they used DFT to find out the second order elastic constants (SOECs) and acoustic Debye temperature. Zhang et al. [18] investigated the structure and pressure dependent ultrasonic velocities and second order elastic constants (SOECs).

Due to the high-pressure industrial applications of Hf in harsh conditions, it needs to be extensively investigated for enhancing and modifying its already known mechanical and elastic properties. The ultrasonic non-destructive evaluation (UNDT) is an effective procedure

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https://doi.org/10.1515/zna-2021-0013

https://doi.org/10.1595/205651320x15940360546454 Johnson Matthey Technol. Rev., 2021, 65, (3), 418–430

JOHNSON MATTHEY TECHNOLOGY REVIEW www.technology.matthey.com

Ultrasonic and Thermophysical Studies of Ethylene Glycol Nanofluids Containing Titania Nanoparticles and Their Heat Transfer Enhancements

Next-generation heat transfer nanofluids for industrial applications

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In the present investigation, TiO_2 nanostructures were synthesised *via* a simple sol-gel technique and characterised with X-ray diffraction (XRD), scanning electron microscopy with energy-dispersive X-ray analysis (SEM-EDX), high-resolution transmission electron microscopy (HR-TEM) and ultraviolet-visible (UV-vis) spectroscopy. The temperature and concentration dependence of thermal conductivity enhancement (TCE) and ultrasonic velocity have been explored in ethylene glycol-based TiO_2 nanofluids. The obtained results showed 24% enhancement in thermal conductivity at higher temperature (80°C) of the base fluid ethylene glycol by adding 1.0 wt% of TiO_2 nanoparticles. The behaviour of TCE and ultrasonic velocity with temperature in prepared nanofluids has been explained with the help of existing phenomena. The increase in ultrasonic velocity in ethylene glycol with TiO_2 nanoparticles shows that a strong cohesive interaction force arises among the nanoparticles and base fluid. These results

https://doi.org/10.1595/205651321X16038755164270 Johnson Matthey Technol. Rev., 2021, 65, (4), 556–567

JOHNSON MATTHEY
TECHNOLOGY REVIEW

www.technology.matthey.com

Study of Ultrasonic Attenuation and Thermal Conduction in Bimetallic Gold/Platinum Nanofluids

Effect of thermal conductivity on ultrasonic attenuation of gold and gold/platinum nanofluids

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Here, we report the frequency dependent ultrasonic attenuation of monometallic gold and bimetallic gold/platinum based aqueous nanofluids (NFs). The as-synthesised bimetallic NFs (BMNFs) revealed less resistance to ultrasonic waves compared to the monometallic NFs. Thermal conductivity of both NFs taken at different concentrations revealed substantial conductivity improvement when compared to the base fluid, although gold/platinum showed lesser improvement compared to gold. Characterisation of the as-synthesised nanoparticles (NPs) and fluids was carried out with X-ray diffraction (XRD), ultraviolet-visible (UV-vis) spectroscopy, transmission electron microscopy (TEM) and energy-dispersive X-ray spectroscopy (EDS). The distinct two-phase bimetallic nature of gold/platinum, its two plasmonic band optical absorption features and the spherical morphology of the particles were shown. The findings were correlated with the observed thermal and ultrasonic behaviour and proper rationalisation is provided. It

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https://doi.org/10.1134/S1063771021330022

ISSN 1063-7710, Acoustical Physics, 2021, Vol. 67, No. 5, pp. 584–589. © Pleiades Publishing, Ltd., 2021

PHYSICAL ACOUSTICS

Ultrasonic and Thermophysical Properties of Cobalt Nanowires

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Received September 3, 2020; revised September 2, 2021; accepted November 30, 2021

Abstract—We have estimated elastic, mechanical, thermal and ultrasonic properties, in high temperature regime, of cobalt nanowires (Co-NWs) having a hexagonal close-packed (HCP) structure. The second and third order elastic constants (SOECs and TOECs) have been calculated using the Lennard–Jones potential model at 300 K. These elastic constants are used to find out mechanical properties, ultrasonic velocities, Grüneisen parameters and thermal conductivity of Co-NWs. Further, these properties are used to analyze the stability and bonding properties of the present system. The relaxation time, non-linearity parameter and ultrasonic attenuation have been computed using the associated parameters. The achieved results of the present investigation have been analyzed with other NWs systems.

Keywords: Co-NWs, elastic properties, thermal properties, ultrasonic properties

DOI: 10.1134/S1063771021330022

1. INTRODUCTION

In current years, nanowires have considerable attraction of researchers worldwide due to their brilliant performance in numerous applications. Among these, the cobalt nanowires have fascinated significant care due to their foremost properties and applications such as unresolved magnetic properties [1], high-density magnetic storage media [2, 3], immune magnetic separation [4], gene delivery [5] and as targeted drug carrier [6] etc. A number of studies have been done by several researchers and scientists on the various properties of cobalt nanowires. Li et al. [1] synthesized cobalt nanowires with a mean diameter of about 100 nm by chemical reduction method in an aqueous solution under an external magnetic field and studied the magnetic properties of the same. Yang et al. [7] fabricated ordered arrays of cobalt nanowires by electrodepositing the similar materials into the pores of anodic aluminum oxide (AAO) membranes. Co-NWs of different diameters and lengths were investigated by Lavín et al. [8] using electro-deposition into nanopores of alumina and polycarbonate membranes. Hu et al. [9] constructed EAM-type many-body potentials for ten hexagonal close packed metals. They reported equilibrium density, cohesive energy, five independent SOECs and the vacancy formation energy. They also introduced a modification term for chosen metals with negative Cauchy pressure. Igarashi et al. [10] constructed Finnis–Sinclair (F–S) type many-body potentials for eight HCP metals: Co, Zr, Ti, Ru, Hf, Zn, Mg and Be.

As per the authors' information, no one has studied the Co-NWs for its mechanical, thermal, and acoustical properties. These lacks of information motivated us to investigate these additional properties of the Co-NWs. In present investigation, we computed the SOECs and TOECs using simple Lennard–Jones interaction potential approach. The obtained values of SOECs have been applied to find out the various mechanical modules such as Young's modulus, bulk modulus, shear modulus, Poisson's ratio and Zener's anisotropic factor. The ultrasonic velocity and thermal conductivity have been also evaluated. Further, these evaluated parameters have been used to find out thermal relaxation time, acoustic coupling constant and ultrasonic attenuation due to phonon–phonon (p–p) interaction and thermal relaxation mechanisms. Obtained results have been presented, compared and discussed with available findings of Co-NWs and other reported similar nanowires at room temperature.

J. Pure Appl. Ultrason. 43 (2021) pp. 56-60

Ultrasonic characterization of intermetallic compounds

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A simple interaction potential model has been established to calculate the higher order elastic constants of the intermetallic compounds NdS, NdSe, NdTe in the temperature range from 100-500 K. Debye average velocity, thermal relaxation time and acoustic coupling constant are calculated using the higher order elastic constants and other related parameters. Ultrasonic attenuation due to phonon-phonon interaction and thermoelastic loss are studied as a function of temperature along <111> direction. Important characteristic features well connected to the acoustical parameters are discussed.

Keywords: Ultrasonic propagation, elastic constants, intermetallics

Introduction

Intermetallic compounds are defined as a mixture in specifies proportion of two metallic elements that form a periodic crystalline structure different from those of the original elements. Intermetallic compounds, often called "Bulk Intermetallics" differ in a number of important ways from conventional metal alloys. Conventional alloys consists basically of a disordered solid solution of one or more metallic elements. They do not have any particular chemical formula, and are best described as consisting of a base material to which certain percentages of other elements have been added. Ultrasonic attenuation values are very helpful in the characterization and nondestructive evaluation of materials. Attenuation often serves as a measurement tool that leads to the formation theories to explain physical or chemical phenomena. Ultrasonic velocity and attenuation studies have been made in solids, liquid and liquid crystals. In solids[1,2] there are several causes of ultrasonic attenuation, but the most important being the electron-phonon (e-p) interaction below 80K and phonon-phonon interaction (p-p) interactions above 100K[3,4]. In the present study, Ultrasonic attenuation due to phonon-phonon interaction and thermoelastic loss in Neodymium monochalcogenides (NdS, NdSe, NdTe) from 100-500 K has been made along <111> crystallographic direction.

All the compounds have metallic luster. The sulfides are golden-yellow, the selenides from golden-yellow to copper-red and tellurides from violet-blue to blue. The phase composition of the samples checked by X-Ray diffraction, shown that all samples are practically one phase and have a well formed, NaCl-type structure[5]. These monochalcogenides were synthesized by V. P. Zhuze *et al.*[6,7] using the Iandelli's method8. All materials are extensively used in carbon lighting application especially by the motion picture industry for studio lighting and projection.

Theory

SOEC and TOEC are evaluated following Brügger's definition[9] of elastic constants at absolute zero using Born-Mayer potential[10]. The SOEC and TOEC at different temperatures are obtained by the method developed by Leibfried and Hahn[11], Leibfried and Ludwig[12], Ghate[13] and finally by Mori and Hiki[14] for NaCl type crystals.Themost important for evaluation of ultrasonic absorption due to phonon-phonon interaction also known as Akhieser type damping and Thermoelastic loss is the Grüneisen number. These are related to SOEC

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Indian J Phys
https://doi.org/10.1007/s12648-021-02278-9

ORIGINAL PAPER

Elastic, mechanical and ultrasonic studies of boron monopnictides in two different structural phases

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Received: 05 July 2021 / Accepted: 24 December 2021

Abstract: In the present study, elastic, mechanical, thermo-physical and ultrasonic properties of boron monopnictides BX (X = N, P, As) in both NaCl (B1) and CsCl (B2) phases have been investigated at room temperature. Coulomb and Born–Mayer potential model has been used for the calculation of second- and third-order elastic constants (SOECs and TOECs) of BX in both B1 and B2 phases. The calculated values of SOECs have been applied for the evaluation of the mechanical properties of these compounds using Voigt–Reuss–Hill approximation. The Born stability criteria and Vicker's hardness parameter (H) have been used for the analysis of nature and strength of the chosen materials. Later on, ultrasonic velocities including Debye average velocities have been evaluated utilizing calculated values of SOECs and density of the chosen materials. Thermal properties of the materials such as the lattice thermal conductivity, thermal relaxation time, thermal energy density and acoustic coupling constant have been also computed along < 100 > direction. These computed thermo-physical properties indicate that BP and BAs show metallic behaviour in B1 phase, while BN shows a metallic behaviour in both phases. Finally, ultrasonic attenuation has been estimated for these materials at room temperature along < 100 > direction. The obtained results have been compared with available results and discussed with available findings on these types of materials.

Keywords: Elastic constants; Mechanical property; Thermophysical property; Ultrasonic attenuation

1. Introduction

In the past few years, boron compounds have gained huge interest due to their wide industrial applications [1]. The boron is similar to carbon, having one electron less compared to the latter. When boron is combined with metal atoms, it leads to acquiring stable structured and forms metal-boron cluster compounds, especially with rare earth elements, which are localized with 4f orbitals. The boron is inherently p electron-deficient and has a small core size that causes B-doped molecules to have unique physical properties. Nowadays, these compounds are widely used in electronic, optical and medical fields [2, 3]. For instance, boron-based materials are used to enhance the photophysical properties of compounds, which are making them useful in luminescent and sensor materials. In particular, boron monopnictides with P and As were predicted to improve the thermal conductivity. Among these, boron monopnictides BX (X: N, P, As) are of particular interest for being B as anion and other as the most covalent one which in turn helps to advance the properties of materials. Most of the boron-based compounds possess outstanding physical properties such as high Pugh's indicator, ductility, hardness and thermal conductivity [4–6]. While few of them have attained other properties which include low density, low attenuation and higher resistivity [7, 8].

Various techniques and approaches were used to estimate the physical properties of boron-based compounds in different ambience conditions like pressure, temperature, phase of structure [9, 10]. Some important elastic, thermal and anisotropic properties of boron-based compounds (BP and BAs) were studied and elaborated by Dong et al. [11]

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Published online: 09 February 2022

Studies on flexible and highly stretchable sodium ion conducting blend polymer electrolytes with enhanced structural, thermal, optical, and electrochemical properties

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Received: 8 April 2021
Accepted: 19 June 2021
Published online: 6 July 2021

ABSTRACT

Polymer blend electrolyte films based on polyvinyl alcohol (PVA)–polyethylene glycol (PEG) with dopant sodium nitrate ($NaNO_3$) salt were successfully synthesized by the standard solution casting technique. These blend electrolytes were characterized by XRD, DSC/TGA, FTIR, FE-SEM, UV–Vis, ionic conductivity, Raman spectroscopic study and electrochemical measurements to optimize their structural, thermal, optical, ionic transport and electrochemical properties. XRD and DSC studies showed that the crystalline phase of the PVA–PEG blend polymer matrix decreases significantly with the content of $NaNO_3$ salt, which favours highly flexible polymer backbone and hence providing high ionic conductivity of the polymer blend electrolyte films. The maximum ionic conductivity is found to be 1.53×10^{-5} S cm^{-1} at room temperature (~ 30 °C) for the blend electrolyte film PB30. The ionic transference numbers of these polymeric blend electrolytes are estimated in the range of 0.94–0.97, which showed that ion conduction is purely ionic in nature. The Raman and FTIR spectroscopic analysis confirms the complexation of the cation of dopant salt (Na^+) with the backbone of the blend polymer matrix via Lewis acid–base interactions. The UV–visible analysis showed that optical band gap (direct and indirect band gap), absorption edge, and refractive index of the pristine polymeric blend change significantly with the concentration of dopant $NaNO_3$ salt, and these effects are more noticeable at the higher loading. The electrochemical stability window of the blend polymer electrolytes is observed 3.9 V for the PB 30 films, which confirm their utility as a separator membrane in the high-performance flexible solid-state electrochemical devices.

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https://doi.org/10.1007/s10854-021-06456-7

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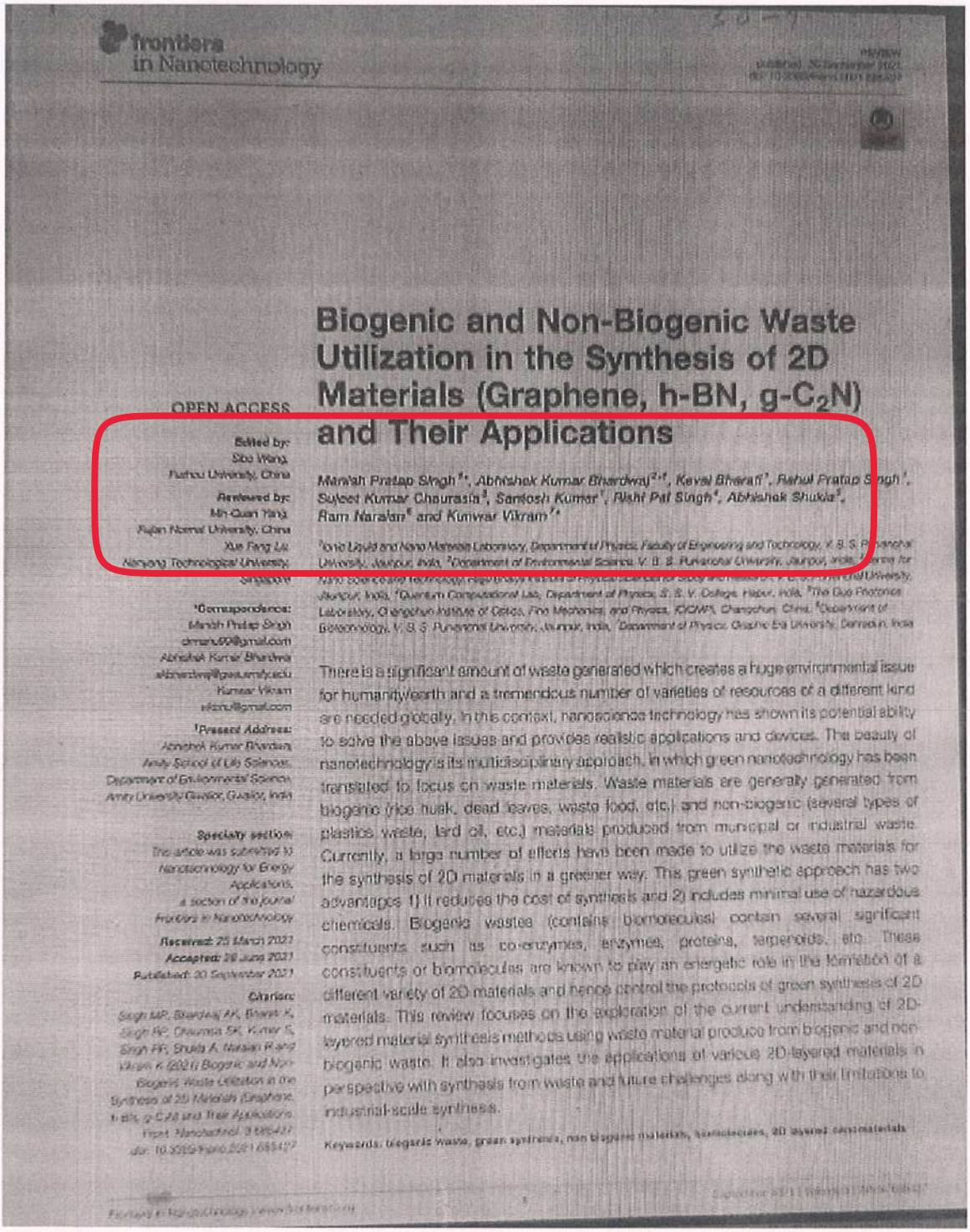
https://doi.org/10.1007/s10854-021-06456-7

frontiers in Nanotechnology



Biogenic and Non-Biogenic Waste Utilization in the Synthesis of 2D Materials (Graphene, h-BN, g-C_2N) and Their Applications

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There is a significant amount of waste generated which creates a huge environmental issue for humanity/earth and a tremendous number of varieties of resources of a different kind are needed globally. In this context, nanoscience technology has shown its potential ability to solve the above issues and provides realistic applications and devices. The beauty of nanotechnology is its multidisciplinary approach, in which green nanotechnology has been translated to focus on waste materials. Waste materials are generally generated from biogenic (rice husk, dead leaves, waste food, etc.) and non-biogenic (several types of plastics waste, lard oil, etc.) materials produced from municipal or industrial waste. Currently, a large number of efforts have been made to utilize the waste materials for the synthesis of 2D materials in a greener way. This green synthetic approach has two advantages 1) it reduces the cost of synthesis and 2) includes minimal use of hazardous chemicals. Biogenic wastes (contains biomolecules) contain several significant constituents such as co-enzymes, enzymes, proteins, terpenoids, etc. These constituents or biomolecules are known to play an energetic role in the formation of a different variety of 2D materials and hence control the protocols of green synthesis of 2D materials. This review focuses on the exploration of the current understanding of 2D-layered material synthesis methods using waste material produce from biogenic and non-biogenic waste. It also investigates the applications of various 2D-layered materials in perspective with synthesis from waste and future challenges along with their limitations to industrial-scale synthesis.

Keywords: biogenic waste, green synthesis, non biogenic materials, nanosheets, 2D layered nanomaterials

OPEN ACCESS

Edited by:
Sibo Wang
Fuzhou University, China

Reviewed by:
Mi-Quan Yang
Fujian Normal University, China
Xue Feng Lie
Nanyang Technological University, Singapore

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Specialty section:
This article was submitted to Nanotechnology for Energy Applications, a section of the journal Frontiers in Nanotechnology

Received: 25 March 2021
Accepted: 28 June 2021
Published: 20 September 2021

Citation:
Singh MP, Bhardwaj AK, Bharati K, Singh RP, Chaurasia SK, Kumar S, Singh RP, Shukla A, Naraian R and Vikram K (2021) Biogenic and Non-Biogenic Waste Utilization in the Synthesis of 2D Materials (Graphene, h-BN, g-C_2N) and Their Applications. Front. Nanotechnol. 3:685427. doi: 10.3389/fnano.2021.685427

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https://doi.org/10.3389/fnano.2021.685427

Studies on the interaction of Na^+ ion with binary mixture of carbonate-ester solvents: A density functional theory approach

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Abstract. The advancement of sodium-ion batteries as an alternative to lithium-ion batteries presents a viable way to make energy storage cost-efficient. However, the inherent properties of Na^+ are not quite well understood as it is for Li^+, which also include solvation of Na^+ in non-aqueous electrolyte for its application in electrochemical devices. Here, a comprehensive study of Na^+ solvation in the binary mixture of ethylene carbonate (EC) and propylene carbonate (PC) in different ratios is reported, using density functional theory calculation. The optimised structure of cluster of binary mixture EC-PC-Na^+ in three different ratios (1:1, 2:1 and 3:1) of EC: PC is analysed. Binding and Gibbs free energy of Na^+ solvated by EC and PC and charge on Na^+ is calculated. The calculated results favour the stability of binary mixtures containing higher concentration of ethylene carbonate. In infrared (IR) vibrational spectra, substantial changes are observed in the IR active modes of the solvent because of cation-solvent interaction.

1. Introduction

Ample amount of research is going on across the globe to encourage sodium-ion batteries (SIBs) as an alternative to lithium-ion batteries (LIBs) as an electrochemical energy storage device [1-2]. These efforts are being made not only to meet the dramatically increasing demands of sustainable resources but also to cut down the cost of electronic devices without compromising the high power density offered by LIBs [1,3]. SIBs are attracting tremendous attention because of their cost-effectiveness and comparable energy density as offered by LIBs [4-5]. Reason for a lesser rate of SIBs is the high sodium concentration in the earth's crust and oceans relative to lithium [6]. Generally, for understanding the fundamental of SIB materials, researchers in the field of sodium-ion batteries (SIB) make use of much know-how and examples from the field of lithium-ion batteries (LIB)[5]. A small but important aspect of these endeavours is modelling of electrolytic system via computer simulations to facilitate the exploration of the optimal electrolyte for SIBs [4,7]. Liquid electrolytes have always been the most widely used electrolyte for LIBs and therefore have gained attention for SIBs as well.

Applied Surface Science Advances 6 (2021) 100167

Contents lists available at ScienceDirect

Applied Surface Science Advances

journal homepage: www.sciencedirect.com/journal/applied-surface-science-advances

Probing on crystallographic structural and surface morphology of hydrothermally synthesized MoS_2 nanoflowers consisting of nanosheets

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ARTICLE INFO

Keywords:
Molybdenum disulfide
Nanoflowers
Nanosheets
Hydrothermal
Structural model
Electron microscopy

ABSTRACT

Hydrothermally synthesized MoS_2 were obtained and their morphological characteristics were ascertained via electron microscopy. Field emission scanning electron microscope (FESEM) micrographs revealed the formation of nano-flowers by accumulation of nanosheets. The Transmission electron microscopy (TEM) revealed the nanosheets to be of ~100 nm length and ~5 nm in edge width. X-ray diffraction pattern analysis showed the formation of 2H polymorph of MoS_2, having a long range stacking of about 14 (002) lattice planes in a single crystallite. The Fourier transform infrared (FT-IR) spectroscopic analysis revealed the presence of bridging S_2^{2-} ligands. Energy dispersive spectroscopy (EDS) analysis associated with the SEM indicates the presence of no other elements except Mo and S in the material. Visualization of atomic structural model and intense lattice plane has been carried out and correlated with crystallographic results. Such findings can be considered as important precursors in both experimental elementary aspects and theoretical approach towards the application-oriented research for crystallographic analysis of nanostructures.

Introduction

Nanostructured transition metal chalcogenides such as metal oxides (cobalt oxide (Co_3O_4), nickel oxide (NiO), vanadium oxides (VO_2, V_2O_5)) and metal sulfides (cobalt sulfides [CoS, Co_3S_4, Co_9S_8], copper sulfides (CuS, Cu_2S), iron disulfide (FeS_2), nickel sulfides (NiS, Ni_3S_4), tin sulfide (SnS_2), tungsten disulfide (WS_2)) have increasingly become an area of special interest in both fundamental research and applied disciplines [1–10]. Largely because of the promise shown by them for a broad range of applications; these materials for decades have captured the attention of the research community. An intriguing aspect of these transition metal chalcogenides is their well-known two-dimensional (2D) structure in which a plane (M) of transition metal element (e.g., Mo, Ta, Ti, V, W, Zr etc.) and two planes (X) of the chalcogenides (e.g., S, Se or Te) are arranged periodically in a hexagonal structure with a layered X-M-X sandwiched composition [11–16]. Similar to graphene these kinds of layers are held together by weak van der Waals's interaction between them and thus the distance between the layers are prone to easy manipulation by methods such as exfoliation [3,11–12]. Amongst various layered transition metal sulphides (LTMSs), nano-structured molybdenum (IV) sulfide (often referred to as molybdenum disulfide; MoS_2) materials have often received the most attention due to their unique physicochemical features such as simple 2D structure, ease of processing, inexpensiveness, and more importantly, close structural analogy to graphene nanosheets and a large number of potential applications [21–27]. The layered structure or 2D morphologies of MoS_2 have found potential for a varieties of applications such as electronic devices [1,5,8,35–39], sodium ion batteries [2,18,19], lithium ion batteries [25], hydrogen evolution reaction [12,22,27,30,34,35], solar cells [14], water filtration [15,24,46], electrochemical capacitors [17,20,23], lubricants [29], sensors [40,41] and in electromagnetic wave absorption [42,43].In fact, shielding from harmful electromagnetic waves is a potential application for such 2D nanostructures with high specific surface area and good carrier mobility [44–47].

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https://doi.org/10.1016/j.apsadv.2021.100167
Received 12 May 2021; Received in revised form 4 September 2021; Accepted 14 September 2021

https://doi.org/10.1016/j.apsadv.2021.100167

Non-functionalized Au nanoparticles can act as high-performing humidity sensor

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Received: 18 June 2020
Accepted: 24 August 2020

ABSTRACT

We synthesized gold (Au) nanoparticles via a rapid chemical route by reducing chloroauric acid by trisodium citrate. TEM micrographs revealed that particles were spherical with well-defined lattice structures and most of them were within the size range of 8–12 nm. A single surface plasmon resonance peak observed at 525 nm indicated the uniformness of the spherical morphology of the particles. XRD analysis showed that the particles were well crystalline. An impedance-based humidity sensor device was fabricated for depositing these gold nanoparticles in their non-functionalized state and the sensor revealed fast response time of 54 s, high stability and repeatability, and an impressive average sensitivity of 7.57 MΩ/% RH within the humidity range of 10–95%. SEM micrographs revealed the presence of cracks on the film surface and our analysis of the sensing mechanism correlated the sensitivity and the surface cracks along with smaller particle sizes. Our results show that gold nanoparticles without further functionalization are able to perform as a well-performing humidity sensor.

1 Introduction

Humidity, which can be defined as the concentration of moisture in air, happens to be an extremely important parameter in our regular livelihood. For a comfortable living condition, the relative humidity (RH) i.e., the ratio between the absolute humidity and the saturation humidity should be between 40 and 60% with the temperature being around 20–25 °C. Higher values of relative humidity results in a feeling of discomfort, whereas lower values cause dryness in skin, eyes, and mouth. Perspiration, one of the most effective biological procedures for animals to control the body temperature, is primarily a function of humidity, or relative humidity to be more exact. However, various applicational necessities could demand specific RH values e.g., the RH value must remain steady at 38% in class 10 clean rooms, 60% in hospital operating

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https://doi.org/10.1007/s10854-020-04338-y
Published online: 19 September 2020

Journal of Applied Physics ARTICLE

Thickness effect on scaling law and surface properties of nano-dimensional SnTe thin films

Cite as: J. Appl. Phys. 130, 175306 (2021); doi: 10.1063/5.0066006
Submitted: 6 August 2021 · Accepted: 14 October 2021
Published Online: 3 November 2021

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ABSTRACT

SnTe is an important material because of its applications in mid-infrared photo-detectors. In the present work, the effects of film thickness on scaling law and surface properties (i.e., morphologies and optical properties) of SnTe thin films have been investigated. SnTe thin films of different thicknesses are prepared by means of e-beam evaporation technique. The surface morphology of each film is analyzed by atomic force microscopy (AFM) as well as a scanning electron microscope. The crystallinity of the films is found to increase with increasing film thickness, as confirmed by x-ray diffraction and Raman measurements. Fractal analysis is performed on AFM images to investigate the irregularity of surfaces. It is found that the surface of the thicker sample is rougher than the thinner sample. The autocorrelation function is applied to investigate the self-affine fractal nature of surfaces. The average roughness, interface width, lateral correlation length, local surface slope, and fractal dimension increased with film thickness. The values of roughness exponent, growth exponent, dynamic exponent, and steepening exponent are calculated and found to be $\alpha = 0.76$–0.96, $\beta = 0.75$, $z = 1.92$, and $\lambda = 0.35$–0.25, respectively. The scaling exponents together with the other parameters such as the local surface slope indicate that the growth is quasi-3D island/mound type with rapid surface roughening behavior and obeys anomalous scaling. The multiple scattering cross sections of light together with Fourier transform infrared spectroscopy data analyses suggest that the higher crystalline film with a smaller number of defects is infrared-sensitive and may be more suitable for advanced mid-infrared detector applications.

I. INTRODUCTION

In the last few decades, metal chalcogenides of the IV–VI group have been the focus of extensive research due to their interesting physical properties.[1–3] In this group, a topological crystalline insulator (TCI) such as tin telluride (SnTe) is a direct narrow bandgap (i.e., 0.35 eV) semiconductor with rock salt structure. SnTe has wide applications in thermoelectric devices, mid-infrared (MIR) detectors, and photodetectors.[4–6] The presence of mirror symmetry of the lattice rather than the time-reversal symmetry in SnTe ensures the existence of robust topological surface states.[7–9] Recently, various methods have been developed to fabricate SnTe nanostructures (i.e., nano-wires, nano-ribbons, nano-plates, and nano-sheets) including vapor deposition, molecular beam epitaxial, mechanical exfoliation, and liquid solution synthesis.[10–12] The influence of material surfaces becomes predominant in the miniaturization of devices, and the stability and morphology of these surfaces may be tuned by thermodynamics.[13] Moreover, topological insulating (TI) properties significantly depend on the precise atomic structure of the surface and the exact location of the Fermi level.[14,15] SnTe always acts as a p-type semiconductor due to high

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https://doi.org/10.1063/5.0066006

Gene Reports 25 (2021) 101377

Contents lists available at ScienceDirect

Gene Reports

journal homepage: www.elsevier.com/locate/genrep

Interleukin-10 (IL-10) gene polymorphisms and prostate cancer susceptibility: Evidence from a meta-analysis

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ARTICLE INFO

Keywords:
Prostate cancer
Interleukin-10
IL-10
Polymorphism
Meta-analysis

ABSTRACT

Prostate cancer is the second most frequent cancer in men. The frequency of the prostate cancer is greatly varies in different populations of the world. Three common polymorphisms in promoter region of interleukin-10 (IL-10) gene viz. -1082A > G, -819C > T and -592C > A are extensively studied in prostate cancer with inconclusive results. So, a meta-analysis was performed to assess the association between these three IL-10 gene polymorphisms and risk of prostate cancer susceptibility. Suitable studies were retrieved by electronic databases search and odds ratios (ORs) with 95% confidence intervals (CIs) were used as association measure. All the statistical analyses were conducted in the Open Meta-Analyst program. In our meta-analysis we included 17 studies (10,718 samples), 12 studies (8810 samples) and 13 studies (7801 samples) for -1082A > G, -819C > T and -592C > A polymorphisms respectively. The result of the -592C > A polymorphism revealed low heterogeneity with no association in the overall analysis ($OR_{Avs.C}$ = 1.05, 95% CI = 0.99–1.12, p = 0.09, I^2 = 35.89%). In ethnicity based stratified analyses, significant association was found in Caucasian population with prostate cancer using allele contrast model ($OR_{Avs.C}$ = 1.10, 95% CI = 1.02–1.18, p = 0.01, I^2 = 19.37%), homozygote model ($OR_{AAvs.CC}$ = 1.32, 95% CI = 1.05–1.67, p = 0.01, I^2 = 0%), and dominant model ($OR_{AA+CAvs.CC}$ = 1.11, 95% CI = 1.00–1.24, p = 0.04, I^2 = 40.75%). No such results were found in the Asian population. In the other two polymorphisms i.e. -1082A > G and -819C > T, no significant association with prostate cancer was observed. In conclusion, results of present meta-analysis suggested that IL-10-592C > A polymorphism plays a role in the etiology of the prostate cancer in the Caucasian population.

1. Introduction

Prostate cancer is the second most common cancer and fifth leading cause of deaths in males worldwide. The worldwide incidence and mortality rate of prostate cancer is 13.5% and 6.7% respectively. The incidence of prostate cancer greatly varies in different regions of the world (highest in Australia/New Zealand and lowest in South Central Asia). While the mortality is highest in Southern Africa and lowest in South Central Asia (Bray et al., 2018). The progression of prostate cancer is often slow and it remains localized firstly and later when the cells of the prostatic tissue abnormally proliferate it may spread to nearby tissues and organs and then metastasizes. The etiology of the prostate is least understood despite being a common cancer. A few genetic factors were identified which are consider as the risk for the prostate cancer including age, family history of prostate cancer and ethnicity. Smoking, diet, androgen, and obesity are the secondary factors that may contribute to the risk of prostate cancer (Hsing and Chokkalingam, 2006).

Recently inflammation has been added to the list of secondary factors as it contributes to proliferation, malignancy, angiogenesis, metastasis, modulation of adaptive immunity, and unresponsiveness to hormones and chemotherapeutic agents (McCarron et al., 2002). Interleukin-10 (IL-10) is an anti-inflammatory cytokine primarily produced by monocytes and to a lesser amount by lymphocytes like- T_H2, $CD4^+$ and $CD8^+$ T cells, macrophages, and dendritic cells (Saraiva and O'Garra, 2010). IL-10 down regulates the cytokine production of the T_H1 cells (Mosser and Zhang, 2008). It enhances the proliferation of B cells, thymocytes, and mast cells and also stimulates the antibody production (Moore et al., 2001; Sabat et al., 2010).

The IL-10 cytokine in humans is coded by interlukin-10 (*IL-10*) gene,

Abbreviations: IL-10, interleukin 10; OR, odds ratio; CI, confidence interval; PRISMA, Preferred Reporting Items for Systematic Reviews and Meta-Analyses; HWE, Hardy-Weinberg equilibrium.

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https://doi.org/10.1016/j.genrep.2021.101377
Received 15 January 2021; Received in revised form 9 August 2021; Accepted 28 September 2021
Available online 4 October 2021

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Ind J Clin Biochem (Jan-Mar 2022) 37(1):3–17
https://doi.org/10.1007/s12291-021-01000-0

REVIEW ARTICLE

Relation Between Methylenetetrahydrofolate Reductase Polymorphisms (C677T and A1298C) and Migraine Susceptibility

Vandana Rai[1] · Pradeep Kumar[1]

Received: 24 January 2021 / Accepted: 17 August 2021 / Published online: 20 September 2021

Abstract Migraine is a neurological disorder which impairs the patient's quality of life. Several association studies investigating the association between MTHFR gene C677T and A1298C polymorphisms and susceptibility to migraine were published. But the results were conflicting, so authors performed a meta-analysis of published case control studies to find out the exact association between MTHFR polymorphism and migraine susceptibility. Four databases were searched for suitable studies up to December, 2018. Odds ratios (OR) with 95% confidence intervals (CI) was calculated adopting additive, homozygote, co-dominant, dominant, and recessive genetic models. Results of MTHFR C677T polymorphism studies meta-analysis showed significant association with migraine risk using allele contrast, homozygote, dominant and recessive genetic models (T vs. C: OR = 1.18, 95% CI = 1.00–1.26, $p = 0.05$; TT vs. CC: OR = 1.24, 95% CI = 1.0–1.5, $p = 0.04$; CT vs. CC: OR = 1.08, 95% CI = 0.97–1.07, $p = 0.25$; TT + CT vs. CC: OR = 1.15, 95% CI = 1.0–1.29, $p = 0.04$; TT vs. CT + CC: OR = 1.97, 95% CI = 1.28–3.42, $p = 0.002$). However, results of MTHFR A1298 polymorphism studies meta-analysis did not show any association with migraine. Subgroup analysis based on ethnicity and migraine types i.e. migraine with aura (MA) and without aura (MO) were also performed. Results of present meta-analysis indicate overall association between MTHFR C677T polymorphism with migraine in total 24 studies, in Asian population and in MA cases but did not show any association with Caucasian population and MO cases.

Keywords Migraine · MTHFR · C677T · A1298C · Polymorphism · Homocysteine · Risk factors

Introduction

Migraine is a highly prevalent neurological disorder affecting up to 20% of the general population [1]. It is characterized by recurrent episodes of headache, nausea, vomiting, photophobia, phonophobia and autonomic nervous system dysfunction [2]. International Headache Society (IHS) defined two major classes of migraine: migraine with aura (MA) and migraine without aura (MO).

Migraine is considered a polygenic multifactorial disease with several genes participating in its pathogenesis through interaction with environmental factors [3, 4]. About 50% of affected individuals have a first-degree relative also suffering from migraine [5–7]. Family and twin studies support the idea of MO and MA being different phenotypes of the same entity, with a heritability ranging from 33 to 57% [6, 8, 9]. The number and types of genes responsible for migraine are still not clearly known.

Among all the genes associated with common migraine and MA, the 5,10-methylenetetrahydrofolate reductase (MTHFR) gene is the most thoroughly studied one. MTHFR gene is located on chromosome 1 (1p36.3) and contains 11 exons. Several polymorphisms are reported in MTHFR gene, but C677T and A1298C polymorphisms are clinically very important and most studied so far. In C677T polymorphism, cytosine at 677 position is substituted by thymine. This substitution makes MTHFR enzyme thermo labile with reduced enzymatic activity. T allele frequency

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Contents lists available at ScienceDirect

Infection, Genetics and Evolution

journal homepage: www.elsevier.com/locate/meegid

Review

*Fok*I polymorphism of the vitamin D receptor (VDR) gene and susceptibility to tuberculosis: Evidence through a meta-analysis

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ARTICLE INFO

Keywords:
VDR
*Fok*I
Tuberculosis
Meta-analysis
Polymorphism

ABSTRACT

Background: Tuberculosis is one of the top ten causes of deaths worldwide. The deficiency of vitamin D was reported to be associated with the increased susceptibility of tuberculosis. Various previous reports were published to check the association of *Fok*I polymorphism of the vitamin D receptor gene with tuberculosis risk. But their results were inconsistent so, we performed a meta-analysis to know the exact relation of the two.

Methods: Different databases were screened up to November 2020 with the keywords "Vitamin D receptor", "VDR", and "*Fok*I", along with "Tuberculosis" and "TB" to find the suitable articles. All the statistical analyses were performed by the Open Meta-Analyst program and all *p*-values were two-tailed with a significance level of 0.05.

Results: No statistically significant association was observed in the allele contrast model ($OR_{fvs.F}$ = 1.11, 95%CI = 0.99–1.24, p = 0.05, I^2 = 73.46%), in the dominant model ($OR_{ff+Ffvs.FF}$ = 1.11, 95%CI = 0.96–1.28, p = 0.14, I^2 = 71.39%), and in the co-dominant model ($OR_{Ffvs.FF}$ = 1.05, 95%CI = 0.92–1.21, p = 0.41, I^2 = 65.97%). However, a significant association was found in the homozygote model ($OR_{ffvs.FF}$ = 1.32, 95%CI = 1.03–1.69, p = 0.02, I^2 = 67.02%) and in the recessive model ($OR_{FF+Ff\ vs.ff}$ = 1.26, 95%CI = 1.03–1.54, p = 0.02, I^2 = 58.01%). Further analysis was performed on the bases of the ethnicity. In Asian population a significant association was found in the homozygote model ($OR_{ffvs.FF}$ = 1.57, 95%CI = 1.12–2.21, p = 0.008, I^2 = 70.37%) and in the recessive model ($OR_{FF+Ff\ vs.ff}$ = 1.43, 95%CI = 1.08–1.89, p = 0.01, I^2 = 63.13%).

Conclusion: In conclusion, a significant association of *Fok*I with tuberculosis susceptibility was found in the overall analysis and in the Asian population.

1. Introduction

Tuberculosis (TB) is an infectious disease caused by the bacterium *Mycobacterium tuberculosis*. TB is one of the top 10 causes of death globally. In the year 2019 an estimated 10 million people fell ill with TB worldwide and nearly 1.4 million people were died worldwide due to TB (WHO, 2020). Although, one third of the population of the world is infected with the bacillus but only a tiny percentage of the people may progress to active TB disease (Delgado et al., 2002). A number of factors are associated with the susceptibility of TB such as- environmental (Hillerdal, 2000), genetic (Newport and Nejentsev, 2004), and HIV infection (Bowen et al., 2000; Raghavan et al., 2012) etc. A number of studies were performed to determine the role of single nucleotide polymorphisms (SNPs) in the susceptibility of TB like- natural resistance–associated macrophage protein 1 (NRAMP1) gene (Borgdorff, 1998), interleukin (IL) genes (Diagbouga et al., 1999; Wilkinson et al., 1999), vitamin D receptor (VDR) genes (Selvaraj et al., 2004a), and tumor necrosis factor (TNF) genes (Selvaraj et al., 2001).

Among them the VDR gene is most studied and it has been considered as a risk factor for the TB development process as it may affect the host immunity. The vitamin D receptor interacts with the 1,25-dihydroxyvitamin D3 and activates the monocytes, stimulate cell mediated immunity and suppress the proliferation of lymphocytes (Tachi et al., 2003), so the susceptibility to TB may be increased by deficiency of 1,25-dihydroxyvitamin D3. The VDR gene is located on chromosome 12 that spans approximately 75 kb of genomic DNA and contains 11 exons (Taymans et al., 1999). The VDR gene of humans has a number of polymorphisms but the most studied of them are *Apa*I G > T (rs7975232), *Bsm*I G > A (rs1544410), *Taq*I T > C (rs731236) and *Fok*I T > C (rs2228570). The *Bsm*I, *Apa*I and *Taq*I SNPs are involved in the regulation of the stability of the VDR mRNA. The *Bsm*I and *Apa*I polymorphisms are located in the intron 8 and *Taq*I is found in the exon 9

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https://doi.org/10.1016/j.meegid.2021.104871
Received 2 March 2021; Received in revised form 15 April 2021; Accepted 20 April 2021
Available online 24 April 2021

Ind J Clin Biochem
https://doi.org/10.1007/s12291-020-00933-2

REVIEW ARTICLE

Catechol-O-methyltransferase (COMT) Val158Met Polymorphism and Susceptibility to Alcohol Dependence

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Received: 30 April 2020 / Accepted: 31 October 2020

Abstract Catechol-O-methyl transferase (COMT) enzyme catalyzes the metabolism of dopamine and other catechols in the brain. Several articles investigated catechol-O-methyltransferase (COMT) Val158Met polymorphism as risk factor for alcohol dependence (AD) but the results were inconclusive. The aim of present meta-analysis was to evaluate the association of Val158Met (COMT) polymorphism with AD. Authors performed keyword search of the 4 electronic databases—Pubmed, Google Scholar, Springer Link and Science Direct databases up to December 31, 2019. Total eighteen studies that investigated the association of Val158Met polymorphism with AD were retrieved. The pooled results from the meta-analysis (2278 AD cases and 3717 healthy controls) did not show association with AD using all 5 genetic models (allele contrast model: OR = 1.02, 95% CI = 0.90–1.14, $p = 0.03$; homozygote model: OR = 1.06, 95% CI = 0.81–1.38, $p = 0.69$; dominant model: OR = 0.99, 95% CI = 0.85–1.14, $p = 0.87$; co-dominant model: OR = 0.97, 95% CI = 0.86–1.11, $p = 0.71$; recessive model: OR = 1.05;95% CI = 0.85–1.29, $p = 0.61$). Results of subgroup analysis showed that Val158Met is not risk for AD in Asian and Caucasian population. In conclusion, COMT Val158Met is not a risk factor for alcohol dependence.

Keywords Alcohol dependence · AD · COMT · Val158Met · Meta-analysis · Polymorphism

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Introduction

Alcohol dependence (AD) is a common, chronic, relapsing neuropsychiatric disorder and isone of the leading causes of the global burden of disease [1–3]. It has been demonstrated that among those who drink alcohol, only a minority (~ 15%) eventually become dependent on it [4] (Hasin et al. 2007). Heritability estimates are as high as 40–60%, with involvement of multiple genes [5, 6] (Stacey et al. 2009; Bienvenu et al. 2010). Chronic alcoholics have suffered with different psychiatric comorbidities, such as antisocial personality disorder, anxiety, depression, and attention deficit hyperactivity disorder [7] (Ducci et al. 2007).

Dopamine is a main neurotransmitter in the development of addiction behaviour [8] (Hyman et al. 2006). Catechol-O-methyl transferase (COMT) enzyme catalyzes the metabolism of dopamine and other catechols in the brain [9, 10]. In the striatum and nucleus accumbens, dopamine is removed from the synaptic cleft by reuptake through dopamine transporter (DAT) and subsequent oxidation by monoamine oxidase [11]. In prefrontal cortex (PF), COMT mainly controls the dopaminergic transmission, because DAT density is low in PF [12, 13]. So, the gene repeatedly implicated in PFC dopamine function is *COMT*. COMT enzyme metabolizes dopamine, adrenalin and noradrenalin, and is the main factor controlling dopamine levels in the PFC.

COMT gene is present on chromosome 22q11.2, contains 6 exons, and expresses at high levels in many tissues including the brain, liver, kidney, and breast etc. Several polymorphisms are reported in the COMT gene, but the most studied and cinicay significant is a single base pair G–A substitution at position 472 in exon 4 (G472A), results in substitution of valine by methionine (Val158Met) in

Published online: 02 January 2021

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AIMS Neuroscience, 8(2): 212–225.
DOI:10.3934/Neuroscience.2021011
Received: 22 November 2020
Accepted: 22 November 2020
Published: 27 January 2021

http://www.aimspress.com/journal/neuroscience

Research article

Methylenetetrahydrofolate reductase (*MTHFR*) gene C677T (rs1801133) polymorphism and risk of alcohol dependence: a meta-analysis

Running title: MTHFR and alcohol dependence

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Abstract: Alcohol dependence is a complex neuropsychiatric disorder. Numerous studies investigated association between *MTHFR* gene C677T (rs1801133) polymorphism and alcohol dependence (AD), but the results of this association remain conflicting. Accordingly, authors conducted a meta-analysis to further investigate such an association. PubMed, Elsevier Science Direct and Springer Link databases were searched for studies on the association between the *MTHFR*C677T polymorphism and AD. Pooled odds ratio (OR) with 95% confidence interval (CI) was calculated using the fixed- or random-effects model. Statistical analysis was performed with the software program MetaAnayst and MIX.A total of 11 articles were identified through a search of electronic databases, up to February 28, 2020. The results of the present meta-analysis did not show any association between MTHFR C677T polymorphisms and AD risk (for T vs. C: OR = 1.04, 95% CI = 0.88–1.24; CT vs. CC: OR = 1.02, 95% CI = 0.62–1.68; for TT+CT vs. CC: OR = 1.10, 95% CI = 0.94–1.29; for TT vs. CC: OR = 1.01, 95% CI = 0.66–1.51; for TT vs. CT+CC: OR = 0.97, 95% CI = 0.66–1.40). Results of subgroup analysis showed no significant association between *MTHFR* C677T polymorphism with AD in Asian as well as in Caucasian population. In conclusion, C677T polymorphism is not a risk factor for alcohol dependence.

Keywords: alcohol dependence; AD; *MTHFR*; C677T; polymorphism; homocysteine; meta-analysis

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Contents lists available at ScienceDirect

Transfusion and Apheresis Science

journal homepage: www.elsevier.com/locate/transci

The association of ABO blood group with the asymptomatic COVID-19 cases in India

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ARTICLE INFO

Keywords:
India
Blood group
Asymptomatic
COVID-19
Coronavirus

ABSTRACT

The COVID-19 pandemic resulted in multiple waves of infection worldwide. The large variations in case fatality rate among different geographical regions suggest that the human susceptibility against this virus varies substantially. Several studies from different parts of the world showed a significant association of ABO blood group and COVID-19 susceptibility. It was demonstrated that individuals with blood group O are at the lower risk of coronavirus infection. To establish the association of ABO blood group in SARS-CoV-2 susceptibility, we for the first time analysed SARS-CoV-2 neutralising antibodies among 509 individuals, collected from three major districts of Eastern Uttar Pradesh region of India. Interestingly, we found neutralising antibodies in a significantly higher percentage of people with blood group AB (0.36) followed by B (0.31), A (0.22) and lowest in people with blood group O (0.11). We further estimated that people with blood group AB are at comparatively higher risk of infection than other blood groups. Thus, among the asymptomatic SARS-CoV-2 recovered people blood group AB has highest, whilst individuals with blood group O has lowest risk of infection.

1. Introduction

COVID-19 has impacted life of billions because of its virulence. The extensive ongoing research revealed the complex nature of this novel SARS-CoV-2 virus transmitted to the humans [1–6]. With the growing knowledge about this disease, it is clear that there are certain risk factors associated with morbidity and mortality [7–9]. More importantly, many of the studies have found strong association of the ABO blood group and COVID-19 with morbidity and mortality [6,10–14], whilst, a few studies have also found no association of COVID-19 with the ABO blood group 10,15,16]. In the past, there have been several studies suggesting the association of ABO blood group with diseases. For example, individual with the blood group O were reported to be more susceptible to the Cholera in Gangetic plain populations [17] and *Helicobacter pylori* infection [18]. However, blood group O was found to be less susceptible for Dengue [19,20] and SARS (Severe Acute Respiratory Syndrome) viruses [14,21].

The ABO blood type is administered by the gene *ABO*, located at chromosome 9 [22]. Studies have found that the this gene modulates the COVID-19 susceptibility directly or indirectly [23–25]. Several genetic variants of this gene affect morbidity and mortality in COVID-19 and many other diseases. For example, it affects red blood related physiology [26,27], venous thromboembolism [28], type 2 diabetes [29], ischemic stroke [30], heart related functions [31] and coronary artery disease [31–33]. Thus, studying the association of ABO blood type with SARS-CoV-2 infection, it is feasible to ascertain the factors influencing

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https://doi.org/10.1016/j.transci.2021.103224
Received 29 May 2021; Received in revised form 22 July 2021; Accepted 27 July 2021
Available online 30 July 2021

Ind J Clin Biochem
https://doi.org/10.1007/s12291-019-00862-9

ORIGINAL RESEARCH ARTICLE

Distribution of Methionine Synthase Reductase (MTRR) Gene A66G Polymorphism in Indian Population

Upendra Yadav[1] · Pradeep Kumar[1] · Vandana Rai[1]

Received: 17 May 2019 / Accepted: 25 November 2019

Abstract Methionine synthase reductase (MTRR) is an important enzyme of the folate/homocysteine pathway. It is responsible for regulation of methionine enzyme by reductive methylation. A common variant A66G is reported in the FMN-binding domain of the *MTRR* gene, which leads to substitution of isoleucine by methionine (I22M) in MTRR enzyme with reduced activity. Reduced catalytic activity of enzyme leads to high homocysteine concentration in blood and increases risk for numerous diseases. The frequency of A66G polymorphism varies in different ethnic groups. The present study has been designed to evaluate the frequency of *MTRR* A66G gene polymorphism in the Eastern UP population by PCR–RFLP method. Along with this we also performed a meta-analysis to evaluate the global prevalence of this polymorphism. Databases were screened to identified the eligible studies. The prevalence of the G allele and GG genotype was determined by the use of prevalence proportion with 95% CI. Open meta-analyst software was used for the meta-analysis. Total 1000 blood samples were analyzed, the frequencies of A and G alleles were 0.35 and 0.65 respectively. Meta-analysis results revealed that the prevalence of G allele and GG genotype were 49.4% (95% CI 40.6–58.1, $p \leq 0.001$) and 24.3% (95% CI 17.8–30.9, $p \leq 0.001$) respectively. In sub-group meta-analysis, the lowest frequency of G allele was found in South America (32.7%; 95% CI 14.1–51.3, $p \leq 0.001$), and highest in Asia (56.4%; 95% CI 39.5–73.3, $p \leq 0.001$). The results of the meta-analysis showed that the Asian population has the highest frequency of G allele and highest frequency of the GG genotype was found in the European population.

Keywords Methionine synthase reductase · MTRR · A66G · Polymorphism · Genotyping

Abbreviations

MTRR	Methionine synthase reductase

Introduction

Folate has important role in pregnancy and cell replication, because it is essentially required for DNA methylation, synthesis and repair. Chronic folate deficiency in vivo and in vitro has been associated with abnormal DNA methylation [1–3], DNA strand breaks [4], altered chromosomal recombination [5] and aberrant chromosome segregation [6]. The exact mechanisms by which these anomalies are related with the folate pathway are not fully elucidated but it is believed that the insufficient methylation of crucial metabolites or direct toxicity of homocysteine play some role in these abnormalities [7]. Folic acid pathway is governed by the dietary/environment and genetic factors and the genetic polymorphisms of the pathway genes regulated the folic acid pathway. Methionine synthase reductase (MTRR) is one of the crucial enzymes of folic acid pathway.

MTRR gene is mapped on chromosome 5*p*15.2–15.3 and has 15 exons [8]. MTRR is an electron transferase enzyme of FNR (ferredoxin-NADP(+) reductase) family. It is

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Published online: 30 November 2019

Austin Hematology

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Rapid Communication

Molecular Screening of Hemoglobin E Variant in Anemia Patients of Eastern UP Population, India

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Received: October 22, 2021; **Accepted:** November 16, 2021; **Published:** November 23, 2021

Abstract

Hemoglobinopathy is one of the most common monogenic disorders. This is prevalent in South East Asia. More than 700 heboglobinopathies are reported worldwide, out of which HbS and HbE are also prevalent in India. The objective of the present study is to determine the frequency of HbE in Eastern UP population. After taking written consent, blood samples was collected from 350 individuals and genomic DNA was extracted from all the collected blood samples. PCR-RFP method was used to analyze the HbE mutation. Out of 350 samples analyzed, one individual was Heterozygous (HbE/N) and one individual was Homozygous (HbE/E) for HbE mutation. In conclusion, the β^E allele frequency was observed as 0.42% in Eastern UP population. Percentage of both heterozygous and homozygous genotypes were 0.28%.

Keywords: Hemoglobin; Hemoglobinopathy; HbE; Globin gene

Introduction

Hemoglobin E (HbE) is the most common hemoglobinopathy in Asia and the second most common hemoglobinopathy in the world. It has been estimated that approximately 50 million people in the South East Asia alone carry the gene for hemoglobin E. It occurs at up to 50% in Khmer people living on the borders of Laos, Thailand and Cambodia which have been known as "Hb E triangle". The hemoglobin E has a wide spread distribution, being most frequent in the Eastern and Far Eastern Region in the India [1]. However, sporadic reports are also available from other parts of the country. Average gene frequency has been found to be 10.9% for North Eastern states of India.

HbE is caused by a substitution of glutamic acid by lysine at 26th position of β-globin protein, and G-->A substitution in β-globin gene (β^{26} Gluà Lys; GAGàAAG). The mutation underlying HbE creates an abnormal splicing site and thereby drastically reduces the formation of functional β-globin mRNA, this gene is similar to β ± thalassemia gene [2,3]. HbE has a weekend a/b interface, leading to some instability during conditions of increased oxidant stress [4]. Heterozygotes for HbE are microcytic, minimally anemic, and asymptomatic, however, homozygotes are clinically anemic. No reports of HbE frequency was available from Uttar Pradesh, hence we have screened anemic patients for HbE mutation.

Methods

The present study was approved by the Institutional Ethics Committee of VBS Purvanchal University, Jaunpur, India and all participants gave their written informed consent. 2 ml blood sample was collected from 350 anemia patients. Subjects for the present study selected from the three districts of Eastern UP like Varanasi, Allahabad and Jaunpur. Genomic DNA was extracted using the standard method of Bartlett and White [5]. And HbE mutation analysis was done by PCR-RFLP method of Tachavanich et al. [6].

Figure 1: Gel picture showing 444bp of HbE amplicon.

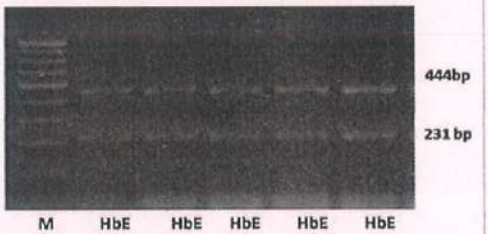

Figure 2: Gel picture showing MnlI digested HbE amplicon.

Results and Discussion

Out of 350 samples, 50 samples were of Muslims, 100 from Scheduled cast, 100 from Brahmin and 100 samples from OBC. HbE specific primers amplified 444 long DNA amplicon (Figure 1). In case of normal β-globin allele, MnlI enzyme cleave 444 bp long amplicon in to five fragments of 231/89/56/35/33bp long. HbE mutation (GAGàAAG) abolishes the MnlI restriction site and 444p long amplicon remained uncut after restriction digestion (Figure 2). Out of 350 samples, one individuals was heterozygous (β^A / β^E) and one individual was homozygous (β^E / β^E). Both individuals

Citation: Rai V, Yadav U and Kumar P. Molecular Screening of Hemoglobin E Variant in Anemia Patients of Eastern UP Population, India. Austin Hematol. 2021; 6(3): 1042.

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Molecular Screening of Hemoglobin S Variant in Anemia Patients of Eastern UP Population

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Abstract:

Hemoglobinopathies are the most common type of inherited disease in human. in India the most frequent and clinically significant hemoglobin structural variants are HbS, HbD and HbE. The HbS mutation, in which a glutamic acid at position 6 in the β chain is substituted for valine Sickle cell disease is a major health problem in some parts of India. 2 ml blood sample was collected from 350 anemia patient and PCR-RFLP method was used for hemoglobin S analysis. Out of 350 samples, in four individuals, HbS mutation was found in homozygous (β^6/β^6) condition. All four individuals are Sickle cell cases. In conclusion, the percentage of Sickle cell disease was observed as 1.14% in Eastern UP anemic patients.

Keywords:
Hemoglobin S, PCR, DdeI, Amplicon, Restriction enzyme

Introduction:

Abnormalities of hemoglobin (hemoglobinopathies) are the most common type of inherited disease in human. These variants are usually the result of point mutations in globin genes, commonly in β gene. However, in India the most frequent and clinically significant hemoglobin structural variants are HbS, HbD and HbE. The HbS mutation, in which a glutamic acid at position 6 in the β chain is substituted for valine (Codon 6 A–>T; β^6 Glu→Val), is responsible for sickle cell disease. Sickle cell disease affects the oxygen-carrying capacity of red blood cells. Valine is a hydrophobic amino acid, while glutamic acid is a hydrophilic amino acid. So this substitution creates a hydrophobic spot on the outside of the protein structure that sticks to the hydrophobic region of an adjacent hemoglobin molecule's beta chain. This clumping together or polymerization of HbS molecules into rigid fibres causes the 'sickling' of red blood corpuscles (RBCs).

The highest frequency of HbS allele has been found 22.2% in Orissa followed by Madhya Pradesh (20%) Tamilnadu (20%), Assam (19.3%), Andhra Pradesh (18.3%) and Uttar Pradesh (9%) (Balgir, 1996). Now it is apparent that the sickle cell gene is not confined only to certain pockets of central and south India as previously postulated (Saha and Baneerji, 1973; Sharma,

Annals of Hematology & Oncology

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Short Communication

Molecular Screening of Hemoglobin D Variant in Anemia Patients of Eastern UP Population, India

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Received: January 25, 2021; **Accepted:** February 26, 2021; **Published:** March 05, 2021

Abstract

Hemoglobinopathy is the commonest inherited monogenic disorders, which are highly prevalent in India. The three most predominant hemoglobinopathies are HbS, HbE, the aim of the present study is to determine the frequency of HbD in Eastern UP population. After taking written consent, blood samples was collected from 350 individuals and genomic DNA was extracted from a the collected blood samples. PCR-RFP method was used to analyze the mutation. Out of 350 samples analyzed, one individual was heterozygous (Hb^{β^D}) and two individuals were homozygous (Hb^{β^D}) for Hb D mutation. In conclusion, the overall β^D allele frequency in Eastern Uttar Pradesh was observed as 0.71%.

Keywords: Hemoglobin D; HB D; PCR-RFLP; EcoRI

Introduction

Inherited hemoglobin disorders are important health problem in developing countries including India. The cumulative gene frequency of haemoglobinopathies in India is 4.2% [1-3]. The commonest hemoglobin variants are HbS, HbE and HbD. The incidence of hemoglobin D as a whole is relatively low in India. The average prevalence of hemoglobin D gene is around 1% [3,4]. The mutation responsible for HbD is point mutation in β-globin chain (β^{121} G-->C). The gene frequency varies between 0.1% to 3.6% in different populations of India, the highest being represented by the states of Punjab (3.65), Jammu and Kashmir (3.3%), and Uttar Pradesh (2.3%) [3]. In this study, we aimed to determine the HbD mutation in the Eastern UP state population.

Materials and Methods

The study was approved by the Institutional Ethics Committee of VBS Purvanchal University, Jaunpur, India and all participants gave their written informed consent. 2ml blood sample was collected from 350 anemic patients from three districts of Eastern Uttar Pradesh-Jaunpur, Varanasi and Allahabad. Out of 350 samples, 50 samples were of Muslims, 100 from Scheduled cast, 100 from Brahmin and 100 samples from Other Backward Caste (OBC). Genomic DNA was extracted using the standard method of Bartlett and White [5]. HbD mutation analysis was done by PCR-RFLP method. PCR was carried out using codon 121 specific PCR primers and amplicon was subsequently digested by EcoRI restriction enzymes. 2ug of template DNA, 4pM of each oligonucleotide primer (Forward: 5' CAATGTATCATGCCTCTTTGCACC 3'; Reverse: 5' 5'-GAGTCAAGGCTGAGAGATGC AGGA-3'), 250μM dNTP mix, 1.5U Taq buffer, 1 unit of Taq DNA polymerase and 0.1% Triton X 100 (Bangalore Genei Pvt. Ltd., India) in a total volume of 15 ul. The thermal cycling was carried out for denaturation of template DNA at 94°C for 1 min., primer annealing at 65°C for 1 min and primer extension at 72°C for 1 min for 30 cycles. In the last cycle, primer extension was prolonged for 3 min. The PCR products were subjected to electrophoresis using agarose (Sigma Co., USA). The purified PCR product was digested by restriction enzyme EcoRI and electrophoresed using 2% agarose gel and analyzed on a UV-trans-illuminator.

Results and Discussion

HbD (codon 121) specific primers amplified 861 bp long DNA amplicon (Figure 1). In case of normal β-globin allele, EcoRI enzyme cleave 861 bp long amplicon in to 552 and 309 bp long fragments. HbD mutation demolished EcoRI site. β^D allele remain uncut after EcoRI digestion (Figure 2). Out of 350 anemia samples, in one individual, HbD mutation was found in heterozygous (Hb^{β^D}) condition and two individuals were homozygous for HbD mutation (Figure 2). The overall β^D allele frequency in Eastern Uttar Pradesh was observed as 0.71%. Mutant homozygous (β^D/β^D) and heterozygous (β^A/β^D) genotype percentage was 0.57% and 0.28% respectively. Out of two

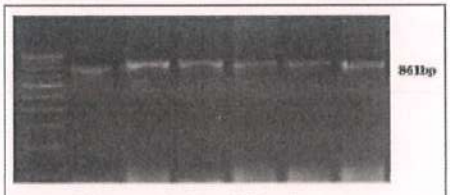

Figure 1: Gel picture showing 861bp of HbD amplicon.

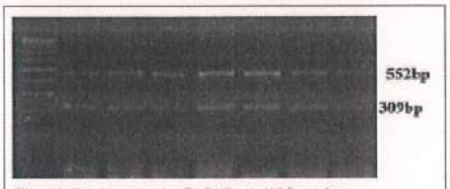

Figure 2: Gel picture showing EcoRI digested HbD amplicon.

Citation: Rai V, Yadav U, Kumar P, Mishra OP. Molecular Screening of Hemoglobin D Variant in Anemia Patients of Eastern UP Population, India. Ann Hematol Oncol 2021; 8(2): 1380.

V.B.S. Purvanchal University
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3 Biotech (2021) 11:445
https://doi.org/10.1007/s13205-021-02992-5

REVIEW ARTICLE

Cyanobacteria as biochemical energy source for the synthesis of inorganic nanoparticles, mechanism and potential applications: a review

Abhishek Kumar Bhardwaj[1] · Ram Naraian[2]

Received: 13 April 2021 / Accepted: 10 September 2021 / Published online: 23 September 2021

Abstract
Green synthesis of nanoparticles (NPs) has gained great concern among researchers due to their unique properties, excellent applications and efficient route of synthesis. From the last decades, the number biologicals such as plants, fungus, bacteria, yeast, algae, and cyanobacteria and their products are using by various researchers for the synthesis of different NPs. However, the pillar of green chemistry keeps touching new heights to improve the performance. This review paper unveils almost recent cyanobacteria-assisted greener NP synthesis technique, characterization and application. The enormous potency of cyanobacteria in NP synthesis (silver, gold, copper, zinc, palladium, titanium, cadmium sulfide, and selenium) and significance of reducing enzymes were summarized. The extracellular and intracellular entity such as metabolites, enzyme, protein, pigments in cyanobacteria play a significant role in the conversion of metal ions to metal NPs with unique properties discussed briefly. The green synthesis of nanomaterials is valuable because of their cost-effective, nontoxic and eco-friendly prospects as well as the potential application metal NPs such as antibacterial, antifungal, anticancerous, catalytic, drug delivery, bioimaging, nanopesticide, nanofertilizer, sensing properties, etc. Therefore, in the present review, we have systematically discussed the mechanisms of synthesis and applications of cyanobacteria-assisted green synthesis of NPs.

Keywords Cyanobacteria · Green synthesis · Extracellular NPs · Intracellular NPs · Application of NPs

Abbreviations

AAS	Atomic absorbance spectrometry
AFM	Atomic force microscopy
Ag	Silver
AgNPs	Silver nanoparticles
Au	Gold
BET	Brunauer–Emmett–Teller
BGA	Blue Green algae
CdS	Cadmium sulfide
CFU	Colony forming unit
C-PE	C-phycoerythrin
Cu	Copper
CuO	Copper oxide
DLS	Dynamic light scattering
DNA	Deoxyribonucleic acid
EDX	Energy-dispersive X-ray spectroscopy
EELS	Electron energy-loss spectroscopy
ESBL	Spectrum beta lactamases
FTIR	Fourier-transform infrared spectroscopy
IC-50	Inhibitory concentration
ICP-MS	Inductively coupled plasma mass spectrometry
ICP-OES	Inductively couple plasma optical emission spectrometry
MB	Methylene blue
MBC	Minimum bactericidal concentration
MIC	Minimum inhibitory concentration
NAD^+	Nicotinamide adenine dinucleotide
NMs	Nanomaterials
NPs	Nanoparticles
Pd	Palladium
Pt	Platinum
ROS	Reactive oxygen species
Se	Selenium
SEM	Scanning electron microscope
TEM	Transmission electron microscopy

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Register
V.B.S. Purvanchal University
Jaunpur

DOI: 10.1007/s12291-019-00862-9

Received: 28 March 2021 | Revised: 6 July 2021 | Accepted: 2 September 2021
DOI: 10.1002/ldr.4090

REVIEW ARTICLE

WILEY

Developing sustainable measures to restore fly-ash contaminated lands: Current challenges and future prospects

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Abstract

Land degradation is one of the major global environmental issues that need serious attention. The land itself is a complex system regulating myriads of processes. Any perturbation in these processes would undoubtedly lead to the stimulation of land degradation. Among these, fly ash (FA) dumping is one of the usual practices, which has been adopted to overcome land-use disruption and other health hazards. However, this practice has become a driving factor for FA-induced land degradation. Therefore, in purview to tackle this issue, the present article aimed to identify and suggest sustainable practices to restore and manage FA-contaminated sites. As a preliminarily it deals with the systematic exploration and identification of FA-based and associated contaminated lands via geospatial technology with a brief focus on assessing its different contaminant profiles in the FA and soil systems. Further, this moreover, the article emphasizes the need to identify identifying the potential local plant species in the FA-contaminated regions that can meet the local people's demands. Following this we suggest appropriate sustainable approaches to expedite the restoration of FA-contaminated lands and highlight the critical bottlenecks during ground implementation. Our article aimed to unravel ways to address the aforementioned bottlenecks to develop an efficient restoration enterprise during the UN Decade on Ecosystem Restoration (2021–2030).

KEYWORDS
ecological restoration, fly-ash management, land degradation, sustainable measures, UN Sustainable Development Goals

1 | INTRODUCTION

The current exploitation of fossil fuels, including coal extraction at the global level, has been underway since the Industrial Revolution. The global coal production has been raised from 3.55 billion tonnes in 1978 to 7.81 billion tonnes in 2018 (www.iea.org). Recent data on coal production by different countries is given in Figure 1. Around 40% of global electricity is derived via coal-based combustion process (Smith et al., 2013). As a result, the process leads to fly ash (FA) generation. FA total production was about 750 million tonnes per year globally in 2012 (Blissett & Rowson, 2012). The composition of FA depends on the mode and stage of coal combustion and coal quality (NRC, 2006). FA contains several types of compounds, which are hazardous to the environment and human health. It contains oxides of metals (i.e., silica, ferric, calcium, zinc, etc.) micro and macro elements (K, P, Mg, Cd, Hg, Pb, Se, As, etc.) and organic compounds such as PAHs and PCBs (Blissett & Rowson, 2012). There are also toxic heavy metals and organic pollutants. FA also possesses various radioactive elements, making it hazardous at higher levels. Therefore, utilizing the FA to reduce its toxicity extent before dumping and landfilling has been suggested. However, only about 26% of FA is used for the formation of bricks, roads, etc., in a few developing and developed nations (Blissett & Rowson, 2012). Subsequently, during its mismanaged disposal, the land gets contaminated during mismanaged FA disposal.

DOI: 10.22541/au.161778535.53589401/v1

Chemosphere 267 (2021) 128916

Contents lists available at ScienceDirect

Chemosphere

journal homepage: www.elsevier.com/locate/chemosphere

Optimization of eco-friendly novel amendments for sustainable utilization of Fly ash based on growth performance, hormones, antioxidant, and heavy metal translocation in chickpea (Cicer arietinum L.) plant

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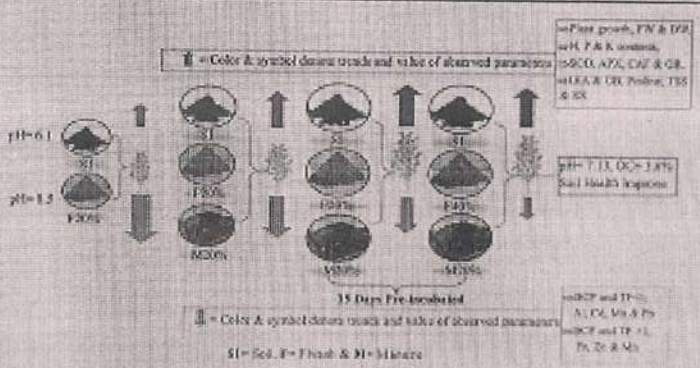
HIGHLIGHTS

- The pre-incubation and application of manure is a novel approach to utilize maximum amount of FA (40%) towards reclamation of slightly acidic soil.
- 15 days pre-incubated 40 % FA supplemented manure in acidic soil significantly enhanced the levels of FW, DW, NPK and antioxidant activities in chickpea after 60 days.
- The levels of IAA, GR, Proline, TSS and RS were copious in T15 (FA: 20%) and T16 (FA: 40%) treated combination with control after 60days.
- Toxic heavy metals present in FA exhibited less BCF and TF values under 15 days pre-incubated FA (40%) supplemented manure in acidic soil treatments.
- FA (40%) enhances growth performance of chickpea plant and promising amendment in acidic soil which could be useful for sustainable agricultural.

GRAPHICAL ABSTRACT



ARTICLE INFO

Article history:
Received 10 September 2020
Received in revised form
25 November 2020

ABSTRACT

The present study has focused on the evaluation of the maximum amount of fly ash (FA) utilization augmentation in the acidic soil (pH 6.1) with the manure during the growth performance and impact of toxic heavy metals under the pot experiment. The 15 days pre-incubated 40% FA treated combination (T16) significantly ($P < 0.05$) influenced growth performance of chickpea plant after 60 days. The dry

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https://doi.org/10.1016/j.chemosphere.2020.129216
0045-6535/© 2020 Published by Elsevier Ltd.

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DOI: 10.1016/j.chemosphere.2020.12921

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Review

Nano-Enabled Products: Challenges and Opportunities for Sustainable Agriculture

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Abstract: Nanotechnology has gained popularity in recent years owing to its established potential for application and implementation in various sectors such as medical drugs, medicine, catalysis, energy, material, and plant science. Nanoparticles (NPs) are smaller in size (1–100 nm) with a larger surface area and have many fruitful applications. The extraordinary functions of NPs are utilized in sustainable agriculture due to nano-enabled products, e.g., nano-insecticides, nano-pesticides, and nano-fertilizers. Nanoparticles have lately been suggested as an alternate method for controlling plant pests such as insects, fungi, and weeds. Several NPs exhibit antimicrobial properties considered in food packaging processes; for example, Ag-NPs are commonly used for such purposes. Apart from their antimicrobial properties, NPs such as Si, Ag, Fe, Cu, Al, Zn, ZnO, TiO_2, CeO_2, Al_2O_3, and carbon nanotubes have also been demonstrated to have negative impacts on plant growth and development. This review examines the field-use of nano-enabled products in sustainable agriculture, future perspectives, and growing environmental concerns. The remarkable information on commercialized nano-enabled products used in the agriculture and allied sectors are also provided.

Keywords: nanotechnology; nano-insecticide; nano-fertilizer; nano-pesticide; health risk; soil; plant

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Citation: Rajput, V.D.; Singh, A.; Minkina, T.; Rawat, S.; Mandzhieva, S.; Sushkova, S.; Shuvaeva, V.; Nazarenko, O.; Rajput, P.; Komaraiah et al. Nano-Enabled Products: Challenges and Opportunities for Sustainable Agriculture. *Plants* 2021, *10*, 2727. https://doi.org/10.3390/plants10122727

Academic Editor: Per Kudsk

Received: 11 November 2021
Accepted: 8 December 2021
Published: 11 December 2021

Publisher's Note: MDPI stays neutral with regard to jurisdictional claims in published maps and institutional affiliations.

1. Introduction

The world's population presently stands at almost 7.9 billion (2021), with a significant proportion residing in developing countries, especially in Asia, with approximately 50%. A large bulk of people here confront daily food shortages owing to environmental effects or political uncertainties, whereas in the industrialized world, the drive is to plant drought- and pest-resistant crops, which also boost yields [1,2]. The annual meeting of the American Physical Society was held on 29 December 1959, at the California Institute of Technology, and Richard Feynman delivered a speech entitled "There's Plenty of Room at the Bottom,

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10.3390/plants10122727

JOURNAL OF BIOMOLECULAR STRUCTURE AND DYNAMICS
https://doi.org/10.1080/07391102.2021.1988711

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Unlocking SGK1 inhibitor potential of bis-[1-N,7-N, pyrazolo tetraethoxyphthalimido{-4-(3,5-Dimethyl-4-(spiro-3-methylpyazolo)-1,7-dihydro-1H-dipyrazolo[3,4-b;4',3'-e]pyridin-8-yl)}]p-disubstituted phenyl compounds: a computational study

Abhishek Kumar Verma[a#], Sk. Faisal Ahmed[b], Md.Shahadat Hossain[b], Ali Asger Bhojiya[c], Sudhir K. Upadhyay[d#], Abhishek K. Srivastava[e], Nripendra Singh[f], Harina[a], Md. Mizanur Rahaman[g] and Newaz Mohammed Bahadur[h]

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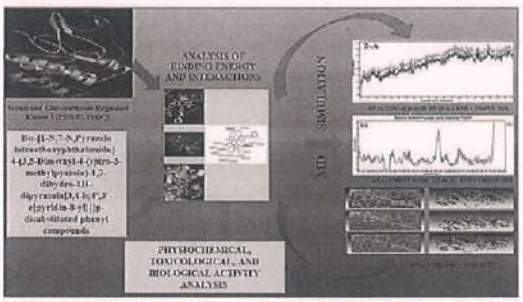
Communicated by Ramaswamy H. Sarma

ABSTRACT

SGK1 (Serum and Glucocorticoid Regulated Kinase 1), a serine/threonine kinase that is activated by various stimuli, including serum and glucocorticoids. It controls inflammation, apoptosis, hormone release, neuro-excitability and cell proliferation, all of which play an important role in cancer progression and metastasis. SGK1 was recently proposed as a potential drug target for cancer, diabetes, and neurodegenerative diseases. In this study, molecular docking, physiochemical, toxicological properties and molecular dynamic simulation of the Bis-[1-N,7-N, Pyrazolo tetraethoxyphthalimido{-4-(3,5-Dimethyl-4-(spiro-3-methylpyazolo)-1,7-dihydro-1H-dipyrazolo[3,4-b;4',3'-e]pyridin-8-yl)}]p-disubstituted phenyl compoundsand reference EMD638683 against new SGK1 target protein. Compared to the reference inhibitor EMD638683, we choose the best compounds (series 2-6) based on the binding energy (in the range from −11.0 to −10.6 kcal/mol). With the exception of compounds 2 and 6, none of the compounds posed a risk for AMES toxicity or carcinogenicity due to their toxicological properties. 100 ns MD simulation accompanied by MM/PBSA energy calculations and PCA. According to MD simulation results, the binding of compounds 3, 4 and 5 stabilizes the SGK1 structure and causes febrile conformational changes compared to EMD638683. As a result of this research, the final selected compounds 3, 4 and 5 can be used as scaffolds to develop promising SGK1 inhibitors for the treatment of related diseases such as cancer.



ARTICLE HISTORY
Received 24 June 2021
Accepted 26 September 2021

KEYWORDS
Serum/glucocorticoid-regulated kinase 1; molecular docking; MM/PBSA; molecular dynamics simulation; cancer; synthetic compounds

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Supplemental data for this article can be accessed online at http://dx.doi.org/10.1080/07391102.2021.1988711

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DOI: 10.1080/07391102.2021.1988711

JOURNAL OF BIOMOLECULAR STRUCTURE AND DYNAMICS
https://doi.org/10.1080/07391102.2021.1944911

Taylor & Francis

Molecular docking and simulation studies of flavonoid compounds against PBP-2a of methicillin-resistant *Staphylococcus aureus*

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Communicated by Ramaswamy H. Sarma

ABSTRACT

Methicillin-Resistant *Staphylococcus aureus* (MRSA), a pathogenic bacterium that causes life-threatening outbreaks such as community-onset and nosocomial infections as emerging 'superbug'. Time and motion study of its virulent property developed resistance against most of the antibiotics such as Vancomycin. Thereby, to curb this problem entails the development of new therapeutic agents. Plant-derived antimicrobial agents have recently piqued people's interest, so in this research, 186 flavonoids compound selected to unmask the best candidates that can act as potent inhibitors against the Penicillin Binding Protein-2a (PBP-2a) of MRSA. Molecular docking performed using PyRx and GOLD suite to determine the binding affinities and interactions between the phytochemicals and the PBP-2a. The selected candidates strongly interact with the different amino acid residues. The 30 ns molecular dynamics (MD) simulations with five top-ranked compounds such as Naringin, Hesperidin, Neohesperidin, Didymin and Eardin validated the docking interactions. These findings are also strongly supported by root-mean-square deviation, root-mean-square fluctuation and the radius of gyration. ADME/T analysis demonstrates that these candidates appear to be safer inhibitors. Our findings point to natural flavonoids as a promising and readily available source of adjuvant antimicrobial therapy against resistant strains in the future.

ARTICLE HISTORY
Received 4 February 2021
Accepted 14 June 2021

KEYWORDS
Penicillin Binding Protein-2a; flavonoids compounds; methicillin-resistant staphylococcus aureus; molecular docking; molecular dynamic simulation; ADME/T properties

1. Introduction

Methicillin-Resistant *Staphylococcus aureus* (MRSA) is such a notorious pathogenic bacterium causing many infections that controlling the bacterium has become a serious issue worldwide (Kuehnert et al., 2005). The high outbreak of MRSA was observed in closed communities such as schools, prisons, sports teams and the disease has mainly been transmitted from fomite to person and from person to person and so on (David et al., 2011; Kokoska et al., 2019). The pathogenicity of the bacteria includes skin and soft tissue infections, bone, joint, implant infections, pneumonia and septicemia, etc. (Monecke et al., 2011). Recent reports have indicated the emergence of multidrug-resistant *Staphylococci* against all classes of β-lactam antibiotics. The antibiotic resistance is mainly due to the expression of PC1 β-lactamase and the acquisition of the mecA gene encoding a penicillin-binding protein, PBP-2a (Bal et al., 2021; Lhanul et al., 2009). Improving the affinity of β-lactams for MRSA-specific PBP-2a has been the purpose of intensive research. Recent work on the structure of PBP-2a and potential blocking β-lactams indicates that the active site of the enzyme is closed in the resting state and thus difficult to reach with the drug. However, when the enzyme is exposed to cell wall precursors or β-lactams with appropriate pharmacophores, allosteric interactions at other portions of PBP-2a trigger the opening of the active site, providing access to the precursors or the blocking drug (Figure 1). The bacteria initially penetrate the host's immune system via epidermal and mucosal epithelia and the antimicrobial peptides play a necessary role in the host's innate immune defence against the initial colonization of bacteria (Ouhara et al., 2008).

Recent studies revealed that strains of MRSA have gained resistance to traditional antibiotics and emerged as multi-drug-resistant superbugs. Hence, there is a huge need for discovering better therapeutic agents. Many medicinal plants

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Supplemental data for this article can be accessed online at https://doi.org/10.1080/07391102.2021.1944911.

Saudi Journal of Biological Sciences 28 (2021) 4022–4028

Contents lists available at ScienceDirect

Saudi Journal of Biological Sciences

journal homepage: www.sciencedirect.com

Original article

Anti-enterococcal and anti-oxidative potential of a thermophilic cyanobacterium, *Leptolyngbya* sp. HNBGU 003

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ARTICLE INFO

Article history:
Received 10 December 2020
Revised 1 April 2021
Accepted 4 April 2021
Available online 20 April 2021

Keywords:
Diethyl ether
GC–MS
Vancomycin-resistant enterococci (VRE)

ABSTRACT

Enterococci, the opportunistic pathogens, pose several serious and life-threatening infections such as urinary tract infections, sepsis, and endocarditis. The situation is worsening due to the development of drug resistance in these pathogens against several antibiotics. The addition of anti-enterococcal compounds with antioxidant activity in fermented and packaged food may help prevent the transmission of food-borne enterococcal infections. Scientists are in continuous search of such compounds from various sources. Hence, the present study has tested the diethyl ether extracts of thermophilic cyanobacteria, selected based on a previous study, against the multidrug-resistant and -sensitive strains of *Enterococcus faecium*. Out of the eleven tested extracts, 72% have shown anti-enterococcal activity against both strains. Among the extracts with anti-enterococcal activity, the diethyl ether extract of *Leptolyngbya* sp. (DEEL-3) inhibited the growth of VRE in a dose-dependent manner with a minimum inhibitory concentration of 2.0 mg mL^{-1}. The DEEL-3 has also shown its antioxidant potential in terms of DPPH scavenging with an IC_{50} of 3.16 mg mL^{-1}. The organism was named *Leptolyngbya* sp. HNBGU 003 based on 16SrRNA sequence homology analysis and morphological features. Further, the GC–MS analysis of the DEEL-3 has revealed the predominance of two phenolic compounds, phenol, 2,4-bis(1,1-dimethylethyl)-, phosphite (3:1) and tris(2,4-di-*tert*-butylphenyl) phosphate, in it. Thus, the anti-enterococcal and antioxidant activity of DEEL-3 may be attributed to these phenolics, which may be isolated and developed as food additives.

1. Introduction

Enterococci have emerged as the third most common source of hospital-acquired bloodstream infections (Oprea and Zervos, 2007). Besides, these organisms can also cause urinary tract infections, sepsis, and endocarditis (Sood et al., 2008). More than twelve species are known to cause enterococcal infections in humans worldwide. However, *Enterococcus faecium* and *Enterococcus faecalis* are the most common species responsible for about 90–95% of enterococcal infections (García-Solache and Rice, 2019). Further, the development of multidrug resistance including vancomycin resistance has left physicians with very limited choices of antibiotics for the treatment of infections caused by *Enterococci* (Karaiskos et al., 2019). The vancomycin-resistant enterococci impose severe economic loss to society as they pose serious threats to the patients admitted in intensive care units (ICUs) as well as those with compromised immunity (MacDougall et al., 2020; Ben Braïek and Smaoui, 2019; Puchter et al., 2018). These organisms have been categorized in the high priority list of antibiotic-resistant bacteria by World Health Organization (Melese et al., 2020).

Enterococci are food-borne pathogens and can be transmitted in humans through the consumption of contaminated food materials. These organisms can colonize in both raw and fermented food products such as meat, vegetables, cheese, and sausages (Giraffa, 2002). The use of natural food additives having both anti-enterococcal and antioxidant properties in food products can easily reduce the transmission of enterococci through the food chain (Lucera et al., 2012). Microorganisms have always been the major source of novel natural products with such bioactive properties

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Peer review under responsibility of King Saud University.

Production and hosting by Elsevier

https://doi.org/10.1016/j.sjbs.2021.04.003
1319-562X/

DOI: 10.1016/j.sjbs.2021.04.00

Environmental Sustainability
https://doi.org/10.1007/s42398-020-00130-0

ORIGINAL ARTICLE

Decolourization of noxious safranin-T from waste water using *Mangifera indica* as precursor

Deepak Pathania[1,2] · Sunil Dhar[2] · Arush Sharma[3] · A. K. Srivastava[4]

Received: 7 August 2020 / Revised: 1 September 2020 / Accepted: 15 September 2020

Abstract

Bark prepared from *Mangifera indica* has been employed for eradication of safranin-T. Structural analysis of bark was attempted using Fourier-transform infrared spectroscopy (FTIR), thermogravimetric analysis (TGA), and scanning electron microscopy (SEM). The effect of several parameters was tested and optimized. The percentage adsorption of dye onto bark was found to increase with temperature and dictate endothermic adsorption. About 87% of dye removal was found at contact time of 80 min. The percentage of safranin-T dye removal increased with adsorbent dosage. Different isotherms like Langmuir, Freundlich, and Tempkin were studied to determine the adsorption mechanism. The adsorption capacity of bark was recorded to be 78.96 mg/g. Langmuir model rightly described the adsorption process with higher regression value (R^2=0.99). The experimental data was found close to using Langmuir isotherm. This confirms the monolayer adsorption of safranin-T dye onto bark. The kinetic study and intra-particle diffusion described that adsorption followed the pseudo-second-order kinetics with greater R^2 value. The study confirmed the chemical adsorption of dye onto adsorbent. The different thermodynamic processes confirmed the feasible, spontaneous and endothermic adsorption of dye using *M. indica* bark.

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Environmental Sustainability
https://doi.org/10.1007/s42398-020-00142-w

REVIEW

Advances in nanoparticles tailored lignocellulosic biochars for removal of heavy metals with special reference to cadmium (II) and chromium (VI)

Deepak Pathania[1,2] · A. K. Srivastava[3]

Received: 27 June 2020 / Revised: 10 October 2020 / Accepted: 24 October 2020

Abstract
Environmental degradation due to heavy metals has been studied worldwide due to their non-biodegradable and persistent nature. Among various heavy metals, chromium (VI) (Cr (VI)) and cadmium (Cd (II)) are toxic and enter into aquatic systems from anthropogenic activities. Therefore, considerable efforts have been made for the growth of a well-organized and cost-effective method for the removal of heavy metals. Among various methods, biosorption is cost-effective, environmentally friendly, and readily available. Biochar is porous, carboneous material produced from biomass by thermal decomposition under a limited supply of oxygen at a temperature below 900 °C. The biomass comprises mainly of 35–50% cellulose, 20–35% hemicellulose, and 10–25% lignin, extractives, and ash. These components are accountable for most of the unique properties of the biochar. Further, the conversion of biomasses into biochar depends upon feedstock, particle size, temperature, reaction time, etc. The biomass with high carbon and lignin content produces biochar with high yield. Biochar has huge affinity for pollutants due to porous arrangement and functional groups such as carboxyl, hydroxyl, and phenolic. Therefore, biochars have been modified with different materials including nanoparticles to improve the removal capacity for pollutants. The sorption efficiency of biochar was found to be improved after modification with nanoparticles. Biochar-based nanocomposite has superior physical and chemical properties that arise due to a combination of advantages of both constituent particles. Thus, the fabrication of biochar based nanomaterials has been reported for the removal of Cd (II) and Cr (VI) from aqueous systems.

Keywords Lignocellulose · Biochar · Nanocomposite · Modification · Cadmium · Chromium · Remediation

Introduction

Heavy metals have been released into the aquatic system from natural and human activities (Demirbas 2008). Heavy metals are carcinogenic and harmful to the environment and living organisms. Hence, their removal from the water has been attempted worldwide. Various methods have been reported for the eradication of toxic pollutants from the environment. However, adsorption using carbon materials has been considered as the perfect method to tackle environmental pollution due to low price, high effectiveness, and ease of operation. Number of methods such as chemical vapor deposition, carbonization, etc. have been used for the preparation of activated carbon, and carbon black (Volotskova et al. 2010; Yang et al. 2012; Jun et al. 2015; Agnieszka et al. 2020). However, drawbacks like tedious synthetic methods, complicated apparatus, high processing temperature, organic solvents, expensive fossil-fuel, etc. limit the utility of carbon materials (Titirici et al. 2012).

The lignocellulosic biomass from different naturally abundant resources have been used as potential raw material for the production of carbon with various functional moieties. In thermochemical pyrolysis process, liquid fuel (bio-oil), and solid residue called biochar is produced from biomass (Lehmann et al. 2006). The carbon of the biochar is used to increase the crop yield, diminishes the greenhouse gas emission, improves the soil quality, and decrease the

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Published online: 18 November 2020

DOI: 10.1007/s42398-020-00142-w

Chemosphere 277 (2021) 130315

Contents lists available at ScienceDirect

Chemosphere

journal homepage: www.elsevier.com/locate/chemosphere

Bio-synthesized Cu–ZnO hetro-nanostructure for catalytic degradation of organophosphate chlorpyrifos under solar illumination

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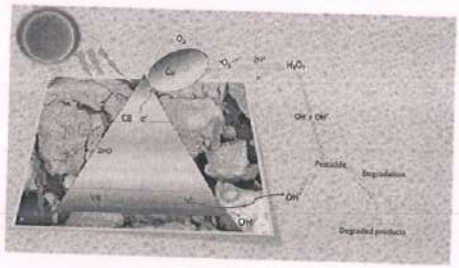
HIGHLIGHTS

- Cu–ZnO nanocomposite was prepared using leaf extract as capping agent.
- The effect of different parameters such as irradiation time, pH and catalyst dosage for the degradation of chlorpyrifos has studied in detail.
- The rate constant value for chlorpyrifos was found to be 0.0126 min^{-1} having R^2 of 0.99.
- LC-MS spectrum has also recorded indicates the absence of any toxic products.
- About 91% of chlorpyrifos was degraded at pH of 6.0.

GRAPHICAL ABSTRACT



ARTICLE INFO

Article history:
Received 7 January 2021
Received in revised form
17 February 2021
Accepted 14 March 2021
Available online 24 March 2021

Handling Editor: Derek Muir

Keywords:
Nanocomposite
Chlorpyrifos
Photodegradation
Kinetics
Characterization

ABSTRACT

In present study, a simple, effective and rapid green method using leaf extract of *Melia* azedarach was explored for the synthesis of Cu–ZnO nano heterojunction particles. The leaf extract of *Melia* azedarach acts as a reducing agent and prevents the agglomeration of nanoparticles. Different standard analytical techniques were used to study the morphology and size of synthesized nanocomposite. The efficiency of the synthesized material was tested as a photocatalyst for the degradation of simulated wastewater having chlorpyriphos pesticide. The different factors have been investigated such as pH of the solution, catalyst dosage and conact time. Approximately, 81% of chlorpyrifos was degraded after 240 min of solar illumination. The generation of hydroxyl radicals at the catalysts surface owing to photo-irradiation contributed to the chlorpyrifos degradation. The maximum photo-degradation (91%) of pesticides was observed at 6.0 pH. The pathway for the degradation of chlorpyriphos has been checked by LC-MS and this hinting the absence of any harmfull side product. The COD removal and TOC was found to be 32.4%

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https://doi.org/10.1016/j.chemosphere.2021.130315

Catalysis

Metal-Free One-Pot Synthesis of 2-(2-Hydrazinyl) Thiazole Derivatives Using Graphene Oxide in a Green Solvent and Molecular Docking Studies

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An efficient, one-pot three-component reaction in the synthesis of a wide range of 2,4-disubstituted hydrazinyl thiazole scaffolds in ethanol at room temperature has been developed by the reaction of carbonyl compounds, phenacyl bromides, and thiosemicarbazide, using graphene oxide (GO) as a catalyst. The present catalytic method has many significant advantages such as shorter reaction time, broad substrate scope, low catalyst loading, environmentally benign solvent media, easy handling, and operational simplicity at room temperature. The products are identified based on their various spectroscopic data. The GO catalyst has a high reusability rate and is simple to recover. A mechanistic study suggests that the reaction takes place *via* a thiosemicarbazone intermediate, which is isolated and confirmed in this study using spectroscopic techniques. Thereafter, a molecular docking study has been performed to evaluate the binding affinity of hydrazinyl thiazole derivative as a possible inhibitor on the protein active site of human α-amylase and glucosamine 6-phosphate synthase

Introduction

Hydrazinyl thiazoles are among the most prevalent heterocyclic scaffolds in medicinal chemistry, with a wide range of applications. Hydrazinyl thiazole and its derivative showed a remarkable pharmacological activity such as anti-tubercular,[1] antibacterial,[2] anti-allergic,[3] herbicidal activity,[4] and anti-HIV.[5] Some well-known commercially available drugs, such as Nitazoxanide (anti-infective drug), 2-(2-hydrazinyl) thiazole (anti-tubercular), 2-amino thiazole (hyperthyroidism), and Tizoxanide (anti-infective drug), include hydrazinyl thiazole as the key structural motifs (Figure 1). In addition to the pharmacological application, hydrazinyl thiazole scaffolds are widely used in a variety of technological applications, including fluorescent chemosensors,[6] organic light-emitting diode (OLED),[7] and semiconducting materials.[8]

An extensive literature review revealed that there are only two ways to achieve hydrazinyl thiazole derivatives in the laboratory. The first method employs a two-step condensation-cyclization sequence between a carbonyl function and thiosemicarbazide to yield thiosemicarbazone, which is then cyclized with α-halo carbonyl compound to produce hydrazinyl thiazole derivatives. In current literature, Reddys,[9] Mokhtary,[10] Hangirgekar,[11] Kannan,[12] Chobe,[13] Chinnaraja,[14] Bhosale,[15] and Iqbal[16] have demonstrated the rapid synthesis of the hydrazinyl thiazole motif utilizing various catalytic models.

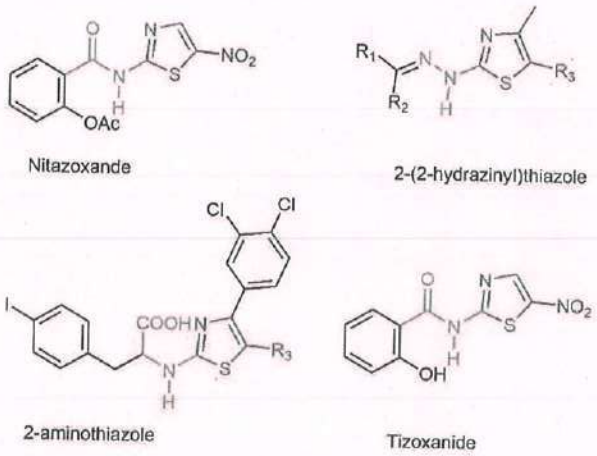

Figure 1. Representative examples of hydrazinyl thiazole derivatives as a potential drugs candidate.

Despite the improved synthetic strategy for making hydrazinyl thiazole derivatives, the process still has substantial flaws, such as harsh reaction conditions, a limited substrate range, low yield, and a long reaction time. The second literature approach, on the other hand, employs α-halo carbonyl function, thiosemicarbazide, and carbonyl compounds in a

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Supporting information for this article is available on the WWW under https://doi.org/10.1002/slct.202102642

Journal of the Indian Chemical Society 98 (2021) 100010

Contents lists available at ScienceDirect

Journal of the Indian Chemical Society

journal homepage: www.editorialmanager.com/JINCS/default.aspx

An intramolecular oxa-Michael addition on prebuilt β-lactam tethered α, β-unsaturated ester: A remarkable synthesis of a unique scaffold of 2,3-fused β-lactam-1,4-dioxepane

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ARTICLE INFO

Keywords:
1,4-Dioxepane
B-lactam
Intramolecular
Michael addition reaction
Conjugate addition
a,b-unsaturated ester
Diol
Oxy-Michael reaction

ABSTRACT

An expeditious base assisted highly diastereoselective intramolecular *oxy*-Michael addition reaction in the synthesis of enantiomerically pure 1,4-dioxepane fused β-lactam has been described. This present study has been portrayed a rapid intramolecular 7-*exo*-*trig* *oxy*-Michael reaction involving chemoselective nucleophilic addition of 2^0 alcohol of the *vic*-diols to an α β-unsaturated ester. Furthermore, the developed methodology elaborates an extremely atom-economical approach in constructing the C–O bond in stereoselective fashion under mild reaction conditions.

Saturated seven-membered *oxy*-cycles are ubiquitous structural motifs often found in a large number of bioactive natural products and a pharmaceutical agent [1,2]. The constraint ring rigidity and three dimensional (3D) spatial arrangement featuring the extended binding affinity to biological receptors, cell permeability, and enhanced bioavailability compared to other ring size system (small and macrocycles) [3]. Despite its well antique past of enriched biological activity, seven-membered ring systems is unobtrusive in drug discovery program, mainly due to the challenge related to its chemical synthesis. There have been many studies performed on the mechanistic approach to understanding the reason behind the difficulties associated with chemical synthesis; specifically, the seven-membered ring reveals that the thermodynamic and kinetic energy transition barrier is the cause of the impedance in their synthesis [4]. The ever-growing interest among the scientific community to find the molecules of therapeutic interest in a rapid and cost-effective approach is inevitable to add a newer strategy in the synthetic toolbox of organic and medicinal chemistry. The fraternity of the synthetic community in the past many decades developed many arsenals, combating the challenge in creating new bonds and functional group transformation as desired. Off course, however, plants, microbes, and marine organisms represent a chief source of natural products that are effective against various life-threatening diseases. The phyllostadimer **A 1** is an important class of compound featuring 1,4-dioxepane ring as a central structural motif and diversely substituted with phenolic aromatic ring isolated from *Phyllostachys edulis*, possess a strong inhibitory effect on ADP/Fe^{3+} induced liposomal lipid peroxidation *via* free radical scavenging and found sixteen times more effective than well-known antioxidant α-tocopherol [5]. The quinazolinone **A 2** having unprecedented spiro fused 1,4-dioxepane ring isolated from streptomyces sp. MBT 27 (actinomycete bacteria) possess an elevated level of glycerol in the biological system [6].

In the past, recent is the witness of many unnatural nucleosides having potential antiviral inhibitory properties against HIV, HSV, and tumor cell [7]. There are several deoxy nucleosides, especially prototypes with oxy-cycle, dioxyphenyl, and the prevalent structural motif as the heterocyclic counterpart. For example, dioxolane T and BCH-189 having two oxygen atoms in the ring of varying ring size Fig. 1. The extensive study reveals that the carbohydrate-based nucleoside having dioxygen in their fused ring imparts interesting biological activities, including *anti*-HIV and anti-neoplastic activities [8].

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https://doi.org/10.1016/j.jics.2021.100010
Received 18 January 2021; Accepted 24 January 2021

Asian Journal of Chemistry; Vol. 33, No. 9 (2021), 2203-2206

ASIAN JOURNAL OF CHEMISTRY

https://doi.org/10.14233/ajchem.2021.23131

Microwave-Induced Surface-Mediated Highly Efficient Regioselective Nitration of Aromatic Compounds: Effects of Penetration Depth

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Received: 13 March 2021; *Accepted*: 17 July 2021; *Published online*: 20 August 2021; AJC-20484

Surface mediated highly regioselective nitration of aromatic compounds under diverse microwave-induced conditions was investigated in this work. The effects of the penetration depth of the surfaces were found to be more crucial than other dielectric parameters. Despite significant progress of microwave-induced reactions, no reports have examined the penetration depth of the surfaces used in these processes.

Keywords: Aromatic compounds, Microwave, Penetration depth, Nitration, Catalyst.

INTRODUCTION

Syntheses of aromatic nitro compounds are important as the derivatives of these compounds can possess significant biological activities [1]. The nitro compounds needed for the synthesis of these derivatives were mainly made by the conventional nitric acid-sulfuric acid or nitronium tetrafluoroborate methods [2,3]. But these conventional methods produced a large amount of acid waste and the disposal of this acid-waste is one of the major concerns in this process. One way to avoid these complications associated with this method was to utilize the nitrating abilities of nitrate-salts under solid-phase conditions for the synthesis of the nitro compounds [4]. Nowadays extensive investigation is going on surface-mediated reactions as they are more ecologically friendly [5,6]. For instance, non-selective nitration of simple aromatic compounds was reported with sulfuric acid supported on silica gel [7]. Montmorillonite has shown considerable hope as solid support in carrying out different chemical reactions. Claycop (montmorillonite clay impregnated with anhydrous cupric nitrate) was used for aromatic nitration reaction [8]. However, a large amount of acetic anhydride was needed when claycop was used as the nitrating agent. Acetyl nitrate was the nitrating species in this case [8]. Likewise, clayfen (clay with ferric nitrate) was also used as the reagent for the nitration of estrone. However, the yields were very poor [9] and extreme precautions were needed for the preparation of these types of reagents [10].

Among the several synthesis methods, methods assisted by microwave irradiation has several advantages compared to conventional methods [11-13]. However, not all the reactions work satisfactorily with microwave irradiation. The reacting materials must have certain dielectric properties to get efficient heating during microwave irradiation. Considering all these facts, in this study we have considered the nitration of aromatic compounds under microwave irradiation with diverse solid surfaces that have different penetration depth values.

EXPERIMENTAL

Chemicals: All chemicals and solvents required to pursue this method were purchased from Aldrich Chemical Company.

Instrumentation: NMR data was recorded in Bruker and IR data was recorded in Perkin-Elmer Instruments. CEM automated microwave with frequency 2.45 GHz and power 300 W was used for irradiation.

Synthesis: The synthesis of nitro compounds by bismuth nitrate under various solid-phase conditions using microwave irradiation is shown in **Scheme-I**. The compound to be nitrated (1 mmol) and solid support were added to a suspension of bismuth nitrate (1 mmol) in THF (5 mL). The solvent was

International Journal of Electrical Engineering and Technology (IJEET)
Volume 12, Issue 7, July 2021, pp. 39-58, Article ID: IJEET_12_07_006
Available online at https://iaeme.com/Home/issue/IJEET?Volume=12&Issue=7
ISSN Print: 0976-6545 and ISSN Online: 0976-6553
https://doi.org/10.34218/IJEET.12.7.2021.006

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NERC'S APPROACH FOR MULTI-AREA DEREGULATED POWER SYSTEM UNDER DIFFERENT CONTRACT SCENARIOS

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ABSTRACT

This paper deals with performance of fuzzy logic and artificial neural network on an electrical power system. A comparison of fuzzy controller and ANN controller based approaches shows the superiority of proposed ANN based approach over fuzzy controller. This paper presents the design of a North American Reliability Council (NERC) standards BAL-001-2 based Adaptive Neuro-Fuzzy Interface System (ANFIS) controller for multi-area deregulated power system under different contract scenarios. The proposed controller is tested on the Indian regional grid system and its control performance standards are compared with the conventional PID controller and ANFIS controller. The major objectives are to find a suitable control for mitigating the diverse LFC problems in a deregulated power.

Key words: Fuzzy controller, Artificial Neural Network Controller, NERC, ANFIS Controller.

Cite this Article: Piyush Kumar Yadav, Jaya Shukla, Rajnish Bhasker, Satyam Kumar Upadhyay, NERC's Approach for Multi-area Deregulated Power System under Different Contract Scenarios, *International Journal of Electrical Engineering and Technology (IJEET)*, 12(7), 2021, pp. 39-58.
https://iaeme.com/Home/issue/IJEET?Volume=12&Issue=7

1. INTRODUNCTION

An artificial neuron is a concept whose components have a direct analogy with the biological neuron. The structure of an artificial neuron, reminds us of an analog summer-like computation. It is also called a neuron, PE (Processing Element), neurode, node, or cell [6] [11]. The signals $X_1, X_2, X_3, \ldots\ldots X_N$ are normally continuous variables but can also be discrete pulses. Each input signal flows through a gain or weight, called a synaptic weight or connection strength, whose function is analogous to that of the synaptic junction in a biological neuron. The weights can be positives (excitory) or negative (inhibitory), corresponding to "acceleration" or "inhibition," respectively of the flow of electrical signals in a biological cell. The summing node accumulates all the input weighted signals, adds the bias signal b, and then passes to the

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DOI: https://doi.org/10.17605/OSF.IO/CS9TD

International Journal of Electrical Engineering and Technology (IJEET)
Volume 12, Issue 9, September 2021, pp. 91-106, Article ID: IJEET_12_09_009
Available online at https://iaeme.com/Home/issue/IJEET?Volume=12&Issue=9
ISSN Print: 0976-6545 and ISSN Online: 0976-6553
DOI: https://doi.org/10.34218/IJEET.12.9.2021.009

PERFORMANCE ANALYSIS OF MULTI-FUNCTIONAL GRID CONNECTED CONVERTER UNDER DIFFERENT OPERATING MODES

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ABSTRACT

The increasing utilization of renewable energy sources (RESs) plays a vital role within the modern grid. The high penetration of the RESs within the electric power network results in challenges to the system's stability. This paper presents a multifunctional grid connected converter, controlled using current loop control. The multifunctional converter acts as an interface between various non-conventional sources and also the grid. The battery is employed to either supply or store power surges or transients. Multifunctional features of the converter includes active power injection, active power compensation, reactive compensation, harmonics compensation and other modes. The validity of the proposed model is verified within the real-time simulation of Typhoon HIL software.

Key words: AC micro grids, Renewable Energy Sources (RESs) Multifunctional converter Power quality, Hardware-in-the-loop simulation

Cite this Article: Vinod Kumar Yadav, Rajnish Bhasker, Satyam Kumar Upadhyay, Performance Analysis of Multi-functional Grid connected Converter Under different Operating Modes, *International Journal of Electrical Engineering and Technology (IJEET)*, 12(9), 2021, pp. 91-106.
https://iaeme.com/Home/issue/IJEET?Volume=12&Issue=9

1. INTRODUCTION

In renewable energy and storage applications that need high power density, the utilization of half-bridge converter is more preferable than the total bridge converter. Also, smart converters must be equipped with multiple functionalities [1-2]. Some advantages of this application are:

1. Converter are often operated in seven different modes using just one simple topology
2. All seven operating modes are embedded in one controller

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International Journal of Electrical Engineering and Technology (IJEET)
Volume 12, Issue 9, September 2021, pp. 145-156, Article ID: IJEET_12_09_013
Available online at https://iaeme.com/Home/issue/IJEET?Volume=12&Issue=9
ISSN Print: 0976-6545 and ISSN Online: 0976-6553
DOI: https://doi.org/10.34218/IJEET.12.9.2021.013

PERFORMANCE ENHANCEMENTS IN GRID CONNECTED PV SYSTEM WITH MODIFIED MPPT

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ABSTRACT

Renewable energy experts are doing their best to meet the world's great need for clean and sustainable energy. Using the Passive Solar Compliant Grid (GCPS) method, integrating solar energy into a grid works well. High-quality inverters are among the most innovative in the solar system. This method has been shown to be effective in extracting a multi-level inverter form, using precise predictor control. This concept is related to HV-linked PV systems that are connected to the H bridge, using the MATLAB Simulink of PV-linked PV-linked systems in the Br Bridge. of MPPT like PSO to help it tuned. It is best to eliminate THD from both gas and current. Based on the data, it appears that the improvement method improves the current and dynamic values of THD.

Key words: THD, Voltage, Current, MPPT, Inverter, Multi-Level

Cite this Article: Raina Kumari, RajnishBhaskar, Satyam Kumar Upadhyay, Performance Enhancements in Grid Connected PV System with Modified MPPT, *International Journal of Electrical Engineering and Technology (IJEET)*. 12(9), 2021, pp. 145-156.
https://iaeme.com/Home/issue/IJEET?Volume=12&Issue=9

1. INTRODUCTION

Both academics and the industry have received a lot of public and private attention in the last few decades due to the diversity of multilevel inverters compared to their traditional counterparts. To understand the aforementioned lists, it is necessary to investigate the characteristics of wave emission forms, minimal electromagnetic interference, and low filtering requirements. Following an increase in the use of renewable energy, there has been a rise in the number of cascaded multilevel inverters (CMLI). Another major advantage of their capabilities is that they are varied and obsolete, and the absence of a capacitor power measurement factor contributes to this. CMLI circuit topologies, with the exception of limited circuit measures, are used for regional expansion and are all intended for regional power expansion. Electrical inputs

International Journal of Electrical Engineering and Technology (IJEET)
Volume 12, Issue 9, September 2021, pp. 76-90, Article ID: IJEET_12_09_008
Available online at https://iaeme.com/Home/issue/IJEET?Volume=12&Issue=9
ISSN Print: 0976-6545 and ISSN Online: 0976-6553
DOI: https://doi.org/10.34218/IJEET.12.9.2021.008

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HYBRIDZATION OF SOLAR WIND RENEWABLE POWER SYSTEMS USING MODELING AND SIMULATION

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ABSTRACT

The modeling, simulation and control strategy of a hybrid power system (HPS) integrating a wind energy conversion system(WECS) and a solar photovoltaic system (SPV). The model includes wind turbine, photovoltaic panels, permanent magnet synchronous generator (PMSG), power converters and maximum power point tracking (MPPT) controllers. A supervisory control unit, designed to execute maximum power point tracking (MPPT), is introduced to maximize the simultaneous energy harvesting from overall power generation under different climatic conditions. Two contingencies are considered and categorized according to the power generation from each energy source, and the load requirement. In PV system Perturb & Observe (P&O) algorithm is used as control logic for the Maximum Power Point Tracking (MPPT) controller and Hill Climb Search (HCS) algorithm is used as MPPT control logic for the Wind power system in order to maximizing the power generated. The dynamic behavior of the proposed HPS is examined under different conditions based on wind speed variation and solar radiations. The developed HPS consists of a 50 W photovoltaic panel and 300 W wind turbine. The resultant model offers a good strategy to ensure power reliability under all conditions using renewable energies. A Simulinkmodel of the proposed Hybrid system with the MPPT controlled Boost converters and Voltage regulated Inverter for stand- alone application is developed in MATLAB.

Key words: wind, power, solar, photovoltaic, reliability, Boost converters, Voltage regulate

Cite this Article: Prashant Gautam, Jaya Shukla, Rajnish Bhasker, Satyam Kumar Upadhaya. Hybridzation of Solar Wind Renewable Power Systems Using Modeling and Simulation. *International Journal of Electrical Engineering and Technology (IJEET)*, 12(9), 2021, pp. 76-90.
https://iaeme.com/Home/issue/IJEET?Volume=12&Issue=9

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यू.एन.एस. इंस्टीट्यूट ऑफ इंजीनियरिंग एण्ड टेक्नोलॉजी
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Editor, IAEME

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V.B.S. Purvanchal University
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International Journal of Electrical Engineering and Technology (IJEET)
Volume 12, Issue 10, October 2021, pp. 41-63, Article ID: IJEET_12_10_003
Available online at https://iaeme.com/Home/issue/IJEET?Volume=12&Issue=10
ISSN Print: 0976-6545 and ISSN Online: 0976-6553
DOI: https://doi.org/10.34218/IJEET.12.10.2021.003

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A NEW APPROACH FOR SOFT SYNCHRONIZATION OF MICRO-GRID USING ROBUST CONTROL THEORY

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ABSTRACT

Today's bulk power system is massive, complex, and very dynamic. The U.S. power grid spans from coast to coast and even as far reaching as Canada. With the addition of new technologies such as renewable energies and power electronics to aid in power conversion and control, the power system grows more complex by the day. The most common approach of analyzing power system stability is through computer modeling and simulation. Due to the vast size and inaccessibility of transmission systems, real time testing can prove difficult. The motivation of this project was to design, simulate, and construct an IEEE 14 bus power system for future use in a lab setting to test, in real time, novel control techniques for various forms of generation and their impacts on the stability of the grid. This Paper presents the theory used to design and construct an IEEE 14-bus power system. A comparison of results from modeling and simulation with actual lab data obtained from the constructed test set up.

Keywords: Microgrid, IEEE 14 BUS system, DC power.

Cite this Article: Shashank yadav, Rajnish Bhasker, Saurabh V Kumar and Satyam Kumar Upadhyay, A New Approach for Soft Synchronization of Micro-Grid Using Robust Control Theory, *International Journal of Electrical Engineering and Technology (IJEET)*, 12(10), 2021, pp.41-63.
https://iaeme.com/Home/issue/IJEET?Volume=12&Issue=10

1. INTRODUNCTION

1.1 History of the Grid

In 1822, Edison lit up Pearl Street Station with the first complete electric power system. Pearl Street station was a DC system that served 59 customers in a 1.5 km radius. However, by 1866, the limitations of DC power systems became apparent. Due to high line losses due to increased currents, higher voltage levels were needed to transmit power further distances. These higher voltage levels needed were not acceptable by both generation and consumption at the time, and an easier way to transform voltages was needed. With the invention of the transformer by L. Gaulard and J.D. Gibbs in 1881, and the purchase of the idea by Westinghouse, the United States AC power system was born.

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International Journal of Electrical Engineering and Technology (IJEET)
Volume 12, Issue 10, October 2021, pp. 1-30, Article ID: IJEET_12_10_001
Available online at https://iaeme.com/Home/Issue/IJEET?Volume=12&Issue=10
ISSN Print: 0976-6545 and ISSN Online: 0976-6553
DOI: 10.34218/IJEET.12.10.2021.001

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LOAD FREQUENCY HYBRID INTELLIGENT CONTROL FOR MULTI- AREA INTERCONNECTED POWER SYSTEM

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ABSTRACT

In this research work, the power systems with, three areas and four areas hydro-thermal power system connected through tie-lines are investigated. The main purpose of system generation control is to balance the system generation against the load and losses so that the desired frequency and power interchange between neighboring systems are maintained. This dissertation is mainly focused on technical issues associated with load-frequency control (LFC)in structured power systems. The PI & PID controllers are very simple for implementation and give better dynamic response, but their performances deteriorate when the complexity in the system increases due to disturbances like load variation boiler dynamics. Therefore, there is needof a controller which can overcome this problem. The Artificial Intelligent controllers like Fuzzy and Neural control approaches are more suitable in this respect. Fuzzy system has been applied tothe load frequency control problems with rather promising results. The salient feature of these techniques is that they provide a model- free description of control systems and do not require model identification when selecting the specific number of membership function. This has some limitation of selecting membership function and defuzzification methods for unstructured power system, to overcome these above said problems Artificial Neural Network (ANN) and ANFIS controllers are introduced. These have advance adaptive control configuration. The NNs are able to monitor the system frequency as the controller issues its control command. The neural control approach is shown to have several advantages over the basic fixed parameter schemes and the more advanced adaptive control technique that have been recently developed. The proposed ANFIS controller combines the advantages of fuzzy controller as well as quick response and adaptability nature of ANN.The intelligent controllers like Fuzzy logic, ANN and Hybrid Fuzzy Neural Networkapproaches are used for Automatic Generation Control for the two areas, three area and four areas interconnected power systems. Area-1 and area-2 consist of thermal reheat power plant whereas area-3 and area-4 consist of hydro power plant with electric governor. Performance evaluation is carried out by using intelligent (ANFIS, ANN and Fuzzy) control and conventional PI & PID control approaches. To enhance the performance of controller sliding surface i.e. variable structure control is included. The three models of interconnected power

International Journal of Electrical Engineering and Technology (IJEET)
Volume 12, Issue 10, October 2021, pp. 81-96, Article ID: IJEET_12_10_006
Available online at https://iaeme.com/Home/issue/IJEET?Volume=12&Issue=10
ISSN Print: 0976-6545 and ISSN Online: 0976-6553
DOI: https://doi.org/10.34218/IJEET.12.10.2021.006

POWER MANAGEMENT SYSTEM IN MICROGRID WITH DISTRIBUTED GENERATION THROUGH OPTIMIZATION TECHNIQUES

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ABSTRACT

In addition to the solidness and force thickness, the synchronization and sharing of force between similar inverters are significant capacities to be acted in the microgrid. This undertaking figures out how to appropriate force and use controllers to restrict force and amount deviations. Voltage soundness and recurrence frequently embrace hang control with advancements intended to expand the appropriation of force (proficient and successful) of conveyed age (DG) units. Conventional hang controls can't precisely appropriate current yield and force between inverters. A modest quantity of cross breed micro grid (MG) signal examination is additionally thought. With vacillations in wind speed or sun based irradiance, the successful energy yield of circulated power age can shift significantly. In this way, the institutional sharing framework will change definitely. Amazing obtaining control is proposed to add to the adjustment of RES and MG security. The proposed control approach gives a common force intend to oversee RES adaptability and guarantee the control of the voltages and force of every DG. Eigenvalue examination and time region recreations show that under the speed of wind and sunlight based radiation, the pace of decrease of basic mode and the unique exhibition of the DG unit are essentially deferred. Because of the utilization of a solid deceleration regulator, the smooth activity and soundness of the half and half electric vehicle has been worked on under many working conditions, hence guaranteeing the steady activity of MG under sustainable power working conditions. Accordingly, molecule swarm improvement (PSO) can be an essential control procedure to lessen recurrence and force distances, diminish symphonious flows, precisely disseminate power, and take out varieties between inverters or DGs. The consequences of the control plan are confirmed in the recreation utilizing MATLAB/Simulink.

International Journal of Electrical Engineering and Technology (IJEET)
Volume 12, Issue 10, October 2021, pp. 64-72, Article ID: IJEET_12_10_004
Available online at https://iaeme.com/Home/issue/IJEET?Volume=12&Issue=10
ISSN Print: 0976-6545 and ISSN Online: 0976-6553
DOI: https://doi.org/10.34218/IJEET.12.10.2021.004

ELECTRIC SPRING UTILIZATION BY SIMULATION FOR SMART GRID STRUCTURE

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ABSTRACT

The electric spring (ES) as a versatile load request control innovation has been examined. The explanation for this is that enormous scope incorporation of sustainable power in the force framework will mess precariousness up, accordingly decreasing the force nature of the voltage power supply. The further developed control plan of the electric spring (ES) in view of the coordinated turning outline control is to give voltage guideline, dynamic force And proposals for receptive force network power remuneration, power factor revision and twisting decrease. Direct current springs (DCES) are proposed to further develop the force quality and voltage strength of DC microgrids. Circulated agreeable control is applied to various DCESs with novel geographies proposed as of late. The new DCES is made out of a DC/DC three-port converter (TPC), a two-way buck-support converter (BBC) and a battery framework, and the BBC and battery framework comprise the energy stockpiling arrangement of the DCES. Dispersed composed control of various DCES, including fundamental control and auxiliary control, is chiefly used to understand the force circulation of numerous DCES, neighborhood voltage adjustment, and the consistency between DC transport voltage and battery condition of charge (SOC). Essential voltage control, including stage shift control, decoupling control and hang control, is utilized to change the nearby voltage of each DCES. The optional control dependent on the agreement calculation, including the control of the DC transport voltage and battery SOC, can change the DC transport voltage reference to accomplish battery SOC balance between DCES. The MATLAB recreation model outcomes are given to confirm the examination.

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https://doi.org/10.17605/OSF.IO/8BCEV

International Journal of
Electrical Power System and Technology

Review Paper on Hybrid Solar Wind Renewable Power Systems

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Abstract

Solar and wind energy have increased greatly in the past few years. In this study, we proposed a hybrid energy system that combines solar panels with wind turbines to replace traditional sources of electricity, such as thermal and hydropower. Renewable energy is becoming increasingly popular as an unrealistic alternative source of electricity to traditional power generation. Electricity demand is growing every day, and non-renewable energy alone cannot be met. Renewable energy is a new option for meeting energy needs, but it is unreliable because of its probability nature. Hybrid renewable energy systems combine two or more renewable sources of energy, including wind turbines and solar systems. Hybrid renewable energy systems combine two or more renewable sources of energy, including wind turbines and solar systems. The purpose of this document is to conduct a comprehensive review of all aspects of the Commission on Human Rights. In this paper, feasibility study, optimization scale, modeling, management and reliability are discussed. The application of evolutionary technology in hybrid renewable energy is introduced. This study summarizes the whole hybrid system and has comprehensive results in determining the feasibility of the system.

Keywords: Power, hybrid photovoltaic, wind energy, Renewable energy, environmental

INTRODUCTION

Energy is the most important factor in industrial and agricultural development. The use of renewable energy technologies has increased steadily over the past few years to meet energy demand, but the main disadvantage associated with renewable energy systems is that the reliability and waste cannot be guaranteed. Imports of petroleum products are a huge waste of foreign exchange reserves.

Renewable resources are considered the best way to address these problems [2].

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Received Date:
Accepted Date:
Published Date:

Citation: Prashant Gautam, Jaya Shukla, Anurag Singh, Rajnish Bhasker. Review Paper on Hybrid Solar Wind Renewable Power Systems. International Journal of Electrical Power System and Technology. 2021; 7(1): 24-27p.

Renewable energy is becoming increasingly popular as an unrealistic alternative source of electricity to traditional power generation. Wind power has increased significantly in the past few years. A simple and cost-effective management technique is proposed to track the operating points that maximize the power supply of wind turbine systems in a changing environment.

The development of renewable energy has been improving as a result of the industrial fuel crisis, such as oil and gas. As a result, renewable energy has recently become increasingly important [7]. Other reasons include a wide range of usability, sustainability and reuse benefits. There are many renewable sources of energy, including solar,

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International Journal of Electrical Engineering and Technology (IJEET)
Volume 12, Issue 11, November 2021, pp. 26-37, Article ID: IJEET_12_11_003
Available online at https://iaeme.com/Home/issue/IJEET?Volume=12&Issue=11
ISSN Print: 0976-6545 and ISSN Online: 0976-6553
DOI: https://doi.org/10.34218/IJEET.12.11.2021.003

 Scopus Indexed

SIMULATION AND ANALYSIS OF DIFFERENT MPPT ALGORITHMS FOR PV SYSTEM

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ABSTRACT

Photovoltaic (PV) system isa renewable form of energy, using direct sunlight and converting it into electrical power PV cells which are coupled as an array to generate usable electrical energy constitute the most critical parts of this system. Electronic converters are required to transform the output of system current &voltage into an appropriate form if consider the situation of system load & its requirements. The electronic converter more typically employed is a DC-DC converter with a solar cell low voltage generating high voltage. This paper looks at the DC/DC converters & PV system with references to both cases: the first case is, The design of the system as a loop system closed in the first case because the system's scenario is dependent on an different types of algorithm separately for MPPT, that captures the sunlight higher amount to produce the highest optimized electrical power. Although the system was created with MPPT in mind, the simulation was carried out with different a controller such as P&O, PSO, Inc and fuzzy logic. The simulation& execution results for such instances are shown to demonstrate the ability of o/p voltage to return to steady-state if the input voltage impact changed. There is also evidence of a brief settling time & overshoot in the output voltage return and comparative result shown that PSO and fuzzy algorithm found accepted results means best result compassion with the existing algorithm. This optimization was carried out with the assistance of MATLAB 2018(a)

Key words: DC to DC converter, PV system, MPPT, Hill climbing (HC), Incremental Conductance (IC), P&O, PSO.

Cite this Article: Dharmendra Yadav, Maneesh Kumar Gupta and Rajnish Bhasker, Simulation and Analysis of different MPPT Algorithms for PV System, *International Journal of Electrical Engineering and Technology (IJEET)*, 12(11), 2021, pp. 26-37.
https://iaeme.com/Home/issue/IJEET?Volume=12&Issue=11

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Turkish Online Journal of Qualitative Inquiry (TOJQI)
Volume 12, Issue 7, August 2021: 10054 - 10062

Research Article

Impact of Social Media on Youth

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Abstract

Social media are those websites and applications that enable users to create and share content or to participate in social-networking. Social media is not only getting deep rooted in current society but it ia also has become an influential and irresistible tool of the modern world. At time it becomes difficult for a person to prove himself in front of people if you are not at social media. Social media has a strong association with social life of a youth. This study also focused the impact of social media on youth. For analyzing the effects of social media on students, the questionnaire study was designed and by using simple random sampling, sample of 150 students was selected from the college Parmeshwar Singh Memorial Mahavidyalaya Mathura Nagar, Anandnagar, Maharajganj (UP).

Keywords: - Social Media, Youth, Facebook, YouTube, Stress.

Impact of Social Media on Youth

Social media is a set of collective channels for online communications sources dedicated to verities of input, communication, sharing and collaboration. It is especially based on websites, applications, blogging, social networking, social bookmarking, and wikis are the different types of social media.

Social media is a collection of websites applications and other platform that enable us to share or create content and also helps us to participate in social networking. It is not only limited to blogging and sharing pictures, but there are also many vigorous tools that social media provides because it has great influence and is far-reaching. We cannot ignore the fact that social media is one of the biggest elements present in our lives today. We can get any information, talk to anyone in any corner of the world at a fast speed.

Social Media and Youth

Youth is the future of our nation. They can make or break the economy. Social media is one of the most attractive elements that exists in his life today. Social media is having a great impact on the youth, as they are the ones who are most active on social networking sites. Social media plays a big role in our lives today. Everything that is so widely expanded has both positivity and negativity. Media is everywhere. It is an inseparable part of everyone's life. Historically, newspapers were the most common of media, but today cell phones and other electronic devices have taken over all forms of communication. Young people today depend on the media for

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Bull Mater Sci (2020)43:281
https://doi.org/10.1007/s12034-020-02250-z

A facile, low temperature spray pyrolysed tungsten oxide (WO_3): an approach to antifouling coating by amalgamating scratch resistant and water repellent properties

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MS received 8 April 2020; accepted 7 September 2020

Abstract. In this study, a facile spray pyrolysed hydrophobic robust tungsten oxide (WO_3) films were deposited at an annealing temperature of 400°C on inexpensive glass substrates, using clear and homogeneous precursor solution containing tungsten hexachloride and 2-methoxyethanol. The 10 and 15 times sprayed films were polycrystalline with the monoclinic crystal structure, uniform with the submicron-sized grain morphology (size ~320–420 nm), with an average surface roughness ranging from 12 to 17 nm and transparent above 60% in the visible region with a thickness of 380 and 550 nm, respectively. Elemental existence of tungsten and oxygen was recognized on the surface of the films possessing the highest lattice oxygen percentage of 91.1. Increment in the scratch hardness of the films with the number of sprays compared to uncoated glass was identified. The films were hydrophilic in nature (water contact angle <8°), converted to hydrophobic (>120°) by treating chemically with octadecyltrichlorosilane to form a self-assembled monolayer on the top and the hydrophobicity remained same (~120°) even after a year. These films with unique and combined properties of scratch hardness and hydrophobicity can serve in the potential application as antifouling coatings.

Keywords. Spray pyrolysis; tungsten oxide; scratch hardness; hydrophobic.

1. Introduction

In marine fields worldwide, biofouling is a significant concern due to an unwanted accumulation of marine species, such as microorganisms, plants and animals on submerged surfaces [1,2]. Biofouling causes notable operational problems, such as increment in weight and decrement in the speed of the ships, frictional resistance and excess fuel consumption, causing excess emission of harmful greenhouse gases. It also has adverse effects on underwater pipelines, desalination plants and industrial equipment [3]. Tributyltin (TBT) self-polishing copolymer paints, an antifouling material, is applied widely to combat biofouling, but these paints incorporated with environmental toxic biocide materials have affected the nontarget species [2,4]. Other antifouling coatings with triphenyltin (TPT) and organotin compounds (OTC) are also recognized as biocides [3]. The usage of TBT, TPT and other tin contained materials in antifouling coatings is intensively opposed by the International Maritime Organization (IMO) and the Marine Environmental Protection Committee (MEPC) [2,3]. This opposition led to the antifouling paint industries as well as researchers to find the replacement of tin-based antifouling paints. Many alternative approaches for designing antifouling coatings, such as coatings with antimicrobial materials, micro or nanostructured surfaces, etc. are introduced, which have drawbacks in adhesion, uniformity, mechanical weakness, stability and biocompatibility [4]. Recently, superhydrophobic coatings mimicking lotus surface structure, with materials such as carbon nanotubes (CNTs) [5], polystyrene nanoparticles, etc. [6] have emerged as antifouling materials; however, these materials lacked in good mechanical stability [4].

To overcome these challenges, rare earth and transition metal oxides have appeared as an interesting class of materials due to their versatile mechanical, physical and chemical properties. Particularly, tungsten oxide (WO_3), an important transition metal oxide [7], is investigated extensively due to its unique electro-photochromic, electrocatalytic properties, high mechanical durability, excellent corrosive resistance in both acidic, basic conditions [4] and high chemical stability [8]. Phase transition behaviour of tungsten oxide is quite complex and it is highly affected by the synthesis process, initial precursors used [7]. Thin films

Electronic supplementary material: The online version of this article (https://doi.org/10.1007/s12034-020-02250-z) contains supplementary material, which is available to authorized users.

Published online: 17 October 2020

International Journal of Scientific Research in Science and Technology
Print ISSN: 2395-6011 | Online ISSN: 2395-602X (www.ijsrst.com)
© 2021 | IJSRST | Volume 8 - Issue 1

Ultrasonic Wave Propagation in Hexagonal $SrMnO_3$ Compound

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ABSTRACT
In the present study, the ultrasonic attenuation due to phonon-phonon interaction has been investigated in hexagonal $SrMnO_3$ compound. Higher order elastic constants have been computed at temperature dependent following the Lenard-Jones Potentials. Second order elastic constants are used for the determination of other ultrasonic parameters. The temperature variation of the ultrasonic velocities is evaluated along different angles with unique axis of the crystal using the second order elastic constants. Temperature variation of the thermal relaxation time and Debye average velocities is also calculated along the same orientation. The temperature dependency of the ultrasonic properties is discussed in correlation with elastic, thermal and electrical properties. It has been found that the thermal conductivity and thermal relaxation times is the main contributor to the behaviour of ultrasonic attenuation as a function of temperature and the responsible cause of attenuation is phonon-phonon interaction. The mechanical properties of $SrMnO_3$ material at low temperature (50K) are better than room temperatures because at this temperature it has low ultrasonic attenuation
Keywords: Elastic constants, Ultrasonic velocity, Ultrasonic attenuation, Thermal properties

I. INTRODUCTION

Perovskite manganese oxides, commonly represented as $AMnO_3$ (A: rare-earth alkaline earth metals), have been instrumental in condensed matter physics as well as in technical applications. Perovskite $SrMnO_3$ (SMO) is a polymorphism that has complex magnetic ordering and dielectric polarization and thus attracted a lot of attention as a multiferroic material [1, 2]. An inorganic chameleon has been inorganic chameleon because of the great flexibility of the hexagonal perovskite structure. Many different compounds take it or the corresponding structure, as the mother structure is easily deformed or diffused to the relative sizes of the ions of the compounds [3]. The hexagonal $SrMnO_3$ is antiferromagnetic below at Néel temperature. Néel temperatures is reported to be 260 K by Takeda and Ohara [4]. Hexagonal polymorphisms are semiconductors. The hexagonal $SrMnO_3$ when heated in air is stoichiometric at room temperature but loses oxygen at high temperature [5].

In the present work, we have worked diligently to make the relationship between thermo physical and microstructural properties for hexagonal $SrMnO_3$ compound. $SrMnO_3$ compound will help in understanding the mechanical behaviour of this compound and it will play an important role in the illustration of industrial applications with useful physical properties under moderate operating

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International Journal of Scientific Research in Science and Technology
Print ISSN: 2395-6011 | Online ISSN: 2395-602X (www.ijsrst.com)
© 2021 | IJSRST | Volume 8 - Issue 1

Mechanical and Thermophysical Properties of Mg3TH7 (T= Mn, Tc, Re) Complex Hydrides

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ABSTRACT

The Mg_3TH_7 (T= Mn, Tc, Re) compounds are hexagonal ternary complex hydrides. The characteristic features of high-temperature ternary complex hydrides are investigated by the theoretical evaluation of thermophysical and ultrasonic properties at room temperature using interaction potential model approach. From elastic constants calculations, it is noted that Mg_3MnH_7, Mg_3TcH7 and Mg_3ReH_7 brittle. With the help of second order elastic constants other elastic moduli, elastic stiffness constants and Poisson's ration are estimated at room temperature for elastic and mechanical characterization. The ultrasonic velocities and thermal relaxation time of these ternary complex hydrides are evaluated utilizing evaluated values of elastic constants 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 analyzed to explore the characteristic of complex hydrides compounds.

Keywords: Ternary Complex Hydrides, Elastic Properties, Ultrasonic Velocity, Thermal Relaxation Time

I. INTRODUCTION

Ternary complex transition hydrides have been considered to be very attractive candidates and have received significant attention as hydrogen storage materials. These compounds show a higher capacity for hydrogen storage in volume densities than compressed gaseous and liquid hydrogen [1]. In recent decades, research and development of new hydrogen storage materials opened up new possibilities for industrialists. On the other hand, the major challenges in solid state hydrogen storage are improved energy storage density, faster kinetics, and improved cycle life, using readily available elements at reasonable costs, with particular reference to fuel cells and rechargeable batteries [2, 3]. Matar et al. [4] have investigated the electronic structure and bonding of three different complex hydrides Mg3MnH7, Mg3ReH7 and Mg3TcH7 by the pseudo- potentials and computation of all electrons within the DFT. They have shown that both Mg3MnH7 and Mg3ReH7 have desorption energies within the range of MgH2 and are higher than those of covalent-like hydrogenated intermetallic compounds. The complex hydrides Mg3MnH7 and Mg3ReH7 compounds crystallize in hexagonal P63/mmc [5, 6].

In the present work, we have worked diligently to make the relationship between thermo physical and

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Requires Authentication Published by De Gruyter August 26, 2021

DFT study of electronic and thermodynamic properties of gold-rich intermetallic compounds, Ce_2Au_2Cd and $CeAu_4Cd_2$

Jyoti Sagar, Ramu Singh, Vijay Kumar, Sanjay Kumar, Manish P. Singh and Rishi P. Singh

From the journal International Journal of Materials Research
https://doi.org/10.1515/ijmr-2020-7955

Abstract

Gold-rich rare earth intermetallic compounds (viz. Ce_2Au_2Cd and $CeAu_4Cd_2$) show unusual magnetic and physical properties, and they have extensive applications in electronic and mechanical industries due to their good electronic and thermal behavior with high mechanical strength. In the present research article, to take full advantage of technological importance of these materials, we have investigated the structural, electronic and thermodynamic properties of Ce_2Au_2Cd and $CeAu_4Cd_2$ ternary intermetallic compounds using density functional theory (DFT). The electronic band structure and density of state calculations show that Ce-f orbital electrons provide metallic character to both the compounds with strong hybridization of Au-p and Cd-p

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AIJBSR (Annamalai International Journal of Business Studies and Research)

SOCIO- ECONOMIC EMPOWERMENT OF WOMEN IN GLOBAL ERA: WITH SPECIAL REFERENCE TO INDIA

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Vol. 13 Issue 1
Nov. 2021
PP. 69-78

Abstract

Purpose: India has the distinction of developing one of the world's longest continuing cultures, which has continuously adapted to the evolving political and socio-economic material and unique events of its history. It is often presumed that, by an unquestionable lack of work or elevated jobs, women will bear the cost of economic liberalization. but the theory of trade shows that women, particularly in emerging economies can contribute a lot due to trade liberalization and increase in foreign trade, women have proven to be a remarkable cohesive unit of the community, which in the stage of rapid societal changes has demonstrated great resilience and adaptability.

Design/ methodology/ approach: This research is qualitative in nature and based on both primary and secondary data both. Research objective and implications: The research's primary emphasis is to explore the impact of globalization in raising the socio-economic status of women and to highlight the positive as well as the negative impact of globalization on women's livelihood. This paper will be helpful for various policymakers, researchers, government bodies, and various stakeholders of the society to know the contribution of microfinance in rebooting the Indian economy by poverty alleviation.

Keywords : Women Empowerment, Gender Inequality, Globalization Trading, transnational feminism.

Introduction

Women empowerment is the process of making women educationally, mentally, physically, and economically confident. In a broader context, women's advancement applies to strengthening their role in society's power structure. The term empowerment of women basically implies that women also have the strength or ability to regulate their livelihood and raise their status in socio-economic and political terms. India has the distinction of developing one of the world's longest continuing cultures, which has continuously adapted to the evolving political and socio-economic material and unique events of its history. Globalization is indeed a trend that tends through progressive reforms of economic policy (like modernization and privatization) as well as increases in the flow of money, commodities, services, and labor. The economic model of the influence of globalization on development and well-being scarcely differentiates among genders.

In evaluating the impact of globalization on women, there are two schools of thought. The first One is essentially optimistic and with some reservations,

DOI: 10.21844/mijia.16.2.4

Biomedical & Pharmacology Journal, September 2021. Vol. 14(3), p. 1633-1645

Performance based Evaluation of Algorithmson Chronic Kidney Disease using Hybrid Ensemble Model in Machine Learning

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(Received: 07 October 2020; accepted: 03 August 2021)

In medical data science, data classification, pattern generation, data analysis and improving classification accuracy are the important issues in the recent scenario. The main objective of this research to enhanced classification accuracy by four combinations of features techniques separately with Neural Network classifier approach. The neural network is analyzed for chronic kidney disease with the help of features reduction and relevant techniques. In experiment, we used neural network as ensemble model with different features techniques as Pearson Correlation, Chi-Square, Extra Tree and Lasso regularization. In this research paper, we have prepared training model on 300(75%) instances of chronic kidney disease attributes and testing on 100 (25%) instances. We test the dataset on different applied epochs and calculated accuracy with error rate. The summary of this experiment, we used400 instances with 26 attributes of Chronic Kidney Disease and evaluated highest accuracy calculated (0.04%) with less error rate on passing several epochs by Neural Network ensemble with Lasso model.

Keywords: Correlation Features Selection Method; Extra Tree Chi-Square Epochs; Error Rate Accuracy; Features Important; Neural Network; Pearson Correlation; Variable Selection and Regularization Lasso Model.

Chronic kidney failure is not known until its function deteriorates. Kidney function can only be assessed if it is too bad, then kidney transplantation will be only one way to safe human life.

Transplantation will be only one way remains by which can be avoided in this fatal situation. Some symptoms arise when the kidney is unhealthy such as:

- Frequent nausea
- Frequent vomiting
- Loss of appetite
- Fatigue
- Excessive weakness of sleep
- Lack of sleepiness
- Frequent urination changes
- Mentally weak muscles
- Spasms, feeling of tension
- Tension, swelling of feet
- Persistent itching in the body[1].

On the basis of our previous analysis[2-5], we calculated high accuracy on the basis of ensemble method and majority of voting. The machine learning algorithm provides an environment that makes the study of the data set very easy for the analyst. Machine learning has different algorithms for different property patterns. Some algorithms describe the relationship between attributes and

https://dx.doi.org/10.13005/bpj/2264

Turkish Journal of Computer and Mathematics Education *Vol.12 No.6 (2021), 2650-2665*
Research Article

Elimination and Backward Selection of Features (P-Value Technique) In Prediction of Heart Disease by Using Machine Learning Algorithms

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Abstract:
Background: Early speculation of cardiovascular disease can help determine the lifestyle change options of high-risk patients, thereby reducing difficulties. We propose a coronary heart disease data set analysis technique to predict people's risk of danger based on people's clinically determined history. The methods introduced may be integrated into multiple uses, such for developing decision support system, developing a risk management network, and help for experts and clinical staff.
Methods: We employed the Framingham Heart study dataset, which is publicly available Kaggle, to train several machine learning classifiers such as logistic regression (LR), K-nearest neighbor (KNN), Naïve Bayes (NB), decision tree (DT), random forest (RF) and gradient boosting classifier (GBC) for disease prediction. The p-value method has been used for feature elimination, and the selected features have been incorporated for further prediction. Various thresholds are used with different classifiers to make predictions. In order to estimating the precision of the classifiers, ROC curve, confusion matrix and AUC value are considered for model verification. The performance of the six classifiers is used for comparison to predict chronic heart disease (CHD).
Results: After applying the p-value backward elimination statistical method on the 10-year CHD data set, 6 significant features were selected from 14 features with $p < 0.5$. In the performance of machine learning classifiers, GBC has the highest accuracy score, which is 87.61%.
Conclusions: Statistical methods, such as the combination of p-value backward elimination method and machine learning classifiers, thereby improving the accuracy of the classifier and shortening the running time of the machine.

Key Words: p-value technique, Statistical Method, Chronic heart disease, Confusion matrix, Machine learning, ROC, AUC.

1. Introduction

Identifying the evidence of risk factors that increase the incidence of cardiovascular illness is one of the significant achievements in the study of disease transmission in the 20th century (Einarson et al. 2018). In addition, analysts can choose to establish multivariate risk prediction calculations to help clinicians perform risk assessment. In the last 10 years, the author has proposed many risk scores (Sofi et al. 2014). These are all created for hazard assessment in a limited time of ten years or less. In order to meet this demand, some reports have introduced the whole life risks of CVD, CHD and stroke. Some experts work to calculate life span and long-opportunities in a class or class of hazardous variables (WHO 2012). Their findings emphasize the importance of the level of risk factors in early adulthood to the risk of CVD, just as CVD risk factors have a huge impact on all-cause mortality. They also pointed out that ten years of work might reduce the real dangers, especially among young people and ladies. These outcome highlight require for continuing models of CVD threat expectations that are very important for young adults and represent a competitive reason for non-CVD mortality (Singh et al. 2020). In any case, obviously, no calculation method has been proposed to measure the direct ability of 10-year CVD risk as a risk factor. The trouble of finding a long enough and thoroughly developed methodological complexity associated with integrating competing death risks into multivariate risk assessments for various reasons (Proust-Lima et al. 2016).
This exploratory article clarifies a procedure for assessing the 10-year risk of hard CVD function among people liberated from baseline conditions. Our risk scale will consider changes to the serious danger of non-CVD deaths, and will utilize standard danger factors that can be gathered during doctor visits. This process depends on the

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DOI: 10.17762/turcomat.v12i6.5765

SN Computer Science (2021) 2:67
https://doi.org/10.1007/s42979-021-00465-3

ORIGINAL RESEARCH

SN

Stacking-Based Ensemble Framework and Feature Selection Technique for the Detection of Breast Cancer

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Received: 29 April 2020 / Accepted: 9 January 2021 / Published online: 2 February 2021

Abstract
Breast cancer is the second most common cancer in women worldwide. The uncontrolled growth of breast cells is called breast cancer. The treatment of human breast cancer is a very critical process, and sometimes certain indicators may produce negative results. To avoid this misleading outcome situation, a reliable and accurate breast cancer diagnosis system must be available. The machine learning (ML) method is a modern and accurate technique that researchers have recently applied to predict and diagnose breast cancer. In this research article, we developed stack-based ensemble techniques and feature selection methods for the comprehensive performance of the algorithm and comparative analysis of breast cancer datasets with reduced attributes and all attributes. In this article, we first take the SVM, k nearest neighbors, Naive Bayes and perceptron as four ML algorithms as sub-models that have been trained and predicted from, and then combine them to make a new model called blending (stacking). Finally, logistic regression is used to predict the stacked model. It is significant that sub-models produce different results that are not correlated predictions. The stacking technique is best when all the sub-models are skillfully combined together. This article uses the five-feature selection technique because it affects the overall performance of the model. Unrelated or moderately related features may adversely affect the behavior of the model. After applying the feature selection method, now we have data set with reduced features as well as all features. We implemented logistic regression on a dataset with all features and a dataset with reduced features. Finally, we see that the dataset with reduced features has got improved accuracy.

Keywords Breast cancer · KNN · Perceptron · SVM · Naïve Bayes · Stacking · Machine learning · Feature selection

Introduction

Among women, malignant breast growth is the most well-known disease. Consistently, 2.1 million women are influenced by the illness and cause more deaths, therefore. Early finding and screening is the best way to conquer this disease [1]. AI gives an effective technique for creating intricate, robotized, and target strategies to dissect high-dimensional and multimodal clinical data. This current article's exploration centers around some cutting edge propel. Clarification in the article has been the improvement of a more inside and out understanding and speculative examination of huge issues identified with algorithmic structure and learning hypothesis. These incorporate compromises for boosting rearrangements execution, utilization of truly pragmatic limitations, and coordination of earlier information and vagueness. This investigation depicts the most recent improvements in AI, with attention on administered and unaided, which significantly affects ailment discovery and analysis. In this exploration article, stack procedures are utilized to assess calculations. Stacking is a basic strategy, like a pail of the model method, where two degrees of arrangement are utilized. The preparation informational index is partitioned into two sections A and B. The split of the preparing dataset

This article is part of the topical collection "Computational Biology and Biomedical Informatics" guest-edited by Dhruba Kr Bhattacharyya, Sushmita Mitra and Jugal Kr Kalita

Supplementary Information The online version contains supplementary material available at https://doi.org/10.1007/s42979-021-00465-3.

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https://doi.org/10.1007/s42979-021-00465-3

Prediction of Presence of Breast Cancer Disease in the Patient using Machine Learning Algorithms and SFS

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Abstract. Breast cancer disease is recognized as the common extensive malignant tumor in between women. Identification of the initial stage of malignant growth may treatment of this disease. Early treatment helps to alleviate the disease and helps anticipate its recurrence in women. Experts have used some fast checks and different medical methods or equipment to improve the accuracy of conclusions in clinical medical service management. In this article, it extensively discussed the implementation of data mining strategies to detection as well as prediction of breast malignant tumors, including random forest (RF), support vector classifier (SVC), k-nearest neighbors (KNN), linear discriminant analysis (LDA), Gradient Boosting Classifier (GBC), Decision Tree (DT) In addition, principal component analysis (PCA) to underline changes and show strong patterns in the informational index. The connection framework is likewise used to show the level of close relationship between attributes. The sequential feature selection (SFS) method is used for comparing the accuracy of a data set with all features and the accuracy of a classifier with selected features. The results show that RF_sfs, KNN_sfs, SVC_rbf and SVC_sfs have the highest and equal accuracy, which is 97.66%. They perform well and can predict the growth of harmful malignant tumors.

Keywords. Breast cancer, Machine learning, Clinical, Medical, SFS, PCA, Correlation matrix

1. Introduction

Breast malignant growth may be the deadliest disease among women. When cells in bosom tissue develop abnormally, they structure a mass of tissue called a tumor. The basic characteristics of these tumors are malignant or benign, the malignant tumors that are harmful and the benign tumors are non-cancerous. Tumors that can live with benign breasts are not dangerous and will not increase to all parts of the body. Harmful tumors are life-threatening, they can extend to different body parts, and after removal, and we often see dangerous tumors recurring anyway. Disease cells continue to divide from breast tumors and can go from side to side lymphatic veins to arrive at different body parts. It might associate with various tissues in different body parts and form into another tumor with a structure that may impede by and large limit. Some tests were performed to analyze the patients, and careful biopsies were performed where the experience activities were required. Today, the application of information mining expanded in the clinical sector [1]. The two perspectives that uphold the utilization of information mining in the welfare section that promote to avoid malignant growth, such

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DOI 10.1088/1757-899X/1099/1/012003

SN Computer Science (2021) 2:50
https://doi.org/10.1007/s42979-020-00446-y

ORIGINAL RESEARCH

An Experimental Study of Diversity of Diabetes Disease Features by Bagging and Boosting Ensemble Method with Rule Based Machine Learning Classifier Algorithms

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Received: 24 October 2020 / Accepted: 31 December 2020 / Published online: 20 January 2021

Abstract

Energy produces by blood sugar in human body. Diabetes mellitus is a condition in which human body cannot manage energy. Blood glucose, Insulin etc., and their functions become unmanaged in the glucose energy system in blood. This unbalanced system generates many dangerous diseases as like blood pressure, diabetes etc., in body. Many different recourses of energy are available in the nature. In this paper we present dataset with their pattern by box whisker plot, histograms and extract nine best features by Chi-Square and plot correlation matrix for correlation of each feature with their heat_map. We have applied rule-based classification algorithms as Decision table, OneR and JRIP on prepared dataset. In proposed work we have managed these three selected algorithms by Bagging and Boosting ensemble methods. These ensemble methods calculate Classification Accuracy, Precision, Recall and F1-Score for diabetes UCI dataset. The summary with the results, finally we concluded that the highest accuracy (98%) of Bagging Ensemble Method and the accuracy, precision, recall and f1-score of the Decision Table, OneR, Jrip and Boosting algorithms were carrying less.

Keywords Feature selection methods: Chi-square, Plot correlation matrix · Rule based classification algorithms: Decision table, OneR, JRIP · Ensemble methods: Bagging, Boosting

Introduction

The correct level of glucose is most requiring for every human body. Diabetes mellitus is divided into two parts:

- Type-1
- Type-2

Type-1

Type-1 Diabetes mellitus is known as diabetes reliant on the measure of insulin. Insulin creation relies upon the pancreas in the human body. The sort 1 diabetes mellitus insulin is not delivered by the pancreas and the invulnerable arrangement of the body is likewise incapable to stay safe, that is, it is crushed. In this diabetes mellitus, insulin is adjusted through the skin by infusion to keep insulin adjusted.

Type-2

Type-2 Diabetes mellitus cannot adjust the measure of insulin like Type-1. Some measure of insulin is delivered by the pancreas yet this amount is additionally not adequate to meet the body's prerequisite so type-2 Diabetes mellitus is known to cause insulin opposition diabetes, otherwise called cells in it are impervious to insulin.

Some symptoms of diabetes mellitus are as follows:

- Excess of thirst
- Overweight incidence
- Excess of urine
- Excessive hunger is why cells have hunger
- Excess of fatigue
- It takes longer for the wound to heal

This article is part of the topical collection "Computational Statistics" guest edited by Anish Gupta, Mike Hinchey, Vincenzo Puri, Zeev Zalevsky and Wan Abdul Rahim.

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DOI:10.1007/s42979-020-00446-y

International Journal of Big Data and Analytics in Healthcare
Volume 6 • Issue 1 • January-June 2021

Analysis of Heart Disease Using Parallel and Sequential Ensemble Methods With Feature Selection Techniques:

Heart Disease Prediction

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ABSTRACT

This paper has organized a heart disease-related dataset from UCI repository. The organized dataset describes variables correlations with class-level target variables. This experiment has analyzed the variables by different machine learning algorithms. The authors have considered prediction-based previous work and finds some machine learning algorithms did not properly work or do not cover 100% classification accuracy with overfitting, underfitting, noisy data, residual errors on base level decision tree. This research has used Pearson correlation and chi-square features selection-based algorithms for heart disease attributes correlation strength. The main objective of this research to achieved highest classification accuracy with fewer errors. So, the authors have used parallel and sequential ensemble methods to reduce above drawback in prediction. The parallel and serial ensemble methods were organized by J48 algorithm, reduced error pruning, and decision stump algorithm decision tree-based algorithms. This paper has used random forest ensemble method for parallel randomly selection in prediction and various sequential ensemble methods such as AdaBoost, Gradient Boosting, and XGBoost Meta classifiers. In this paper, the experiment divides into two parts: The first part deals with J48, reduced error pruning and decision stump and generated a random forest ensemble method. This parallel ensemble method calculated high classification accuracy 100% with low error. The second part of the experiment deals with J48, reduced error pruning, and decision stump with three sequential ensemble methods, namely AdaBoostM1, XG Boost, and Gradient Boosting. The XG Boost ensemble method calculated better results or high classification accuracy and low error compare to AdaBoostM1 and Gradient Boosting ensemble methods. The XG Boost ensemble method calculated 98.05% classification accuracy, but random forest ensemble method calculated high classification accuracy 100% with low error.

KEYWORDS

AdaBoost, Chi-Square, Decision Stump Algorithm, Gradient Boosting, J48 Algorithm, Pearson Correlation, Random Forest Classifiers, Reduced Error Pruning, XGBoost

DOI: 10.4018/IJBDAH.20210101.oa4

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DOI: 10.4018/IJBDAH.20210101.oa4

Machine learning algorithms using binary classification and multi model ensemble techniques for skin diseases prediction

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Abstract: Skin disease has more touchiness as compared to any other disease. Regular skin issues are dermatitis. The main focus of this research paper will be on dermatology database which contains different eryhemato-squamous diseases class as psoriasis, seboreic dermatitis, lichen planus, pityriasisrosea, cronic dermatitis and pityriasisrubrapilaris. Each record is a collection of 33 attributes which are linear values and one attribute of them is nominal. The 75% of the dataset utilise for demonstrating and keep down 25% for approval. The purpose of this article is to achieve the best-performing classifier that will communicate in the collection of dermatological information. Therefore, k-nearest neighbours and support vector machines are used. By using ten-fold cross validation and assess calculations utilising the accuracy metric. This is a gross metric which will prove the developed model is best one.

Keywords: eryhemato-squamous; k-nearest neighbours; KNN; classification and regression trees; CARTs; support vector machines; SVMs; ensemble methods.

Reference to this paper should be made as follows: Chaurasia, V. and Pal, S. (2020) 'Machine learning algorithms using binary classification and multi model ensemble techniques for skin diseases prediction', *Int. J. Biomedical Engineering and Technology*, Vol. 34, No. 1, pp.57–74.

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Journal of Pharmaceutical Research International

33(55B): 81-89, 2021; Article no.JPRI.77704
ISSN: 2456-9119
(Past name: British Journal of Pharmaceutical Research, Past ISSN: 2231-2919, NLM ID: 101631759)

Formulation & Evaluation of Effervescent Tablet of Verapamil Hydrochloride

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Authors' contributions

This work was carried out in collaboration between both authors. Both authors read and approved the final manuscript.

Article Information

DOI: 10.9734/JPRI/2021/v33i55B33849

Open Peer Review History:
This journal follows the Advanced Open Peer Review policy. Identity of the Reviewers, Editor(s) and additional Reviewers, peer review comments, different versions of the manuscript, comments of the editors, etc are available here: https://www.sdiarticle5.com/review-history/77704

Original Research Article

Received 05 October 2021
Accepted 11 December 2021
Published 13 December 2021

ABSTRACT

The chief aim of the present investigation is to study the Formulation & Evaluation of Effervescent Tablet of Verapamil Hydrochloride. The floating tablets of verapamil hydrochloride were prepared by direct compression technique. For each tablet formulation, drug, HPMC-K15M, karaya gum, sodium bicarbonate, and diluents were blended homogeneously for 10 min followed by addition of magnesium stearate. The total weight of each tablet was 300 mg. The amount of karaya gum used was in the range of 40–90 mg, whereas HPMC was used in the range of 20-40 mg. The powder mixture was further mixed for 5 min in a mortar. The resultant mixture was compressed into tablets using a Rimek rotary tablet machine. After preparation, the formulations were evaluated by various parameters. The friability of the tablet formulation varied between 0.3 ± 0.0063 to 0.59 ± 0.0076%. The weight variation of prepared tablet formulation complies with USP limits. The thickness was found to be in the range of 4.1 ± 0.48 to 4.2 ± 0.76 mm. The assay for drug content varied between 96.53 ± 0.36 to 102.03 ± 0.52%. The B1, B5, B6, B9, and B10 exhibited more than 75% drug release at 12 h. The B1 exhibited a maximum of 30 % drug release in the 1st hour and constant release for almost up to 12 h. B8 showed the least drug release among all other formulations; this may be due to the formation of a thick gel barrier on the tablet. Tablets were prepared by direct compression. Technological characteristics of floating tablets were within the Pharmacopoeial limit. Tablets floated for more than 8 h. Complete swelling was achieved by the end of 8 h, so percent swelling was determined at the end of 8 h for all the developed formulations.

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DOI: 10.9734/jpri/2021/v33i55B33849

JOURNAL OF BIOMOLECULAR STRUCTURE AND DYNAMICS
https://doi.org/10.1080/07391102.2021.1988711

Taylor & Francis

Unlocking SGK1 inhibitor potential of bis-[1-N,7-N, pyrazolo tetraethoxyphthalimido{-4-(3,5-Dimethyl-4-(spiro-3-methylpyazolo)-1,7-dihydro-1H-dipyrazolo[3,4-b;4′,3′-e]pyridin-8-yl)}]p-disubstituted phenyl compounds: a computational study

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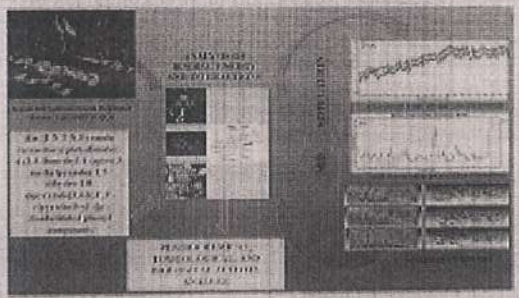
Communicated by Ramaswamy H. Sarma

ABSTRACT

SGK1 (Serum and Glucocorticoid Regulated Kinase 1), a serine/threonine kinase that is activated by various stimuli, including serum and glucocorticoids. It controls inflammation, apoptosis, hormone release, neuro-excitability and cell proliferation, all of which play an important role in cancer progression and metastasis. SGK1 was recently proposed as a potential drug target for cancer, diabetes, and neurodegenerative diseases. In this study, molecular docking, physiochemical, toxicological properties and molecular dynamic simulation of the Bis[1-N,7-N, Pyrazolo tetraethoxyphthalimido{-4-(3,5-Dimethyl-4-(spiro-3-methylpyazolo)-1,7-dihydro-1H-dipyrazolo[3,4-b;4′,3′-e]pyridin-8-yl)}]p-disubstituted phenyl compoundsand reference EMD638683 against new SGK1 target protein. Compared to the reference inhibitor EMD638683, we choose the best compounds (series 2-6) based on the binding energy (in the range from −11.0 to −10.6 kcal/mol). With the exception of compounds 2 and 6, none of the compounds posed a risk for AMES toxicity or carcinogenicity due to their toxicological properties. 100 ns MD simulation accompanied by MM/PBSA energy calculations and PCA. According to MD simulation results, the binding of compounds 3, 4 and 5 stabilizes the SGK1 structure and causes febrile conformational changes compared to EMD638683. As a result of this research, the final selected compounds 3, 4 and 5 can be used as scaffolds to develop promising SGK1 inhibitors for the treatment of related diseases such as cancer.

ARTICLE HISTORY
Received 24 June 2021
Accepted 26 September 2021

KEYWORDS
Serum/glucocorticoid-regulated kinase 1; molecular docking; MM/PBSA; molecular dynamics simulation; cancer; synthetic compounds



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Supplemental data for this article can be accessed online at https://doi.org/10.1080/07391102.2021.1988711

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https://doi.org/10.1080/07391102.2021.1988711

ISSN 0974-3618 (Print)
0974-360X (Online)
www.rjptonline.org
RJPT

RESEARCH ARTICLE

Evaluation of Anti-inflammatory Activity of Ethanolic Extract of *Populus deltoides*

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ABSTRACT:
The ethanolic leaves extract of *P.deltoides* was tested for the presence of various phytoconstituents using standard procedure and study was designed to evaluate the anti-inflammatory activity in rodents. Anti-Inflammatory activity of leaves extract of *P.deltoides* (250 and 500mg/kg) was studied in carragenin induced paw edema and cotton pellet granuloma in rat. The ethanolic leaves extract of plant revealed the presence of variety of chemical constituents like terpenoids, alkaloids, flavonoids, tannins, saponins, amino acids and glycosides. Leaves extract of *P.deltoides* significantly showed anti-Inflammatory activity in carrageenin induced paw edema by reducing paw volume in rats. From our study we concluded that leaves extract of *P.deltoides* has potential to anti-inflammatory and suggests that it can be used in the management of inflammation, thus providing a scientific basis for its traditional use.

KEYWORDS: Anti-Inflammatory, alkaloids, flavonoids, tannins, saponins, *P.deltoides*.

INTRODUCTION:

Inflammation is part of the complex biological counter stand of vascular tissues to injurious stimulus, such as pathogens, damaged cells, or irritants. The classical signs of acute inflammation are pain, heat, redness, swelling, and loss of function. Inflammation is a protective effort by the organism to remove the injurious stimulus and to initiate the healing process[1]. Inflammation is not a synonym for infection, even in cases where inflammation is caused by infection. Although infection is caused by a microorganism, inflammation is one of the responses of the organism to the pathogen. However, inflammation is a stereotyped response, and therefore it is considered as a mechanism of innate immunity as compared to adaptive immunity which is specific for each pathogen[2].

Received on 04.02.2020 Modified on 12.03.2020
Accepted on 08.04.2020
Research J. Pharm. and Tech. 2021; 14(3): 1645-1650.
DOI: 10.5958/0974-360X.2021.00292.4

Progressive destruction of the tissue would compromise the survival of the organism. However, chronic inflammation can also lead to a host of diseases, such as hay fever, periodontitis, atherosclerosis, rheumatoid arthritis, and even cancer (e.g., gallbladder carcinoma). It is the reason that inflammation is normally closely regulated by the body[3].

Causes of inflammation:

The principal cause of inflammation is a pure mechanical pressure, including blunt trauma, foreign bodies vibrations and chronic pressure of low intensity. The basic mechanism of causing inflammation by pressure is most probably through tissue hypoxia[4]. Namely, tissue oxygen as a liposoluble substance is distributed mainly in lipids and hydrophobic proteinaceous matter. Exposed to pressure, the volume of tissue water and hydrophilic components as virtually incompressible remains unchanged, while hydrophobic matter is compressed with oxygen being squeezed out. Upon cessation of pressure, due to its imperfect elasticity the tissue remains more or less shrunk and therefore with a significantly diminished oxygen content for a certain period. Concomitant vascular changes may contribute to hypoxia especially if larger blood vessels are involved. Hypoxia may then generate inflammatory changes

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Indian Journal of Natural Sciences
Vol.12 / Issue 66 / June / 2021
International Bimonthly
www.tnsroindia.org.in ©IJONS
ISSN: 0976 – 0997

RESEARCH ARTICLE

Experimental Study of Ethanolic Extract of *Populus deltoides* Leaves to Evaluate the Antipyretic Activity in Mice

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Received: 05 Mar 2021 Revised: 07 Apr 2021 Accepted: 11 May 2021

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ABSTRACT

The occurrence of different phytoconstituents in the ethanolic leaves extract of *Populus deltoides* was examined, and the analgesic effect in mice was evaluated. Brewer's yeast mediated pyrexia was used to test the antipyretic effect of ethanolic leaves extract of *P. deltoides* (250 and 500 mg/kg). *P. deltoides* leaves extract contained a wide range of chemical constituents, including alkaloids, saponins, flavanoids, terpenes, and steroids. The rats given *P. deltoides* leaves extract were compared to the control (normal saline) group and standard (Paracetamol). The yeast elevated rectal temperature was found to be significantly reduced. We concluded from our research that the leaves extract of *P. deltoides* has antipyretic potential. This research shows that it can be used in management of temperature and provides a scientific foundation for its conventional use.

Keywords: Antipyretic, Paracetamol, Flavanoid, *P. deltoides*, Brewer's yeast.

INTRODUCTION

Fever is characterized as an increase in core body temperature above normal; the average oral temperature in healthy adults is 37°C (98.6°F). A single temperature of more than 38.3°C (101°F) or three temperature readings (at least one hour apart) of more than 38.3°C (100.4° F) was considered important in oncology practice[1]. Lower temperature elevations are found rare in the very young and elderly, as well as in people taking steroids or other immune suppressants. Fever of uncertain origin (FUO) is described as a febrile fever lasting more than three weeks, with temperatures above 38.3°C on several occasions, with no conclusive diagnosis after one week of hospital assessment [2].

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DOI:10.26452/iirps.v11i4.3252

Available online at www.jmpas.com

DOI: 10.22270/jmpas.V10I3.1167

ISSN NO. 2320-7418

REVIEW ARTICLE

VASAKA - A BOON TO THE INDIAN TRADITIONAL SYSTEM OF MEDICINE

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ABSTRACT

Adhatoda vasica (L.) (Acanthaceae) has vital medicinal roles, and it is widely used in the indigenous medicine system in India. One of the important goals of the present study is to make report on the phytochemical and different in-vitro/in-vivo pharmacological activity of plant Adhatoda vasica. This study will help to find specific bioactive compounds of vasaka, and their suitable use for human welfare. The bioactive compound vasicine have been isolated from alcoholic extract of vasica leaves using column chromatography. In this review article covered all the reported pharmacological activities of vasaka plant, and their chemical constituents. In-addition; chemical constituents of vasaka has been found active against many diseases such as antimicrobial activity, hepatoprotective, antitussive, antibacterial, anti-inflammatory and antiulcer, anti-urolithiatic, abortifacient, thrombolytic, radio modulator, cardiovascular protection, hypoglycaemic, antitubercular, antioxidant and anticancer.

KEYWORDS: Adhatoda Vasica, Vasaka, phytoconstituents, pharmacological activity.

DURATION: Received- 31/05/2021, **Reviewed-** 10/06/2021, **Revised/ Accepted-** 16/06/2021

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INTRODUCTION

In the Indian medicine system, a large indefinite number of drugs from plant or mineral origin have been used in various types of diseases and their complications.[1,2] The Vasaka plant perennial, evergreen and highly branched with an unpleasant smell and bitter taste. The Vasaka plant contains stem, leaf, flower, fruit, seeds [3,4], leaves, roots, and young plants. These parts of vasaka plant having quinazoline alkaloids like vasicine, 7- hydroxyvasicine, vasicol, vasicoline, vasicinolone, 3- deoxyvasicine, vasicolinone, betaine, steroids carbohydrate, and alkanes. The flowers of A. vasica contains triterpenes (a-amirine), and flavonoids (Apigenin, astragalin, kaempferol, quercetin, vitexin [3, 5]. Adhatoda vasica, also called as Malabar nut tree. It is part of the Acanthaceae plant family. It is a common small evergreen, sub-herbaceous bush distributed all over India, mostly in the lower altitude of the Himalayas. In the Ayurvedic system of medicine, it is commonly known as ardusi. [7]

Quinazoline alkaloids like vasicine, vasicinone, and vasicinolone vasicol are present in the leaves of Vasaka. Quinazoline alkaloids having various others activities such as bronchodilator effect and expectorant. The antispasmodic effects has been found in combination with ginger (Z. officinale) and Ocimum tenuiflorum [8]. Marketed products are available in market with different names like Spirote, Kada, and Fermiforte. These all marketed products are prescribed in the treatment of respiratory disorder and leucorrhoea [9,10]. A. vasica may also be prescribed in the treatment of diseases like expectorant, antispasmodic, breathlessness, anthelmintic, bronchial antiseptic, idiopathic thrombocytopenic purpura, Antioxidant, Antibacterial, Antifungal Activity, Hepatoprotective Activity, Antiviral activity, Antidiabetes activity, Anti-tuberculosis Activity, Hepato suppression, Anticestodal activity, Immunomodulatory activity, Uterine activity, anti urolithiatic and bronchodilator in combination with other plants. Vasika has been utilized as a basic constituent in various formulations. The leaves have been exhibited diuretic activity. It is minimize the bulge in the kidney and ultimately clear urination passage. Individuals abiding from bleeding piles or diarrhea, go along with bleeding, and women enduring from polymenorrhea may take vasika juice 2 to 3 times a day for better activity [11].

Plant specifications: The different parts of A. vasica (root, leaves, and flowers) is used in the form of juice and decoction to provide relief in fever, intrinsic hemorrhage, cough, asthma, consumption, glucoma, kustha, obesity, edema, skin diseases, pradara, difficult labor, vomiting, piles, pox, retention of urine, diseases of the mouth and as Rasayana in different systems of medicine (Ayurveda, Siddha, Unani, Folk, Homeopathy, Sowa Rigpa and Chinese, Modern).

Vernacular names:

English: adhatoda

Hindi : basinga, basute, basuti, rus, rusa, vasaka Kannada: adusoge, aduthoda, alasoge, atusoge, byalada, edmuttanditappu, edumuttanditappu, yedumuttanditappu

Marathi : adulsa, arusa, bakas, vasuka, adoolsa, adoosa, baksa, adaso, adulsi, adulso,

Sanskrit: vajidanta, vajidantaka, vajidanti, vansa, vasakah, vasha, vasika, vrisha, vrishasinhamukhi, vrsa, vrsah, vrsaka

Tamil: attacaram, atutota ilai, kattumurungai, vachai

Telugu: adda saramu, adda-sarap, addasaramu, addasarapaku, atarushamu, adasaram, addasaram

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Mainstream media and Adivasi

(With Reference of Chhattisgarh)

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ABSTRACT

In 2011 census, the population of Chhattisgarh was 2 crore 55 lakh 45 thousand 198 out of which tribals are about 30 percent i.e. about 78 lakh 22 thousand 902. Tribal community has a good presence in the social and political systems of the state, but despite this, the tribal community in the state is socially and economically backward with employment, education, health as compared to other communities. According to the hypothesis of the research paper, the issues of the tribal community get relatively less prominence in the mainstream journalism or most of the issues of the tribal community find place in the mainstream media only when a major event or issue takes place. The objective of the present paper is to find out the reasons why tribal issues are being ignored by the mainstream media.

Keywords: tribals, Journalists, mainstream media, Naxal violence

INTRODUCTION

Amidst the neglect of tribal issues from the mainstream media, a big question is who will talk about the benefits of tribals in the right way, whether they are not tribals themselves or those who are tribals.

This argument should not be taken to mean that the mainstream media is being accused of any kind of bias. Due to non-representation of tribal community journalists in the mainstream media, local problems of tribals and all their big and small issues are not finding place in newspapers, channels and web media as much as issues of other community. What are the real issues of the tribals, it is very important for the journalists to understand this and this thing the journalists of the tribal community can understand in a better way and can bring those issues in front of the world in the right way.

3- Research Objectives

1-To study about the position and situation of tribal journalists working in Chhattisgarh.

2-To find out actual representation of tribal community Journalist in mainstream media of state.

3- To Study about the coverage of tribal issues in mainstream media.

4-HYPOTHESIS:

H1) Tribal issues being given less importance by mainstream media.

H2) The reason for the low importance of tribal issues by the mainstream media is being less number of tribals in the mainstream media as compare to other community.

H3). The tribal students who study journalism do not come in that proportion in the field ofjournalism.

5- Tribals ignored in journalism

To understand the neglect of tribals from the media, an article by Anil Chamdia, published in the BBC about three years ago, is enough to understand how sensitive the mainstream media is to the tribals. "On the occasion of International Tribal Day in 2018, when a press conference was held at the Constitutional Club in the country's capital New Delhi, not a single mainstream reporter came to cover

International Journal of All Research Education and Scientific Methods (IJARESM), ISSN: 2455-6211
Volume 9, Issue 2, February -2021, Impact Factor: 7.429, Available online at: www.ijaresm.com

A Study of tribal Journalists in Journalism: Problems and Prospects

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ABSTRACT

The aim of this research was to find out the real problems facing by tribal community journalists from working in Chhattisgarh state of India. Government has made various plans and schemes to up streams tribal community that's results in terms of better performance in education and jobs. If we talk about political scenario, government has reserved some seats in Parliament and legislative assemblies and Panchayati polls as well. 47 seats are reserve in lower house of parliament (Loksabha) for schedule tribes. Despite of all those things still there are various fields in which tribes are backward from other communities in India. Media is also one of them in which tribal representation is negligible in terms of numbers. This unbalance ratio makes a question of reporting of tribal issues related to their problems and other issues like education, health, accommodations because these issues can be well raised by the local journalists in front of authorities. If we look at Chhattisgarh state where approximate 30 percent population is from tribal community. In which maximum living in Maoist affected areas. Keeping all these issues it is must to find out the exact representation of tribal community in main stream Journalism of national and state level as well. Desideration in terms of cast and community stops the opportunities for marginalized people of tribal and backward area. All the fields like education, healthcare and employment and sometimes basic livelihood becomes harder to attain for tribal people. It seems that there is a need to increase in representation of tribal people in mainstream journalism to portrayed real and relatively genuine issues of tribal community because only they can better realize problems of their community and present it in front of government and administration as well. By this research proposal researcher will try to find out the reasons that why representation of local level tribal and backward class people in mainstream journalism is relatively less to others.

Keywords: tribes, Journalists, Marginalized, Tribal community.

INTRODUCTION

India is a democratic country, our constitution allows freedom of survival, getting Proper education, and getting food, religious practices and many more things and activities to every community reside in India. Schedule tribe community is relatively backward as we compare it to other General and OBC category in terms of education, job and living standards as well. If we talk about overall tribal census in India it is 8.6 percent of Indian population that is approximately 104 million in census of 2011 and 68 million in 1991 census. In India there are some states containing 30 to 90 percent population of tribal. Out of all 35 states including union territories 11 states are of big contribution of tribal in terms of total percentage of population. These states are Chhattisgarh, Odisha, Madhya Pradesh, Jharkhand, Meghalaya, Tripura, Mizoram, Manipur, Nagaland, Arunachal Pradesh, Sikkim.*

After 70 years of independence, when we are dreaming of becoming a Global guru, on the other hand a blurry picture of rural India is seen in which 65.53 percent of the people live**. Where many caste, religions and groups of people live and one of them is the tribal. According to the 2011 data of the United Nations, it is 13 percent of the total population in India, that is, about 100 million. There are 705 tribal groups residing in India which are found in abundance in Chhattisgarh, Jharkhand and Madhya Pradesh But, who represents them? Who makes their voice? Who talks about their rights? All these are big questions. We all know that Media represent the Society as a bridge to Govt and administration for their betterment in different fields. We call media as a fourth pillar of democracy it means it should represent all communities residing in India with a balanced representation in terms of coverage of different issues related to them. The question arises whether the media is doing this in real. Lot of sectors has a sufficient community wise representation in govt and private sector as well. Tribal people are doing well in different sectors of education, business, administration, armed forces, medical, engineering etc. What are the reasons that they are not having a sufficient representation in mainstream journalism?

International Journal for Research in Applied Science & Engineering Technology (IJRASET)
ISSN: 2321-9653; IC Value: 45.98; SJ Impact Factor: 7.429
Volume 9 Issue II Feb 2021- Available at www.ijraset.com

Impact of Open Defecation on Women in India

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Abstract: *Sanitation is usually a concept that deals with the disposal of liquid and solid waste, hygiene of an individual and foods they consume, household and environmental hygiene. The root cause of various health problems, particularly in rural areas of the country, is the inadequate sanitation. Most of the people still defecate in the open space, most of the villages lack waste disposal and drainage systems and many in the villages are unaware of the effects of poor sanitation and unhygienic conditions. As a result, many people suffer from diseases caused by poor personal and environmental hygiene practices and even die due to them. At present the extent of sanitation coverage in India is around 16 percent of all rural households. This figure is one of the lowest in the world, at par with countries like Niger and Afghanistan and possibly lower than Bangladesh. The absence of safe sanitation contributes significantly to the poor quality of life. In this paper, we have discussed about the overall concept of sanitation and open defecation and its impact on the lives of women all over India. Along with that various issues related to open defecation are also discussed in brief.*

Keywords: *Healthy Environment, Open defecation, Rural India, Sanitation, Women Safety.*

I. INTRODUCTION

'The day every one of us gets a toilet to use, I shall know that our country has reached the pinnacle of progresses. This quote from Pt. Jawaharlal Nehru explains a lot about the importance of sanitation, cleaning and hygiene habits for any society. Access to safe drinking water, sanitation and hygiene is the key element of the life. When it comes to sanitation, the public health problems associated with clean drinking water and proper treatment and disposal of human excreta and sewage are referenced. Preventing contact with feces, or hand washing with soap, is indeed a part of hygiene and sanitation.

Sanitation systems aim at protecting human health through a clean environment, in particular through a fecal oral route that prevents disease transmission. Diarrhea, for example, may be minimized by hygiene, a significant cause of malnutrition and the delayed development of infants. There are several other diseases that can quickly spread in environments with low rates of sanitation, including ascariasis, cholera, hepatitis, schistosomiasis and trachoma (type of intestinal worm infection or helminthiasis). Inadequate and poor quality sanitation infrastructure is the major concern for developing country.

The use of the word "sanitation" amongst countries and organizations often vary widely. Sanitation is not an easily understandable phenomenon [1]. The World Health Organization defines the term "sanitation" as follows:

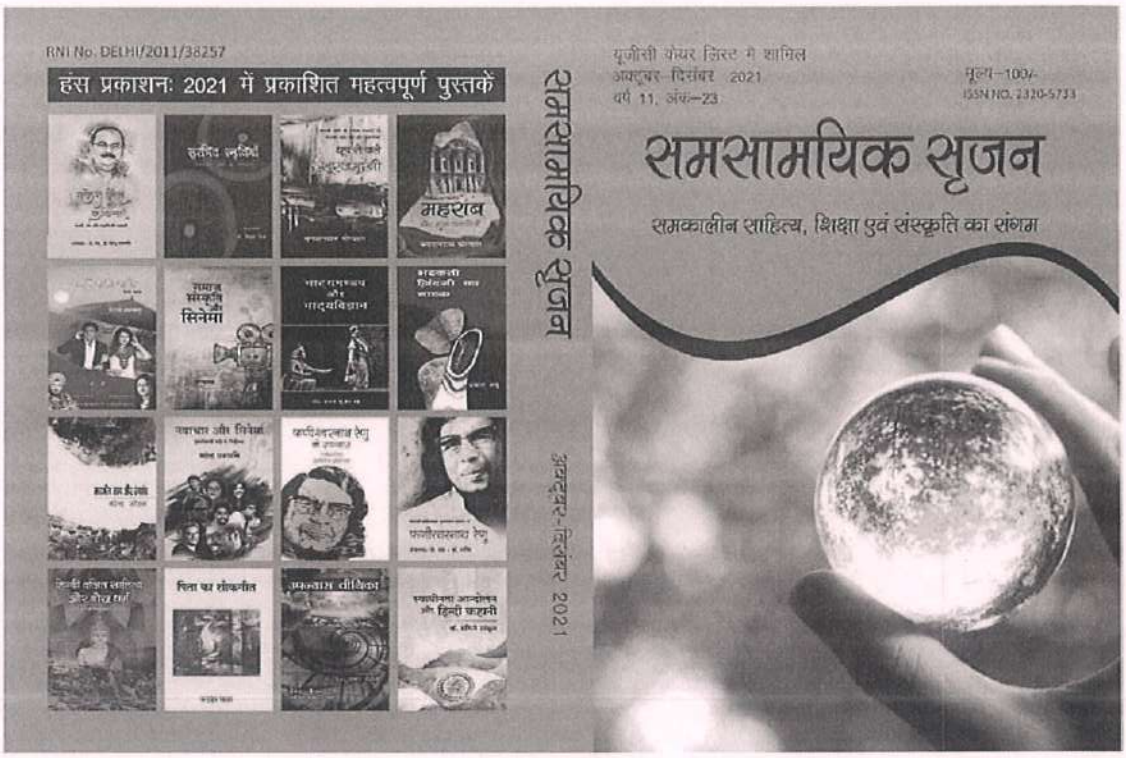
"Sanitation generally refers to the provision of facilities and services for the safe disposal of human urine and feces. The word 'sanitation' also refers to the maintenance of hygienic conditions, through services such as garbage collection and waste water disposal."[2]

All four of these technical and non-technical systems include sanitation: excreta management systems waste water management systems (which include waste water treatment plants), solid waste management systems as well as rainwater runoff systems, also known as storm water. However, many in the WASH sector only include excreta management in their definition of sanitation. The development of sanitation is considered by different people as most significant part of health and wellbeing. The Water Supply and Sanitation Collaborative Council defines sanitation as:

"The collection, transport, treatment and disposal or reuse of human excreta, domestic wastewater and solid waste, and associated hygiene promotion" [3].

Despite the fact that sanitation includes wastewater treatment, the two terms are often used side by side as "sanitation and wastewater management". Another definition is in the DFID guidance manual on water supply and sanitation programmes from 1998:

"For the purposes of this manual, the word 'sanitation' alone is taken to mean the safe management of human excreta. It therefore includes both the 'hardware' (e.g. latrines and sewers) and the 'software' (regulation, hygiene promotion) needed to reduce faecal-oral disease transmission. It encompasses too the re-use and ultimate disposal of human excreta. The term environmental sanitation is used to cover the wider concept of controlling all the factors in the physical environment which may have deleterious impacts on human health and well-being. In developing countries, it normally includes drainage, solid waste management, and vector control, in addition to the activities covered by the definition of sanitation"[4].



लोकतंत्र में मीडिया की भूमिका

डॉ. सुनील कुमार

शोध सार

लोकतंत्र में मीडिया की तीन डिमेन्शनालिटी है। पहला, सत्ताधर्म लोगों पर कड़ी नजर रखना। दूसरा, समाज को पूरे दिन की महत्वपूर्ण सामाजिक और राजनीतिक सूचनाओं पर शिक्षाप्रदीप जानकारी प्रदान करना और तीसरा, निष्पक्ष सभी को उजागर करना। इसीलिए मीडिया को लोकतंत्र का चौथा स्तम्भ कहा जाता है। इसी वजहित का सबसे और लोगों के बीच के सेतु के रूप में देखा जाता है। मीडिया एक सशक्त लोकतंत्र को आकार देने में एक महत्वपूर्ण भूमिका निभाता है। यह बुनियादी में रत रही विभिन्न सामाजिक, राजनीतिक और गतिविधियों के बारे में हमें जागरूक करता है। यह एक दर्पण की तरह जीवन के कड़वे सत्य और कठोर वास्तविकताओं को अभिव्यक्ति करता है। सभी की तरह राजनीतिक घटनाओं में भी मीडिया एक महत्वपूर्ण भूमिका निभाता है।

प्रस्तावना:

मीडिया अथवा जनसंचार माध्यम किसी भी समाज का देश की सामाजिक स्थिति के प्रतिबिंब होते हैं। देश के सामाजिक, राजनीतिक, आर्थिक और सांस्कृतिक पक्षक पर क्या कुछ घटित हो रहा है, इससे आम जनमानस मीडिया के द्वारा ही परिचित होता है। जनसंचार माध्यमों के विभिन्न रूपों ने आज मुनिया के लगभग हर कोने तक अपनी पहुँच बना रखी है। मीडिया की शक्ति का आकलन उसकी व्यापक पहुंच से किया जा सकता है। मीडिया को किसी हताती शक्तियों एवं व्यवस्था की जगह से मीडिया को देश और समाज के प्रति कई महत्वपूर्ण जिम्मेदारी भी है, इसीलिए लोकतंत्र में व्यवस्थापिका, कार्यपालिका और न्यायपालिका के बाद मीडिया को चौथा स्तम्भ माना जाता है।

सामान्यतया लोकतंत्र की तीन विशेषताएँ होती हैं – जनता का प्रतिनिधित्व, जनता के हितों का संरक्षण तथा जनता के प्रति उत्तरदायित्व। व्यवस्थापिका जनता का प्रतिनिधित्व करती है। किंतु जनता के जागरूक न रहने पर ऐसे व्यक्तियों का चुनाव कर सकती है, जो कुर्सी से जनता के हितों की बात करते हों किंतु सत्ता में अपने लाभ के लिये चुनाव लड़ रहे हों। जनता अशिक्षित होकर भी किसी बाहुबली या अपराधी का चुनाव करने को विवश हो सकती है। जनता को अपने हितों को समझना भी जरूरी है। अशिक्षित आर्थिक और सामाजिक संरचना में जनता को सकीर्ण जातिगत या क्षेत्रीय हितों के विरुद्ध राष्ट्रीय अथवा सम्पूर्ण समाज के विशाल हितों के बीच अंतर करना होता है और संसद कोई भी गलत निर्णय जटिल समस्याएँ खड़ी कर देता है। इस प्रकार सशक्त लोकमत का निर्माण आवश्यक हो जाता है। लोकमत के निर्माण में मीडिया की भूमिका सार्थक संवाद और महत्वपूर्ण होती है।

मीडिया से तात्पर्य जनसंचार के माध्यमों–समाचार पत्रों, पत्रिकाओं, रेडियो, टेलीविजन तथा सम्बन्धित से है। समाचार-पत्र विभिन्न घटनाओं, समस्याओं एवं विचारों के संबंध में जनता को सूचना प्रदान करने का कार्य करते हैं और साधारणतया समाचार-पत्रों में प्रकाशित सामाजिक, आर्थिक–राजनीतिक और अंतर्राष्ट्रीय सूचनाओं के आधार पर ही जन–साधारण सार्वजनिक क्षेत्र से सम्बंधित विभिन्न पहलुओं पर अपने विचार का निर्माण करता है। इसकी अतिरिक्त, प्रत्येक समाचार पत्र के सम्पादकीय अंश द्वारा पाठकों के विचारों को प्रभावित रूप से प्रभावित करने का कार्य किया जाता है।

शोध का उद्देश्य –

प्रस्तुत शोध का मुख्य उद्देश्य लोकतंत्र में मीडिया की भूमिका को आकलन करना है।

शोध की पद्धतियां–

प्रस्तुत शोध 'लोकतंत्र में मीडिया की भूमिका' के अध्ययन में निम्नलिखित शोध की पद्धतियां प्रयोग की गई है।

शोध प्रस्ताव– शोध की प्रस्तावना विश्लेषणात्मक है।

शोध प्रविधि– इस शोध को पूरा करने में आवश्यक विश्लेषण प्रविधि का प्रयोग किया गया है। इस शोध कार्य में ऐतिहासिक अभिलेखों का प्रयोग किया गया है।

विश्लेषण:

समाचार-पत्र जनता की बात को शासन तक और शासन संबंधी तथ्यों को जनता तक पहुँचाने का काम करते हैं। विश्व के प्रसार के साथ ही सार्वजनिक क्षेत्र की गतिविधियों पर जनता नजर रखना चाहती है और समाचार-पत्र इसके लिए भरपूर सूचना सामग्री जनता तक पहुँचाते हैं। सामाजिक, पत्रिका और साहित्यिक पत्रिकाओं में राजनीतिक जीवन और सामाजिक–आर्थिक विषयों का विस्तृत विवेचन होता है जिसे पढ़कर जनता लोकतांत्रिक प्रक्रिया में अभिरुचिक भागदारी ग्रहण करती है।

जहाँ तक समाचार पत्रों का सवाल है, तो इन्होंने शुरू से ही मानव के दृष्टिकोण एवं विचारों को प्रभावित किया है। दुनिया के समाज देशों में हुई सामाजिक एवं राजनीतिक क्रांतियों के अलावा भारत के स्वतंत्रता संघर्ष में समाचार-पत्रों ने अभूतपूर्व भूमिका निभाई। पुनर्जागरण के अग्रदूत और भारतीय पत्रकारिता के जनक, राजाराम मोहनराय सहित अन्य सुधारकों ने भी अपने सुधार कार्यक्रमों को विस्तार देने तथा उसे जन–जन तक पहुंचाने के लिए समाचार-पत्रों को माध्यम बनाया। इसके अलावा लोकमान्य बाल गंगाधर तिलक ने 'मराठा' एवं 'केसरी', सुरेन्द्रनाथ बनर्जी ने 'बंगाली', मोतीलाल घोष ने 'अमृत बाजार पत्रिका', लाला लाजपत राय ने 'यंग इंडिया', अरविंद घोष ने एवं महात्मा गांधी ने 'यंग इंडिया' एवं 'हरिजन' के माध्यम से तथा अन्य महान नेताओं ने विभिन्न भाषाई समाचार-पत्रों के माध्यम से ब्रिटिश शासन

Social Media Influencers or Influenza?

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**Dr Digvijay Singh Rathor

1. INTRODUCTION

Social media as we all know are the platforms which allow the users to connect with each other and share pictures, videos, thoughts or any other content and participate in social networking. With the digital era, everyone makes great use of social media to share news, information about subjects that matter to them. Social media not only helps people to share their personal thoughts or updates about life, but it also allows various business entities to connect with their customers and create awareness about the products they sell or the services that they provide. With this brand awareness the business houses easily boost their sales. Over the last decade we have seen social media grow rapidly in importance. According to a 'we are social' report dated January 2019, 3.484 billion people actively are using social media – this number constitutes to 45% of the world's population. But is social media just about sharing our daily life updates or to connect with our kith and kin? No, with the digital era and everything getting digitalized, social media is just not limited till connecting people. Users look forward to a lot of information about news, fashion, politics, sports, memes and a lot more on social media. But with all this comes another interesting use of social media which is the promotion and brand awareness done by the companies for their products or services.

Social media marketing (SMM) is the use of social media platforms and social networks to advertise the goods and services of a business. Social network marketing offers businesses with the means to attract potential consumers, connect current customers and encourage their preferred culture, mission or sound. Often known as "digital marketing" and "e-marketing," social media marketing has purpose-built data analytics tools that allow marketers to monitor how effective their efforts are. Social networking platforms enable advertisers to use a wide variety of techniques and methods to encourage and engage with content. Many social networks encourage users to provide comprehensive geographic, demographic and personal information that would allow advertisers to customise their content to what is most likely to resonate with users. Since Internet viewers can be better segmented than more conventional media platforms, marketers can ensure that they spend their efforts on the demographic they want to attract. Although social media marketing may offer advantages, it can also build challenges that businesses would not have had to contend with otherwise. For example, a viral video alleging that a company's product

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Register
V.B.S. Purvanchal University
Jaunpur

ISSN - 2229-3620
UGC CARE LISTED JOURNAL
NIS
SHODH SANCHAR Bulletin
January-March, 2021
Vol. 11, Issue 41
Page Nos. 67-71
AN INTERNATIONAL BILINGUAL PEER REVIEWED REFEREED RESEARCH JOURNAL

RELATIONSHIP BETWEEN DISPOSITIONAL MINDFULNESS AND PSYCHOLOGICAL WELL-BEING AMONG ADULTS

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ABSTRACT

Mindfulness refers to the process of paying a specific level of attention to moment-to-moment experience (Kabat-Zinn, 1990). Few have disposition to Mindfulness. The aim of the present study was to find out the relationship between dispositional mindfulness and psychological Well-Being among early adults in Hindi speaking states of India between the ages of 18-25 years. A total of 500 adults were included in the study who filled questionnaire online. Our findings indicate that dispositional mindfulness is positively associated with psychological well-being, and its different dimensions given by Carol Ryff.

Keywords : Dispositional Mindfulness, Psychological Well-Being, Adults

For the maintenance and promotion of well-being, many, psychological, philosophical & spiritual traditions highlight the relevance of awareness quality (Wilber, 2000). Still the concept of being mindful or benefits of staying focus in present is less explored. Mindfulness is the ability of an individual to remain focused in present situation without judging or weighing it as wrong or right.

Glomb, Duffy, Bono, and Yang (2011) defined mindfulness as "a state of consciousness characterized by receptive attention to and awareness of present events and experiences, without evaluation, judgment, and cognitive filters" (p. 119).

Mindfulness is age old technique in Buddhism which has immense importance in present day life. Practicing mindfulness is not related to Buddhism, but it focus on peaceful and harmonious relation with oneself and with everything in the world, It emphasise on exploring who we are, questioning our perspective of the outside world and our relation with place in it, and creating a sense of gratitude for each and every moment we are living (Kabat-Zinn, J. (1994). On the other hand mindlessness is absence of awareness, such as when anybody refuses to recognize or focus to a thought, feeling, purpose, emotion or on an object (Brown & Ryan, 2003).

Several studies have supported that being mindful leads to better mental functioning and enhance psychological wellbeing. Depression, anxiety, and psychological wellbeing were all highly linked to mindfulness and certain of its aspects (Brown & Ryan, 2003).

A lot of clinical psychology studies used mindfulness to investigate a variety of psychological problems. Research on Mindfulness, has been shown to be linked with enhanced self-esteem, successful self-regulation, emotional stability, including decreased reaction to emotional stimuli (Brown & Ryan, 2003; Giluk, 2009; Masicampo & Baumeister, 2007; Rasmussen & Pidgeon, 2011).

Psychological well-being (PWB) can be defined as "a generalised feeling of happiness" (Schmutte and Ryff, 1997, p. 551). Ryff (1997) has defined it as "progressions of continued growth across the life course" (p. 99). He gave a six factor model of PWB which are

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Turkish Online Journal of Qualitative Inquiry (TOJQI)
Volume 12, Issue 7, July 2021: 10033 - 10043

Research Article

Validation of the Factor Structure of Acceptance and Action Questionnaire-II (AAQ-II) in the Indian Context

Anna Tyagi[1] and Alpna Agarwal[2]

Abstract

Psychological inflexibility, is the rigid dominance of psychological reactions over chosen values, in guiding action. It as a faulty self-regulation process linked to poor mindfulness, avoidance of certain inner experiences, and a lack of clarity and commitment to personal ideals which results in mental health issues. The Acceptance and Action Questionnaire-II (AAQ-II) is a broadly used measure of psychological inflexibility. The present study aims to validate AAQ-II in Indian context and then evaluate its psychometric properties and factor structure. In this study, 7 items of the AAQ-II, developed by Bond et al. (2011), were translated in the Hindi language and adopted in the Indian context. A total of 1000 Hindi speaking adults (18 above) from different Hindi speaking states were included in the study. An Exploratory Factor Analysis and a Confirmatory Factor Analysis were performed to test the factorial structure of the AAQ-II, and the internal consistency of the scale was studied. The result supported the scale's unidimensionality. The obtained Cronbach's alpha revealed satisfactory internal consistency with a value of 0.84. Based on the psychometric properties obtained, it is concluded that AAQ-II is a reliable measure to assess psychological inflexibility among adults in India.

Keywords: Acceptance and Action Questionnaire-II (AAQ-II), Indian Adaptation, Exploratory Factor Analysis, Confirmatory factor analysis

There is a large and growing Body of Evidence that the mental health and behavioural performances of an individual depends more on how they deal with their thoughts and feelings. If they have rigidity that is in-flexibility in their thoughts it results in several psychological issues and on the other hand if they are flexible in their thinking pattern it results in less distress.

Psychological flexibility is the ability to be aware of and accept one's actual state without attempting to avoid or manage negative events is referred to as psychological flexibility. (Mc Cracken & Vowels, 2007; Hayes et al., 2006)It is a broad term that encompasses a variety of dynamic processes that take place over time. This can be seen in how a person (1) adjusts to changing situational demands, (2) re-allocate mental energy (3) transforms viewpoint, and (4) manages conflicting interests, desires, and life domains. Rather than focusing on particular content

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Original Research Article

Study of Inter-Relationship Between Perceived Workplace Discrimination, Job Stress, Mental Well-Being, And Job Performance of Teachers

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ABSTRACT

Background: This study was planned to investigate the consequences of perceived workplace discrimination on job stress, mental well-being, and teachers' job performance in higher education. A conceptual model was proposed to illustrate the relationship between the study variables.
Methodology: A correlational research design was adopted, and convenience sampling was used for data collection of 200 teachers. The participants of this study represented different streams of science and arts and were asked to fill questionnaires to collect relevant information on the subject matter.
Results: Results show that (a) workplace discrimination is significantly positively related to perceived job stress, negatively related to mental well-being and overall job performance. Further, stepwise regression analysis shows that perceived job stress, job tenure, and workplace discrimination explain significant contributions (job stress emerged as best predictors of job performance) to the job performance of teachers and while job stress and gender explain significant contributions (job stress again emerged as best predictors of mental well-being) to the mental well-being of teachers. Results have been discussed in light of previous studies.

Keywords: Workplace Discrimination, Perceived Job Stress, Mental Well-Being, Job Performance.

(Paper received – 28th August 2021, Peer review completed – 15th September 2021)
(Accepted – 28th September 2021)

INTRODUCTION

The workplace is still a venue for discrimination
Unknown

Workplace discrimination is a persistent problem worldwide, despite legislation designed to prohibit and discourage these practices. According to the Equal Employment Opportunity Commission, 33,937 charges of race-based workplace discrimination, 24,582 age-based, 28,372 sex-based, and 10,601 charges related to national origin were filed in the 2008 fiscal year [1]. These U.S. estimates mark a record high informal complaint and a 15% increase over those filed in 2007 [1].
However, these statistics likely underestimate such occurrences because minority group members often minimize these experiences [2] and are notably reluctant to file formal charges [3]. Workplace discrimination can range from the systematic denial of people's rights based on their gender, sexual orientation, religion, ethnicity, age or other criteria to more informal verbal abuse that orient such characteristics. In general,

ANVESAK
ISSN : 0378 – 4568
UGC Care Group 1 Journal

COLLECTIVE ACTIONS, SOCIAL DISTANCING AND BELIEF IN SCIENCE IN THE AGE OF COVID-19: A CORRELATIONAL STUDY

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ABSTRACT

The purpose of the study was to investigate the patterns of relationships between collective actions, social distancing and belief in science among general population in India. The study was conducted on a sample of N=235 (167 male and 68 female) general population in India. Participants' responses were obtained on questionnaires, which measured collective actions, social distancing and belief in science. Results indicated that collective actions were significantly, positively correlated with their belief in science and collective actions significantly, positively predicted 6.1 percent of variance in belief in science. Findings also showed that social distancing was significantly, positively correlated with their belief in science and social distancing significantly, positively predicted 17.6 percent of variance in belief in science among general population in India.

Keywords: *Collective Actions, Social Distancing, Belief in Science*

Introduction

Collective Actions, Social Distancing and Belief in Science

Moreover, this millennium has already suffered three pandemics (Namely Swine Flu in 2009, Middle East Respiratory Syndrome (MERS), Severe Acute Respiratory Syndrome (SARS)) and Covid-19 may not be the last. Yet, the global community has failed to develop a comprehensive, concerted plan of action, to combat this terror. Global war against the virus will require much more global collective efforts. This is because, as long as the virus is alive in some corner of the world, it can strike back and turn into a pandemic again. Further, national shutdowns have saved lives from the assault of Covid-19, but it poses the risk of losing lives to starvation and malnutrition, somewhere in the world if adequate steps were not taken. However, global collective action has been until now remained inadequate. Speaking of focus –east, west, north and south – COVID-19 has dominated and is dominating conversations at all levels of society. The trickle-down effect from high and inter-governmental dialogue to finding medical, economic and social solutions is being discussed by family and friends as well.

As the COVID-19 outbreak in India enters the community transmission phase, the country needs to introduce community-wide steps to increase physical distancing, government and media should clearly, transparently and regularly communicate the risks, health advice and response measures, including postponing gatherings and curtailing movement; as well as a continuation of essential health services and socioeconomic support for those in need, especially the most vulnerable. Again we would expect to see people in situation COLLECTIVE ACTIONS to get block or lessen virus spreads through destroy or kill them using hand sanitizers and face mask.

In the month of March, the Prime Minister had addressed the nations twice-on March 19 and

Original Research Article

Impact of psychological distress due to COVID-19 pandemic on spouse interpersonal relationships

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ABSTRACT

Background: The novel virus, COVID-19, has proven to be a stressor on many levels due to factors like health, economic disruptions, lockdown, and stay-at-home orders. However, one of the significant stressors has been on relationships, primarily the intimate ones, like between spouses. To investigate the correlation between psychological distress and quality of spouse interpersonal relationships.
Methodology: The mixed research design (i.e., qualitative and quantitative methods) was employed on 119 participants between 22-62 years of age, followed by a semi-structural interview of 12 participants, all through virtual snowball mode due to the COVID-19 scenario. Socio-demographic profile, psychological distress scale, and the quality of spouse interpersonal relationships scale and a semi-structural interview schedule were used for data collection.
Results: The present study shows that psychological distress is negatively correlated with certain aspects like conflict, criticism, resentment, pressure, dominance, relative power, and exclusion of the quality of spouse interpersonal relationships. On the other hand, a positive correlation was observed with affection, emotional support, reliable alliance, satisfaction, companionship, and approval aspects of the quality of spouse interpersonal relationships. Qualitative results shows that argument with each other, disagreement, point out faults, pressurization for intimation, and violence with partner are some of the most prominent negative effects in their present life while developed understanding to each other, sense of trust, feel good, received love and affection, care for each other, emotional support, help in other household errands, and take care of children and parents are some of the positive aspects seen instead of the psychological distress perceived during this pandemic.
Conclusions: COVID-19 has had considerable effects on spousal interpersonal relationships and needs further study.

Keywords: COVID-19, Psychological distress, Spouse interpersonal relationships, Stressor.

(Paper received – 16th October 2020, Peer review completed – 8th December 2020)
(Accepted – 15th December 2020)

INTRODUCTION

COVID-19 pandemic has drastically affected not just the physical but also the overall mental health of humans. In the past, pandemics like SARS have shown extreme psychological difficulties, like stress, anxiety, etc. and the effects are carried over post-outbreak too. The fear of family members being infected by the virus permeates all levels and is an excellent cause of perceived stress. Xiang et al. highlighted that

ISSN 1061-933X, Colloid Journal, 2020, Vol. 82, No. 6, pp. 649–660. © Pleiades Publishing, Ltd., 2020.

Influence of Magnetic Field on Micropolar Fluid Flow in a Cylindrical Tube Enclosing an Impermeable Core Coated with Porous Layer

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Received June 3, 2020; revised June 23, 2020; accepted June 25, 2020

Abstract—In this research work, we have investigated the Stokesian flow of a micropolar fluid in a cylindrical tube enclosing an impermeable core coated with porous layer in the presence of magnetic field. The axis of the cylinder is taken along the direction of fluid flow and the uniform magnetic field is applied in the direction perpendicular to the axis of the cylinder. Using appropriate boundary conditions, fluid velocities, microrotational velocities and stresses are evaluated for corresponding fluid flow regions. Expressions for volumetric flow rate through the annulus and the filtration velocity are obtained. Graphs of linear velocities, microrotational velocities and flow rate for various values of different parameters are plotted and discussed.

DOI: 10.1134/S1061933X20060022

INTRODUCTION

Micropolar fluids are the fluids consisting of rigid, randomly oriented particles suspended in a viscous medium, where the deformation of fluid particles is ignored. However, in animal blood, polymeric suspensions, liquid crystals, and other such complex fluids, particles may be of different shape, may shrink or expand, or change their shape, or they may rotate. The most applications of micropolar fluids are in the theory of lubrication and porous media [1]. Micropolar fluids are a subclass of microfluids with microstructure, termed as micromorphic fluids. A class of theories in which both the effects of couple stresses and microstructure are simultaneously taken into account in a systematic manner has developed by Eringen [2]. The ideas and results of the classical theory of micropolar-elasticity which constitutes one of particular cases of Cosserats' theory, investigated by Nowacki [3]. The micropolar theory is of the current and emerging interest of mechanicians, physicians, materials scientists as well as engineers as its limits and possibilities are not fully established that is a serious constraint for applications [4]. Eringen and Okada [5] reported a nonlocal lubrication theory of fluids with microstructure to present a fundamental concept for calculating the rate at which a thin film of liquid drains. Magnetohydrodynamics (MHD) is concerned with the interactions of free currents and magnetic fields with fluid matter, liquids and gases [6]. Eringen and Suhubi [7] formulated the boundary value problem with the state of stress in two normally intersecting circular cylindrical shells.

Khanukaeva and Filippov [8] considered the flow of a micropolar liquid in a Brinkman porous medium for different forms of constitutive equations and reviewed the possible applications of the micropolar theory. Stokes paradox exists neither in case of polar liquid nor non-polar liquid by considering a problem of micropolar fluid flow past an infinite porous cylinder, i.e. a non-trivial solutions exists, reported by Khanukaeva and Deo [9]. Thermo-micropolar fluids [10] can have translatory and rotory motions with spin inertia and microelements of these fluids can stretch and contract. Yadav et al. [11] investigated the micropolar fluid flow through the membrane composed of porous cylindrical particles by considering the fluid flow parallel to an axis of cylinder. Applying the cell model technique, Khanukaeva et al. [12, 13] reported the micropolar fluid flow through a membrane modeled as a swarm of solid cylindrical particles and discussed the effect of various parameters on hydrodynamic permeability of membrane. Deo and Shukla [14] investigated Stokes flow of micropolar fluid past a sphere with non-homogeneous boundary condition for microrotation vector and determined the drag force experienced by sphere. Sherief et al. [15] investigated the quasisteady two-dimensional micropolar fluid flow between two coaxial cylinders in which the inner cylinder is solid while the outer one is fictitious. Micropolar fluid flow problems parallel to the cylin-

ISSN 1061-933X, Colloid Journal, 2021, Vol. 83, No. 6, pp. 662–673. © Pleiades Publishing, Ltd., 2021.

Effect of Magnetic Field on Hydrodynamic Permeability of Biporous Membrane Relative to Micropolar Liquid Flow

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Received March 13, 2021; revised May 31, 2021; accepted June 11, 2021

Abstract—This work concerns the effect of magnetic field on hydrodynamic permeability of biporous membrane relative to the flow of micropolar liquid using four known cell models. The governing equations of micropolar liquid are expressed in modified form using Nowacki's approach. Fluid velocity, microrotation vectors, shear stresses and couple stresses, which are combinations of modified Bessel functions of first and second kinds, are investigated. Arbitrary integration constants are determined by applying analyticity condition at origin, continuity of velocities (both linear and microrotational), continuity of stresses (both shear and couple) at the porous interfaces along with an equivalent condition to Happel, Kuwabara, Kvashnin and Mehta–Morse models at the cell surface. Expressions of volumetric flow rate, superficial/filtration velocity and hydrodynamic permeability are reported. The graphs of hydrodynamic permeability, fluid velocity and microrotation are plotted under the effect of micropolar parameter, Hartmann number, permeability parameters and conductivity ratio parameters, and discussed for different values of these parameters.

DOI: 10.1134/S1061933X21060119

INTRODUCTION

Micropolar fluids [1] consisting of dumbbell shaped molecules and each volume element has microrotation about its centroid. The theory of micropolar elasticity has been described systematically by Nowacki [2]. Effects of couple stresses can be observed by considering that fluid will not have any microstructure [3]. Micropolar fluids are fluids with microstructure belong to a class of fluids with nonsymmetric stress tensor and consisting of rigid, randomly oriented particles suspended in a viscous medium by ignoring the deformation of fluid particles [4]. The theory of micropolar liquids was reviewed for different forms of constitutive equations and boundary conditions by Khanukaeva and Filippov [5]. Steady Stokes flow of a micropolar fluid past a sphere coated with an immiscible Newtonian fluid layer was investigated in [6]. Stokes flow past an infinite porous cylinder was studied for the micropolar liquid and obtained that a non-trivial solution can be found either in nonpolar or in polar liquid [7]. The fundamental principle of the cell model suggests that a system of randomly oriented cylindrical/spherical particles is substituted by a periodic array of cylinders/spheres embedded in identical cylindrical/spherical liquid shells. The boundary conditions on the hypothetical cell surface are assumed to take into account under the influence of surrounding particles at the center of the shell. Happel [8] and Kuwabara [9] proposed cell models in which both particle and outer hypothetical cell are cylinders/spheres. On applying different boundary conditions on the cell surface another two cell methods/models have been suggested by Cunningham [10] and latter used by Mehta and Morse [11], and Kvashnin [12]. Drag force experienced by a porous cylinder for fluid flow past a swarm of porous circular cylinders with cell methods, was evaluated by Deo [13]. Applying the cell model technique, hydrodynamic permeability of a membrane simulated by a swarm of impermeable cylinders covered with a porous layer was evaluated by Vasin and Filippov [14]. Stokes flow through an aggregate of concentric clusters of porous cylindrical particles and variation of hydrodynamic permeability with different parameters was investigated in [15]. Deo et al. [16] investigated the hydrodynamic permeability of membranes composed by porous cylindrical/spherical particles with impermeable core using different cell methods. Influence of the magnetic field on the hydrodynamic permeability of a membrane of solid cylindrical particles coated with porous layer was reported earlier by Tiwari et al. [17]. Yadav et al. [18] investigated the hydrodynamic permeability of biporous membrane built up by porous cylindrical particles embedded in another porous

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https://doi.org/10.1134/S1061933X21060119

Hindawi
Mathematical Problems in Engineering
Volume 2021, Article ID 2861820, 11 pages
https://doi.org/10.1155/2021/2861820

Hindawi

Research Article

Some Summation Formulas for the Generalized Kampé de Fériet Function

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Received 9 June 2021; Accepted 30 August 2021; Published 15 September 2021

Academic Editor: Abdullahi Yusuf

The aim of this manuscript is to establish several finite summation formulas (FSFs) for the generalized Kampé de Fériet series (GKDFS). Moreover, the particular result for confluent forms of Lauricella series in n variables and four generalized Lauricella functions are obtained from the finite summation formulas for the GKDFS.

1. Introduction

Special functions are essential tools in several equations arising in natural science. The hypergeometric series and its generalizations are appeared in many mathematical problems and their applications. The theory of hypergeometric functions in many variables by the fact that the solutions of partial differential equations appearing in several applied problems of mathematical physics has been presented in terms of such hypergeometric functions [1–4].

Since 2012, Brychkov and Saad [5–8] have obtained many finite summation formulas of Appell's functions F_1, F_2, and F_3. Later, Wang established some infinite summation formulas of double hypergeometric functions [9]. In 2016, Wang and Chen [10] derived FSFs of double hypergeometric functions involving some summation theorems. In 2019, Sahai and Verma [11] gave FSFs for the Srivastava's general triple hypergeometric function [12]. For instance, works of Lauricella functions [13] and Srivastava's triple hypergeometric functions [14, 15] have been provided. These works generalized and unified several results in [10] for the three-variable hypergeometric function. In view of the abovementioned works, our motivation is to present here several FSFs for the GKDFS. Also, some particular cases yielding to FSFs for four generalized Lauricella functions and confluent forms of Lauricella series in n variables are given.

The multivariable generalization of Kampé de Fériet function is given as [2, 3]

$$F_{l:\nu_1,\ldots,\nu_n}^{p:\mu_1,\ldots,\mu_n}\left[\begin{matrix}(a_p):(b_{\mu_1}^{(1)});\ldots;(b_{\mu_n}^{(n)}):\\ (a_l):(\omega_{\nu_1}^{(1)});\ldots;(\omega_{\nu_n}^{(n)}):\end{matrix}\tau_1,\ldots,\tau_n\right] \tag{1}$$

$$=\sum_{s_1,\ldots,s_n=0}^{\infty}\Lambda(s_1,e,s_n)\prod_{i=1}^{n}\frac{\tau_i^{s_i}}{s_i!},$$

where

https://doi.org/10.1155/2021/2861820

Computer Modeling in Engineering & Sciences

Tech Science Press

DOI: 10.32604/cmes.2022.016924

ARTICLE

Some Formulas Involving Hypergeometric Functions in Four Variables

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Received: 10 April 2021 Accepted: 16 August 2021

ABSTRACT

Several (generalized) hypergeometric functions and a variety of their extensions have been presented and investigated in the literature by many authors. In the present paper, we investigate four new hypergeometric functions in four variables and then establish several recursion formulas for these new functions. Also, some interesting particular cases and consequences of our results are discussed.

KEYWORDS

Recursion formula; quadruple hypergeometric functions; pascal; identity
AMS Subject Classification: 15A15; 33C65

1 Introduction

In recent years, many researchers introduced and studied several extensions and generalizations of various special functions due to its applications in diverse areas of mathematical, physical, engineering, etc. Agarwal et al. [1,2] established some properties for generalized Gauss hypergeometric functions, which were introduced by Özergin et al. Later, Agarwal et al. [3] and Çetinkaya et al. [4] introduced and investigated further extensions of Appell's hypergeometric functions of two variables and Lauricella's hypergeometric functions of three variables by using the generalized Beta type function. Purohit et al. [5] investigated Chebyshev type inequalities involving fractional integral operator containing a multi-index Mittag-Leffler function in the kernel. Suthar et al. [6] introduced certain generalized forms of the fractional kinetic equation pertaining to the (p, q)-Mathieu-type power series using the Laplace transforms technique. Chandola et al. [7] defined a new extension of beta function using the Appell series and the Lauricella function. The interested

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DOI: 10.32604/cmes.2022.016924

Advances in Difference Equations
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RESEARCH Open Access

Recursion formulas for certain quadruple hypergeometric functions

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Abstract

A remarkably large number of hypergeometric (and generalized) functions and a variety of their extensions have been presented and investigated in the literature by many authors. In this paper, we introduce five new hypergeometric functions in four variables and then establish several recursion formulas for these new functions. Some interesting particular cases and consequences of the main results are also considered.

MSC: 15A15; 33C65

Keywords: Recursion formula; Quadruple hypergeometric functions

1 Introduction and preliminaries

The ordinary hypergeometric functions have been the subject of extensive researches by several prominent mathematicians. These functions play a crucial role in mathematical analysis, physics, engineering and applied sciences. Most of the special functions, which have various physical and technical applications and are closely connected with orthogonal polynomial and problems of mechanical quadrature, can be expressed in terms of generalized hypergeometric functions. Agarwal et al. [1, 2] established some properties for the generalized Gauss hypergeometric functions, which were introduced by Özergin et al. Rahman et al. [3] defined further extensions of hypergeometric and Appell's hypergeometric functions. Very recently, Saboor et al. [4] defined a new extension of Srivastava's triple hypergeometric functions, and the authors presented some of their properties such as integral representations, derivative formulas, and recurrence relations.

Many modern mathematics and theoretical physics problems lead to the study of the hypergeometric functions of several complex variables (see, e.g., [5–16]). These include, for example, problems in the representation theory, combinatorics, number theory, analytic continuation of integrals of the Mellin–Barnes type, and algebraic geometry. Moreover, hypergeometric-type functions are seen in several applications of physical and chemical problems [17–20].

In [21], Exton defined 21 complete hypergeometric functions in four variables denoted by the symbols $K_1, K_2, \ldots, K_{21}$. In [22], Sharma and Parihar introduced 83 complete quadruple hypergeometric functions, denoted by $F_1^{(4)}, F_2^{(4)}, \ldots, F_{83}^{(4)}$. Bin-Saad and Younis [23, 24] introduced 30 new quadruple hypergeometric functions written as

Springer

https://doi.org/10.1186/s13662-021-03561-z

A mathematical model for the novel coronavirus with effect of lockdown

No Access

Vinay Verma, Manju Agarwal and Ashish Verma

https://doi.org/10.1142/S1793962323500058 | **Cited by:** 0

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Abstract

This paper delineates the mathematical modeling and dynamics of a novel coronavirus (COVID-19) an outbreak, and it is a control measurement; the effect of lockdown in terms of lakhs of cases and deaths. The lockdown effect is studied with a different lockdown success rate and also describes the multiple transmission route in the infectio dynamics, and pushes the role of the environmental reservoir in the transmission and the spread of this disease. In this situation, mathematical models are an important tool to assign an impressive strategy in order to fight against this pandemic. We exhibit the boundedness of the system, the local stability analysis and global

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https://doi.org/10.1142/S1793962323500058

Hindawi
Mathematical Problems in Engineering
Volume 2021, Article ID 9926176, 11 pages
https://doi.org/10.1155/2021/9926176

Hindawi

Research Article

On the Kampé de Fériet Hypergeometric Matrix Function

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Received 18 March 2021; Revised 25 March 2021; Accepted 30 July 2021; Published 18 August 2021

Academic Editor: Sergio Ortobelli Lozza

In this study, we derive recursion formulas for the Kampé de Fériet hypergeometric matrix function. We also obtain some finite matrix and infinite matrix summation formulas for the Kampé de Fériet hypergeometric matrix function.

1. Introduction

The theory of special functions is closely related to the theory of Lie groups and Lie algebras, as well as certain topics in mathematical physics. Symbolic computation and engineering problems usually recognize the majority of special functions. Recently, there has been a surge in the study of recursion formulas for multivariable hypergeometric functions. Recursion formulas for the Appell function F_2 have been investigated by Opps et al. [1], followed by Wang [2], who presented the recursion relations for all Appell functions. Furthermore, recursion formulas for variant multivariable hypergeometric functions were presented in [3–6]. One can refer to various sources [7, 8] for the in-depth study of the hypergeometric functions for several variables.

The theory of generalized matrix special functions has witnessed a rather significant evolution during the last two decades. The reasons of interest have a manifold motivation. Restricting ourselves to the applicative field, we note that for some physical problems, the use of new classes of matrix special functions provided solutions hardly achievable with conventional analytical and numerical means. Special matrix functions appear in the literature related to statistics [9], Lie theory [10], and more recently in connection with the matrix version of Laguerre, Hermite, and Legendre differential equations and the corresponding polynomial families [11–13]. In [14], recursion formulas and matrix summation formulas for Srivastava's triple hypergeometric matrix functions are obtained.

The study is organized in the following manner. In Section 2, we list basic definitions that are needed in the sequel. In Section 3, we obtain recursion formulas for the Kampé de Fériet hypergeometric matrix function (its abbreviation is K de FHMF). In Section 4, we present finite matrix summation formulas for the (K de FHMF) by applying a derivative operator. Finally, in Section 5, we establish infinite matrix summation formulas for the (K de FHMF).

2. Preliminaries

Let $\mathbb{C}^{r\times r}$ be the vector space of r square matrices with complex entries. For any matrix $H \in \mathbb{C}^{r\times r}$, its spectrum $\sigma(H)$ is the set of eigenvalues of H. H in $\mathbb{C}^{r\times r}$ is called a positive stable matrix if $\Re(\lambda) > 0$ for all $\lambda \in \sigma(H)$.

The reciprocal gamma function $\Gamma^{-1}(\theta) = 1/\Gamma(\theta)$ is an entire function of the complex variable θ. The image of $\Gamma^{-1}(\theta)$ acting on H, denoted by $\Gamma^{-1}(H)$, is a well-defined matrix. If $H + \ell I$ is invertible for all integers $\ell \geq 0$, then the

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DOI:10.1155/2021/9926176

Hindawi
Journal of Function Spaces
Volume 2021, Article ID 7638597, 6 pages
https://doi.org/10.1155/2021/7638597

Research Article

Generating Functions for Some Hypergeometric Functions of Four Variables via Laplace Integral Representations

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Received 30 May 2021; Accepted 7 July 2021; Published 15 July 2021

Academic Editor: Mohsan Raza

Generating functions plays an essential role in the investigation of several useful properties of the sequences which they generate. In this paper, we establish certain generating relations, involving some quadruple hypergeometric functions introduced by Bin-Saad and Younis. Some interesting special cases of our main results are also considered.

1. Introduction

The hypergeometric series is the most useful and important special function, and it has been studied to solve various problems in many areas of mathematics, physics, statistics, and engineering [1–5]. Hypergeometric series in several variables appear in numerous fields of applied mathematics, mathematical physics, and chemistry. Very recently, Bin-Saad and Younis [6] introduced thirty new hypergeometric functions of four variables $X_i^{(4)}(i = 1, 2, \cdots, 30)$, eight of them are defined below

$$X_{11}^{(4)}(a_1, a_1, a_1, a_2, a_1, a_2, a_3, a_3 ; c_1, c_1, c_2, c_3 ; x, y, z, u) = \sum_{m,n,p,q=0}^{\infty} \frac{(a_1)_{2m+n+p}(a_2)_{n+q}(a_3)_{p+q}}{(c_1)_{m+n}(c_2)_p(c_3)_q} \frac{x^m}{m!} \frac{y^n}{n!} \frac{z^p}{p!} \frac{u^q}{q!}; \quad (1)$$

$$X_{12}^{(4)}(a_1, a_1, a_1, a_2, a_1, a_2, a_3, a_3 ; c_2, c_1, c_1, c_3 ; x, y, z, u) = \sum_{m,n,p,q=0}^{\infty} \frac{(a_1)_{2m+n+p}(a_2)_{n+q}(a_3)_{p+q}}{(c_1)_{n+p}(c_2)_m(c_3)_q} \frac{x^m}{m!} \frac{y^n}{n!} \frac{z^p}{p!} \frac{u^q}{q!}; \quad (2)$$

$$X_{16}^{(4)}(a_1, a_1, a_1, a_1, a_1, a_2, a_3, a_2 ; c_1, c_1, c_2, c_3 ; x, y, z, u) = \sum_{m,n,p,q=0}^{\infty} \frac{(a_1)_{2m+n+p+q}(a_2)_{n+q}(a_3)_p}{(c_1)_{m+n}(c_2)_p(c_3)_q} \frac{x^m}{m!} \frac{y^n}{n!} \frac{z^p}{p!} \frac{u^q}{q!}; \quad (3)$$

$$X_{17}^{(4)}(a_1, a_1, a_1, a_1, a_1, a_2, a_3, a_2 ; c_2, c_1, c_1, c_3 ; x, y, z, u) = \sum_{m,n,p,q=0}^{\infty} \frac{(a_1)_{2m+n+p+q}(a_2)_{n+q}(a_3)_p}{(c_1)_{n+p}(c_2)_m(c_3)_q} \frac{x^m}{m!} \frac{y^n}{n!} \frac{z^p}{p!} \frac{u^q}{q!}; \quad (4)$$

$$X_{21}^{(4)}(a_1, a_1, a_2, a_1, a_1, a_2, a_3, a_2 ; c_1, c_1, c_2, c_3 ; x, y, z, u) = \sum_{m,n,p,q=0}^{\infty} \frac{(a_1)_{2m+n+q}(a_2)_{n+p+q}(a_3)_p}{(c_1)_{m+n}(c_2)_p(c_3)_q} \frac{x^m}{m!} \frac{y^n}{n!} \frac{z^p}{p!} \frac{u^q}{q!}; \quad (5)$$

$$X_{22}^{(4)}(a_1, a_1, a_2, a_1, a_1, a_2, a_3, a_2 ; c_2, c_1, c_1, c_3 ; x, y, z, u) = \sum_{m,n,p,q=0}^{\infty} \frac{(a_1)_{2m+n+q}(a_2)_{n+p+q}(a_3)_p}{(c_1)_{n+p}(c_2)_m(c_3)_q} \frac{x^m}{m!} \frac{y^n}{n!} \frac{z^p}{p!} \frac{u^q}{q!}; \quad (6)$$

$$X_{27}^{(4)}(a_1, a_1, a_3, a_1, a_1, a_2, a_4, a_4 ; c_2, c_1, c_1, c_3 ; x, y, z, u) = \sum_{m,n,p,q=0}^{\infty} \frac{(a_1)_{2m+n+p}(a_2)_n(a_3)_p(a_4)_{p+q}}{(c_1)_{n+p}(c_2)_m(c_3)_q} \frac{x^m}{m!} \frac{y^n}{n!} \frac{z^p}{p!} \frac{u^q}{q!}; \quad (7)$$

$$X_{28}^{(4)}(a_1, a_1, a_1, a_1, a_1, a_2, a_3, a_4 ; c_1, c_1, c_2, c_3 ; x, y, z, u) = \sum_{m,n,p,q=0}^{\infty} \frac{(a_1)_{2m+n+p+q}(a_2)_m(a_3)_p(a_4)_q}{(c_1)_{m+n}(c_2)_p(c_3)_q} \frac{x^m}{m!} \frac{y^n}{n!} \frac{z^p}{p!} \frac{u^q}{q!}; \quad (8)$$

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DOI: 10.1155/2021/7638597

Hindawi
Journal of Mathematics
Volume 2021, Article ID 5596299, 10 pages
https://doi.org/10.1155/2021/5596299

Hindawi

Research Article

Some Formulas for New Quadruple Hypergeometric Functions

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Received 9 February 2021; Revised 10 March 2021; Accepted 16 March 2021; Published 1 April 2021

Academic Editor: Ahmet Ocak Akdemir

In this paper, we aim to introduce six new quadruple hypergeometric functions. Then, we investigate certain formulas and representations for these functions such as symbolic formulas, differential formulas, and integral representations.

1. Introduction

Hypergeometric functions of several variables play an important role in diverse areas of science and engineering. The developments in applied mathematics, mathematical physics, chemistry, combinatorics, statistics, numerical analysis, and other areas have led to increasing interest in the study of multiple hypergeometric functions. Many authors have studied a number of formulas involving hypergeometric functions (see, e.g., [1–6]).

In [7], Exton presented twenty-one complete hypergeometric functions in four variables denoted by symbols $K_1, K_2, \ldots, K_{21}$. In [8], Sharma and Parihar defined eighty-three complete quadruple hypergeometric functions, namely, $F_1^{(4)}, F_2^{(4)}, \ldots, F_{83}^{(4)}$. Bin-Saad and Younis [9] gave thirty new quadruple hypergeometric functions given by $X_1^{(4)}, X_2^{(4)}, \ldots, X_{30}^{(4)}$. In [10], the authors discovered the existence of twenty additional complete hypergeometric functions in four variables $X_{31}^{(4)}, X_{32}^{(4)}, \ldots, X_{50}^{(4)}$. Each quadruple hypergeometric function in [7–10] is of the form

$$X^{(4)}(.) = \sum_{m,n,p,q=0}^{\infty} \Omega(m,n,p,q) \frac{x^m}{m!} \frac{y^n}{n!} \frac{z^p}{p!} \frac{u^q}{q!}, \quad (1)$$

where $\Omega(m,n,p,q)$ is a certain sequence of complex parameters, and there are twelve parameters in each series of $X^{(4)}(.)$ (eight a's and four c's). The 1st, 2nd, 3rd, and 4th parameters in $X^{(4)}(.)$ are connected with integers m, n, p, and q, respectively. Each repeated parameter in the series $X^{(4)}(.)$ points out a term with double parameters in $\Omega(m,n,p,q)$. For example, $X^{(4)}(a_1, a_1, a_2, a_2, a_3, a_3, a_4, a_5)$ means that $(a_1)_{m+n}(a_2)_{p+q}(a_3)_{m+n}(a_4)_p(a_5)_q$ includes the term. Similarly, $X^{(4)}(a_1, a_1, a_1, a_2, a_1, a_1, a_2, a_3)$ points out the term $(a_1)_{2m+2n+p}(a_2)_{p+q}(a_3)_q$, and $X^{(4)}(a_1, a_1, a_2, a_3, a_1, a_2, a_3, a_4)$ shows the existence of the term $(a_1)_{2m+n}(a_2)_{n+p}(a_3)_{p+q}(a_4)_q$. Thus, it is possible to form various combinations of indices. There seems to be no way of independently establishing the number of distinct Gaussian hypergeometric series for any given integer $n \geq 2$ without explicitly stating all such series. Thus, in every situation with $n = 4$, one ought to begin by actually constructing the set just as in the case $n = 3$ (see [11]).

By using the conventions and notations above, we now introduce further quadruple hypergeometric functions as follows:

https://doi.org/10.1155/2021/5596299

Quaestiones Mathematicae 2021, 44(7): 881–904

https://doi.org/10.2989/16073606.2020.1753123

ON THE INCOMPLETE SRIVASTAVA'S TRIPLE HYPERGEOMETRIC MATRIX FUNCTIONS

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ABSTRACT: The paper proposes to introduce incomplete Srivastava's triple hypergeometric matrix functions through application of the incomplete Pochhammer matrix symbols. We also derive certain properties such as matrix differential equation, integral formula, reduction formula, recursion formula, recurrence relation and differentiation formula of the incomplete Srivastava's triple hypergeometric matrix functions.

Mathematics Subject Classification (2010): 15A15, 33C65, 33C45, 34A05.

Key words: Matrix functional calculus, recursion formula, gamma matrix function, incomplete gamma matrix function, incomplete Pochhammer matrix symbol, Laguerre matrix polynomial, Bessel and modified Bessel matrix function.

1. Introduction. Recently, Srivastava *et al.* [26] have studied incomplete Pochhammer symbols and incomplete hypergeometric functions and discussed applications of these functions in communication theory, probability theory and groundwater pumping modelling. Cetinkaya [4] introduced the incomplete second Appell hypergeometric functions and obtained certain properties of these functions. Also, recently introduced incomplete Srivastava's triple hypergeometrics and investigated certain properties of the incomplete Srivastava's triple hypergeometrics [7, 8]. Srivastava *et al.* [29] have obtained several interesting properties of the incomplete H-functions. On his work on hypergeometric functions of three variables, Srivastava [24, 25] noticed the existence of three additional complete triple hypergeometric functions of the second-order. These functions are known in literature as Srivastava's triple hypergeometric functions H_A, H_D and H_C and are given in [27, 28].

For a wide variety of other explorations involving incomplete hypergeometric functions in several variables, the interested reader may be referred to several recent papers [5, 6, 7, 8, 23, 30, 31].

The matrix theory has become pervasive to almost every area of mathematics, in general and in orthogonal polynomial and special functions, in particular. The matrix analogue of the Gauss hypergeometric function was introduced by Jódar and Cortés [17], particularly the hypergeometric matrix function, plays a very important role in solving numerous problems of mathematical physics, engineering and mathematical sciences [9, 10, 11, 13, 14]. Quite recently, the incomplete hypergeometric matrix functions was introduced by Abdalla [1]. Within the frame, they

Quaestiones Mathematicae is co-published by NISC (Pty) Ltd and Informa UK Limited (trading as the Taylor & Francis Group)

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Jaunpur

MATHEMATICS IN ENGINEERING, SCIENCE AND AEROSPACE
MESA - www.journalmesa.com
Vol. 12, No. 2, pp. 1-14, 2021
© CSP - Cambridge, UK; I&S - Florida, USA, 2021
I&S PUBLISHERS

On the recursion formulas for the matrix special functions of one and two variables

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Abstract. Special matrix functions have recently been investigated for regions of convergence, integral representations and the systems of matrix differential equation that these functions satisfy. In this paper, we find the recursion formulas for the Gauss hypergeometric matrix function (GHMF). We also give the recursion formulas for the two variable Appell matrix functions (AMFs).

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 [4], Lie theory [7] and in connection with the matrix version of Laguerre, Hermite and Legendre differential equations and the corresponding polynomial families [8, 9, 10]. Recently, Abd-Elmageed *et. al.* [1] have obtained numerous contiguous and recursion formulas satisfied by the first AMF, namely F_1. Motivated by this study, in this article, we study recursion formulas for the GHMF and all four AMFs.

Recursion formulas for the Appell functions have been studied in the literature, see [13, 19]. Recursion formulas for several multivariable hypergeometric functions were presented in [14, 15, 16, 17].

Here is elucidated a sectionwise distribution of present work. In Section 2, we list basic definitions that are needed in the sequel. In Section 3, we obtain the recursion formulas for the GHMF. In

2010 Mathematics Subject Classification: 15A15; 33C65; 33C70
Keywords: Matrix functional calculus, Gauss hypergeometric matrix function, Appell matrix functions.

https://doi.org/10.48550/arXiv.2003.0752

INTERNATIONAL JOURNAL FOR COMPUTATIONAL METHODS IN ENGINEERING SCIENCE AND MECHANICS
2021, VOL. 22, NO. 3, 225–234
https://doi.org/10.1080/15502287.2021.1916693

Dynamics of some more invariant solutions of (3 + 1)-Burgers system

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ABSTRACT

This paper is an application of the similarity transformations method *via* Lie-group theory. This method is applied to the (3 + 1)-dimensional Burgers system to derive its invariant solutions. The Burgers system has many physical applications in fluid mechanics, heat conduction, plasma physics, traffic flows, and in some others like acoustic transmission and structure of shock waves. Since Burgers system consists of a system of nonlinear partial differential equations (PDEs), and therefore, it is a difficult task to obtain its exact solution. A system of PDEs is reduced into a system of ODEs and finally solved by making appropriate assumptions and choice of arbitrary functions and constants appeared therein. Hence, the obtained exact solutions compromised multisolitons, kink waves, periodic multisolitons, elastic mutisolitons and stationary waves.

KEYWORDS

Nonlinear PDEs; Burgers system; Lie-group theory; multisolitons

1. Introduction

1.1. Aims and scope

To get the solutions of physically important nonlinear evolution equations (NLEEs) became an intense research area owing to their wide applications in diverse areas notably condensed matter physics, plasma physics and optics, geophysical fluid dynamics, fluid mechanics, and lattice dynamics etc. Therefore, our aim is to attain the analytical solutions of (3 + 1)–dimensional Burgers system that has significant applications in many fields, notably in fluid mechanics, plasma physics, heat conduction, gas dynamics, traffic flows, acoustic transmission and structure of shock waves, for more details, kindly see [1]–[7]. The (3 + 1)–dimensional Burgers system (BS) is governed by the following system of nonlinear PDEs:

$$\begin{aligned} u_t &= 2uu_y + 2vu_x + 2wu_z + u_{xx} + u_{yy} + u_{zz}, \\ u_x &= v_y, \quad u_z = w_y, \end{aligned} \tag{1}$$

where u, v and w are wave functions of variables x, y, z and t. The above system describes about the turbulence that occurred due to propagation of nonlinear waves, non-equilibrium and interface dynamics etc. Moreover, in particular, if u is z-independent (or $z = x$; $w = u$), then the system can be reduced into (2 + 1)-dimensional Burgers equation, i.e., $(u_t = \alpha uu_x + \beta u_{xx} + \gamma vv_x + \frac{\beta\gamma}{\alpha} v_{xy}, u_y = v_x$, where α, β and γ are non-zero constants) which is given in [8] and obtained from the generalized Painlevé integrable Burgers' equations.

Deriving an exact solution of a nonlinear system is extremely difficult and challenging, and therefore, some methods/techniques like generalized (G'/G)-expansion method [9] and (G'/G)-expansion method [10], multilinear variable separation approach [11], [12], extended Riccati equation and Painlevé truncation expansion [13], exp-function method [14], extended mapping approach along with variable separation method [15], [16], Similarity reduction and symmetry transformations [17]–[19], Painlevé anaysis [20], Hirota's bilinear approach [21], Cole-Hopf transformations [22], [23], tanh-coth method [24], optimal sub-algebra of Lie-group and symmetry reductions [25]–[35], and some others are useful to solve the purpose. Therefore, symmetry analysis of nonlinear differential equations such as symmetry reductions and construction of group invariant solutions play a pivotal role in order to extract the analytical solution of such NLEEs.

1.2. Literature review

Since each technique has its own issues and different aspects as far as the analytical solution is concerned, therefore we overview on some interesting literature and contributions addressing to (3 + 1)-BS [10]–[16]

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https://doi.org/10.1080/15502287.2021.1916693

Int. J. Appl. Comput. Math (2021) 7:18
https://doi.org/10.1007/s40819-020-00945-9

ORIGINAL PAPER

Some More Invariant Solutions of (2 + 1)-Water Waves

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Accepted: 11 December 2020 / Published online: 11 January 2021

Abstract

In view of applicability of water waves, the objective of this article is to provide some more analytical solutions of (2 + 1)-dimensional water waves i.e. Boiti–Leon–Pempinelli (BLP) system. A water wave advancing in an infinite narrow channel is described by the BLP system which generally consists of a system of nonlinear partial differential equations, therefore, to get an exact solution would be a difficult task. To solve the purpose, we have converted this system into a system of ordinary differential equations (ODEs) using similarity transformations method via Lie-group theory. The resultant system of ODEs is solved after making appropriate assumptions and choice of arbitrary functions and constants appeared therein. The established results are an extension of our previous findings (Kumar et al. in Comput Math Appl 70(3):212–221, 2015). Hence, the obtained exact solutions compromised elastic single soliton, doubly soliton, multisolitons and flipping of single solitons with passage of time.

Keywords Boiti–Leon–Pempinelli system · Nonlinear partial differential equations · Similarity transformations method · Exact solutions · Lie-group theory

Mathematics Subject Classification 35C08 · 76M60

Introduction

To derive solutions of nonlinear evolution equations (NLEE) has become a very active research area since these equations are extensively used in many areas of science and engineering such as condensed matter physics, mathematical physics, fluid mechanics, plasma physics and optics, etc. However, in general, obtaining an exact solution of NLEEs will be

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https://doi.org/10.1007/s40819-020-00945-9

Indian Journal of Economics and Business
Vol. 20 No. 4 (December, 2021)

http://www.ashwinanokha.com/IJEB.php

Role of Microfinance and Self-Help Group in Women's Financial, Behavioral and Psychological Empowerment

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Received: 28th July 2021
Revised: 29nd September 2021
Accepted: 25th October 2021

Abstract

Purpose: In recent years, the microfinance sector has made great strides. The quantity and volume of MFIs have increased dramatically. Microfinance is thought to play a critical role in poverty alleviation and improving women's economical Condition hence their empowerment.

Objective: The study Primarily aims to study the perceived value creation of women who joined SHGs and availed Microfinance Loan and analyses their status of empowerment apart from its various literature review is intended to highlights of Microfinance and Self-Help Group (Trend Analysis) In Uttar Pradesh.

Research Methodology: The research relies significantly on literature, as well as primary and secondary data. A primary survey was conducted for this aim in order to record the real-life experiences and observations of microfinance women participants in Uttar Pradesh.

Summary: Microfinance activities and involvement in self-help groups have a favourable impact on women participants' income, assets, occupation, savings, access to loans, bank connectivity, knowledge, self-worthiness, and decision-making abilities. The availability of microfinance loans and their constructive use has been found to play a significant effect in women's empowerment.

Keywords: Microfinance, Self-Help Group, Women Empowerment, poverty alleviation, Financial Inclusion.

1. Introduction

Grameen Bank, founded in 1983, was the first microfinance organisation in Bangladesh. Small sums of loans, a lack of physical collateral in favour of social collateral or peer monitoring, and a focus on women borrowers are the main characteristics of micro finance that set it apart from past systems of credit delivery ("Micro Finance and Financial Inclusion of Women: An Evaluation", 2022).Microfinance activities have grown rapidly after 1990and in recent years it is taking even more attention. West Bengal, Tamil Nadu, Bihar, Karnataka, and Uttar Pradesh are the top five states with the most outstanding portfolios as of June

Performance Optimization of Peak to Average Power Ratio in FBMC Waveforms

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Abstract: High spectral efficiency and low computational complexity are requirements of the 5G wireless communication systems. They must also offer low PAPR (peak to average power ratio), low latency, and high throughput. In 5G it is not possible to realize all of these requirements through a single technique. One of the efforts is to look for a suitable technique for 5G. Therefore, a suitable technique Filter Bank Multicarrier (FBMC) emerges. But it has a high complexity, high Peak to Average Power (PAPR) and high out of band (OOB) leakage which results in inter-carrier interference and inter-channel interference. Also, due to high PAPR, mobile batteries are depleted more rapidly. So, a PAPR reduced method is needed. In this paper, a method of Pruned DFT Precoded FBMC to optimize the PAPR for different number of subcarriers has been studied. The performance evaluation in terms of bit error rate (BER) and spectral efficiency of OFDM, FBMC and Pruned DFT Precoded FBMC has been done in this paper. In DFT Precoded FBMC, a DFT spreading matrix is multiplied with FBMC waveform and is transmitted only some part especially half of the DFT precoded matrix and the rest remain zero. Monte Carlo simulation with one tap equalizer is used to validate our results.

Keywords: 5G, FBMC, DFT, PAPR, TDL

(Article history: Received: 9th October2021 and accepted 18th December 2021)

I. INTRODUCTION

As we try to build a waveform with certain required features, the others one fill, and this is why we are improving the engineering of the waveform to provide better features than what existed in the previous generation. Therefore, Filter Bank Multicarrier (FBMC) [1-2] comes into play because of its flexible time and frequency resources. Additionally, it is synchronization dependent compared to OFDM. A OFDM waveform is a Sinc function in frequency domain, so even though the others are orthogonal, the peak occurs at the zero of the neighbouring subcarriers, however, slight offsets cause a severe penalty because of Inter Channel Interference (ICI), with guard interval being small, and channel impulse response extending beyond the Cyclic Prefix (CP). ICI and ISI are present, resulting in performance degradation. FBMC has greater resilience than OFDM, and it has better spectral efficiency because it produces circular pulses. FBMC has a high complexity, high out-of-band leakage, and a high PAPR. This high PAPR calls for power amplifiers with high linear (gain) ranges. But to increase the efficiency of a power amplifier its gain becomes nonlinear, resulting in a distorting of the FBMC signal. Thus, a PAPR reducing technique is needed. Several techniques have been proposed to reduce the PAPR in OFDM, such as selective mapping [3] or partial transmission sequences [4]. Those methods can also be applied to FBMC as in [5-7]. All of these techniques however need highly sophisticated computational capacities. The drawbacks of these systems explain why they are not used in practical systems. For the uplink, 4G LTE uses Single Carrier - Frequency-Division Multiple Access (SC-FDMA) [8], a precoded OFDM system based on DFT. Additionally, the same technique will be used in the Fifth Generation (5G) of wireless communication systems (in addition to CP-OFDM) [9]. In Discrete Fourier Transform spreading based generalized frequency division multiplexing (Pruned DFT Precoded FBMC), simply combining FBMC and a DFT, as in SC-FDMA [10-12]. Ihalainen et.al [10] propose precoding by a filter bank rather than a DFT to improve the performance.

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FR4 Grounded Multiband Micro strip Patch Antenna with Slot and Notch for L, S, and C Band Applications

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Abstract : In this paper a simulated study of slot and notch loaded rectangular patch antenna is presented. This proposed antenna shows the tripple frequency band operation which is depends on the inserted slot and notch on the rectangular patch. It is found the proposed antenna resonates at tripple distinct resonance mode at 2.5GHz, 4.2GHz, and 5GHz for lower and upper resonance frequencies respectively. The designed antenna shows tripple frequency response nature with frequency ratio 1.68 and 1.190. The various characteristics of slot and notch loaded rectangular patch antenna gain (5.7dBi, 5dBi, 6.4 dBi), directivity (5.7dBi, 3.4dBi, 3.9dBi), efficiency (90%, 40%, 90%) and radiation pattern lobes are found in good agreement.

IndexTerms **- Microstrip patch antenna, Multiband, FR4, L, S and C band.**

I. INTRODUCTION

Microstrip patch antennas becomes more popular among the researchers since last two decades due their attractive features such as low profile, light weight, compatibility with various monolithic microwave integrated circuits. Some of these fabulous features of these patch antennas in the field of wireless communication [1] encourage the researchers over the world wide. These antennas have been successfully utilized in many communication systems [2-3] such as satellite communication, cellular communication systems, wireless personal area, wireless local area network and synthetic aperture radar etc. These patch antennas are can be designed by various techniques, in which some popular techniques are based on aperture coupling [4], proximity coupling [5],loading of slots [7-8], loading of notches [9], parasitic elements [10], L-strip feed [11], microstrip line feed [12]. One of the most important techniques is inserting the slots and notches and by which diversion of current takes place over the patch to achieve dual band and multiband frequency response for wireless communication frequency range.

The various contributions of researchers and scientist on slot and notch loaded microstrip patch antennas are reported such as Analysis of slot-loaded rectangular microstrip patch antenna [13], Dualband printed antenna for CDMA/PCS handsets [14], open slot antenna for WLAN/WiMAX operation [15], U-Slot microstrip patch antenna [16]. All the above reported papers are based on the slot and notch loaded rectangular microstrip patch antenna for single or dual band operation.

In this view, the main objective of this paper is to present a simulated design of slot and notch loaded rectangular patch antenna for multiband operation with sufficient amount of gain, directivity, axial ratio, reflection coefficient and good amount of radiation pattern lobes. The proposed antenna is investigated for tripple frequency band operation, so that a single antenna can be utilized for more than one frequency band. The proposed antenna structure is simulated in Zeeland IE3D simulation software.

II. ANTENNA GEOMETRY AND DIMENSIONS

Figure 1 shows the structure of proposed antenna design. The slot and notch loaded rectangular patch antenna with ground plane for L, S and C band application shown in Figure 1. The rectangular patch has a dimension of 20x20 mm whereas the ground plane dimensions are taken order of 20x20 mm. in proposed 20x20 mm patch, 3 parallel slots of dimensions 16x2 mm are inserted in the patch, whereas a single 16x2 mm dimensions vertical notch is inserted in the proposed rectangular patch. A feed point is connected at coordinate $X_f = 0$, $Y_f = 2$ for the excitation of the proposed antenna. The proposed slot and notch loaded rectangular MSA is designed in IE3D simulation media. Figure 1(b) shows the front view of the simulated design of slot and notch loaded rectangular microstrip patch antenna in IE3D simulation software [17]. Figure 1(c) shows the side view of simulated slot and notch loaded rectangular MSA in IE3D simulation media. Firstly the proposed antenna is designed on foam substrate with relative permittivity (ε_r =1.07). Afterwards it was designed with higher relative permittivity material bakellite (ε_r =3.2). Thereafter for final design FR4 (ε_r =4.4) substrate is finally selected in IE3D simulation software and the final design of slot and notch loaded rectangular microstrip patch antenna is simulated. The various geometry parameters are given in Table 1. Where L_{n1}xW_{n1}, L_{n2}xW_{n2}, L_{n3}xW_{n3} are the dimensions of parallel slots over the proposed antenna design. The dimension of vertical notch is denoted with L_vxW_v and dimensions are opted in millimeter (mm).

International Food Research Journal 28(3): 527 - 537 (June 2021)
Journal homepage: http://www.ifrj.upm.edu.my

Introduction of the hypocholesterolemic peptide, LPYPR, to the major storage protein of mung bean [*Vigna radiata* (L.) Wilczek] through site-directed mutagenesis

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Article history

Received: 20 November 2019
Received in revised form: 29 October 2020
Accepted: 2 December 2020

Keywords

site-directed mutagenesis, hypocholesterolemic activity, mung bean, LPYPR, 8Sα globulin

Abstract

The hypocholesterolemic peptide, LPYPR, was successfully introduced into the VR-1, VR-2, and VR-5 regions of the mung bean 8Sα globulin. The mutant protein (MP) has 96.69% structural homology and 97% sequence homology compared to the wild type (WT). Expression of the mutant protein in *E. coli* HMS174(DE3) was 40.66%, which was 144.42% higher than that of the WT. The WT protein and MP had MWs of about 48.4 and 48.7 kDa, respectively. These were purified using HIC and digested with trypsin. UPLC analysis of the tryptic digests of the MP revealed the successful release of the LPYPR peptide. Unlike the WT protein, cholesterol-binding capacity (mg/g sample) of the MP increased over time of tryptic digestion (average growth rate of 9.5% for crude MP and 12.5% for HIC-purified MP) for its undigested form (crude: 220.96 ± 8.65, purified: 214.71 ± 11.91), with maximum values of 380.76 ± 6.61 and 434.44 ± 10.88 were obtained for the 24-h digests of the crude and purified proteins, respectively. Similarly, the sodium taurocholate binding capacity (%) was also found to increase over time of tryptic digestion (average growth rate of 4% for crude MP and 5.67% for HIC-purified MP) for the tryptic digests of the MP. Minimum values for % bound sodium taurocholate was obtained with the undigested samples (crude: 46.71 ± 0.42, purified: 44.49 ± 0.13), while maximum values thereof were obtained with the 24-h digest samples (crude: 59.75 ± 0.30, purified 61.95 ± 0.51).

Introduction

The 8Sα globulin lacks a bioactive peptide that has hypocholesterolemic activity. However, using genetic engineering, it is possible to introduce the oligonucleotide sequence responsible for coding the hypocholesterolemic peptide, LPYPR (Takenaka *et al.*, 2000; 2001). The tool to introduce a short oligonucleotide sequence responsible for coding the bioactive peptide is called site-directed mutagenesis. This technique was previously applied to introduce methionine and cysteine residues into the 8Sα globulin of mung bean to enhance the nutritional quality of the mung bean (Torio *et al.*, 2011; 2012).

Hypocholesterolemic activity is the ability of any substance to lower serum cholesterol. Hypocholesterolemic peptides either prevent cholesterol biosynthesis by inhibiting HMG-CoA reductase (Pak *et al.*, 2007), or prevent the absorption of dietary cholesterol and reabsorption of bile salts in the gastrointestinal tract, thus leading to a decrease in serum cholesterol levels (Sugano *et al.*, 1988; Pak *et al.*, 2007; Sanossian and Ovbiagele, 2008). Hypocholesterolemic peptides can be introduced in various dietary proteins through site-directed mutagenesis, thereby enhancing nutraceutical properties.

LPYPR (MW = 644.36 Da) is one of the hypocholesterolemic peptides first derived from soybean glycinin (11S protein), and has been shown to possess a hypocholesterolemic activity that reduces the serum cholesterol in mice after oral administration (Yoshikawa *et al.*, 2000). LPYPR lowers the serum cholesterol by inhibiting the reabsorption of bile acids from the gastrointestinal tract (Yoshikawa *et al.*, 2000), as well as by inhibiting the HMG-CoA reductase (Kwon *et al.*, 2002). LPYPR interacts with bile acids not only through hydrophobic interactions but also through ionic interactions due to cationic amino acid residues such as Lys and Arg (Howard and Udenigwe, 2013).

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Current Research in Environmental Sustainability 3 (2021) 100063

Contents lists available at ScienceDirect

Current Research in Environmental Sustainability

journal homepage: www.sciencedirect.com/journal/current-research-in-environmental-sustainability

Biofertilizers: A Nexus between soil fertility and crop productivity under abiotic stress

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ARTICLE INFO

Keywords:
Biofertilizers
Chemical fertilizers
Crop yield
Eco-friendly
Sustainable food security

ABSTRACT

High food demand for the world's teeming population necessitates the intensification of crop production in modern agriculture, which requires the extensive use of synthetic fertilizers for higher crop yield. The excessive use of chemical fertilizers, despite the high nutrients contents and ability to grow crops faster, discovered to be dangerous to the health and environment besides polluting the groundwater and atmosphere in the future. The alternative to these, biofertilizers arose today due to their attributes towards eco-friendly, cost-effective, and easy to apply in the agricultural field. Biofertilizers are a batch of diverse microorganisms, which can induce plant growth-promotion activities along with soil health, even under abiotic stress conditions. Biofertilizers maybe plant growth-promoting rhizobacteria, arbuscular mycorrhizal fungi, and as well as the consortia of other beneficial microbes. Biofertilizers can sustain plant growth performance, even in a challenging environment. The performance of perfect-candidate-biofertilizer in the agricultural field depends on crop type, properties of inoculants, technical background, and environmental condition. Biofertilizers can, directly or indirectly, help in attaining food security compared to the harmful effect of chemical fertilizers. A direct mechanism of Biofertilizers refers to phyto-stimulation and nutrient mobility, while an indirect mechanism poses bio-control activity. Direct mechanisms involve phytohormone production and phosphate, potassium, zinc, etc. solubilization. While, indirect-mechanism is HCN production, siderophore production, antibiotic production, etc. The present review elucidates the diversity of microbial inoculants (biofertilizers), their impacts on agricultural production through rising soil fertility, and overall crop yield. In line with related literature worked out by different researchers.

1. Introduction

The sustainability of the agricultural sector is a clef for feeding the emerging population and economic exports of a country; therefore, the growth and survival of a nation indirectly depend on its agriculture. Over the decades, various innovations had elevated by scientists to make the agricultural sector more efficient (Ajmal et al., 2018). The major constraint of crop production in the developing world is characterized by the inaccessibility of the essential plant nutrients due to lack of sufficient quantity and type of fertilizer (Itelima et al., 2018). Fertilizer is defined in many kinds of literature as any material often applied to the soils that provide one or more essential nutrients for plant growth and development (Vanlauwe and Giller, 2006). The use of chemical pesticides and chemical fertilizers virtue of their potential for quick nutrients release and growing the plants more rapidly and efficiently served their purpose up to a point (Sneha et al., 2018). However, the continuous use of chemical fertilizers results in the deterioration of soil quality and gradual loss of soil fertility, which might further lead to the accumulation of heavy metals in plant tissue, affecting the nutritional contents of the yield and edibility (Farnia and Hasanpoor, 2015).

Biofertilizer is the microbial inoculants that contain the culture of dormant or live cells of the effective strains of N-fixing, P-solubilizing/mobilizing, K-solubilizing (Itelima et al., 2018; de Vives-Peris et al., 2020; Fasusi et al., 2021). Microorganisms at their cellular level which is often applied to seeds, soils, or compost material to accelerate the microbial activities by such organisms through their multiplication and enhance the nutrient's availability, which can be easily accessible by the plants (Boraste et al., 2009). The biological activity of microbial

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https://doi.org/10.1016/j.crsust.2021.100063
Received 21 November 2020; Received in revised form 28 June 2021; Accepted 30 June 2021
Available online 9 July 2021

NICE Journal of Business

Promoting and Preserving Business Research

ISSN: 0973-449X

A Peer-reviewed Journal
Listed in *Cabell's Directory, USA*
Included in *EBSCO's Database, USA*
Included in *Ulrich's Directory of Periodicals, USA*

Volume 16, Numbers 1 & 2
January - December, 2021

Shobhit
Institute of Engineering & Technology
Deemed to-be-University
EDUCATION EMPOWERS

HALF-YEARLY JOURNAL OF
SHOBHIT DEEMED UNIVERSITY,
MEERUT (INDIA)

JOURNAL OF COORDINATION CHEMISTRY
https://doi.org/10.1080/00958972.2021.2022128

Taylor & Francis
Taylor & Francis Group

Synthesis, spectroscopic characterization, computational studies, theoretical investigation of NLO properties and antibacterial activities of mixed ligand complexes of Co(II) and Cu(II)

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ABSTRACT

The reaction of Schiff base 2-(4-(dimethylamino)benzylideneamino)phenol (DBAP) and diethylenetriamine/ethylenediamine with cobalt(II) and copper(II) metal ion in equimolar ratio afforded mixed ligand complexes $[M(DBAP)(L)Cl(H_2O)_n]$ (**1–4**), where M = Co(II) **1**, **2**; Cu(II) **3**, **4**; L = diethylenetriamine (**1**, **3**); n = 0 and ethylenediamine (**2**, **4**); n = 1. All the newly synthesized complexes were characterized by elemental analysis, spectroscopic techniques *viz.*, UV-vis, FT-IR, ESR, PXRD and mass spectrometry. The influence of chelation of cobalt(II) and copper(II) ion on nonlinear optical properties of Schiff base (DBAP) were examined with DFT study. The polarizability (α_0) and first-order hyperpolarizability (β) of ligand and their metal complexes were calculated and compared with reference molecule *p*-nitroaniline. The hyperpolarizability of Schiff base and their metal complexes show a good nonlinear optical behavior. Theoretical investigation of the complexes was performed by DFT using B3LYP level of theory on the basis set 6-31 G (d, p)/LanL2DZ. On the basis of spectroscopic data and DFT computation, a six-coordinate geometry is tentatively proposed around the metal ion. *In vitro* antibacterial activities of these complexes were also screened against *V. cholerae* and *E. coli*, and found to have good antibacterial activity.

ARTICLE HISTORY
Received 1 February 2021
Accepted 10 December 2021

KEYWORDS
Transition metal complexes; Schiff base; DFT; NLO properties; antibacterial activities

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Supplemental data for this article is available online at https://doi.org/10.1080/00958972.2021.2022128

SN Computer Science (2021) 2:189
https://doi.org/10.1007/s42979-021-00587-8

ORIGINAL RESEARCH

Hybrid Machine Learning Classifier and Ensemble Techniques to Detect Parkinson's Disease Patients

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Received: 13 October 2020 / Accepted: 11 March 2021 / Published online: 31 March 2021

Abstract

Parkinson's disease is caused by tumors, a progressive nervous system disorder that affects development. Stiffness or slow movement is the basic sign of this problem. There is no cure for Parkinson's disease, but some drugs can improve the condition, and sometimes brain surgery can help patients improve their condition. Using machine learning strategies, we developed a priori model to identify patients affected by Parkinson's disease. By controlling the importance of features, we recognize the most significant indicators of patients who belong to this disease-related estimate. The model-based logic strategies we use include logistic regression (LR), k nearest neighbors (k-NN), support vector classifier (SVC), gradient boosting classifier (GBC), and random forest classifier (RF). The estimated reliability, like the ROC curve and confusion matrix, is five-fold cross-validation. We construct another model that depends on the ensemble method and utilization of majority voting, weighted average, bagging, Ada_boost and Gradient_boosting. The model is also recognized in the five-fold cross-validation and confusion matrix, precision; recall rate and F1 score. The correlation matrix is also drawn to show whether these features are related to each other. Our findings indicate that, compared with different methods, machine learning can provide more reliable clinical outcome assessments for patients with Parkinson's disease. Among the five algorithms, the higher accuracy fluctuates in the middle of 70–95%. Among them, SVC obtains 93.83% accuracy from the five basic classifiers, and Bagging obtains 73.28% accuracy from the ensemble technique.

Keywords Parkinson's · Machine learning · Ensemble · Majority voting · SVC · Bagging · Clinical outcome

Introduction

Parkinson's disease (PD) is a neurodegenerative disease that mainly affects neurons that transmit dopamine in specific areas of the brain. PD affects approximately 1% of individuals over 60, and the increases with age. People with PD experience a series of motor and non-motor side effects. These side effects include rigidity, tumor, slow movement, unstable posture, and aggravated steps, for example, freezing of steps, autonomic instability, emotions Problems, restlessness, and psychological deficits [1]. These side effects especially affect and reduce personal satisfaction related to health [2]. PD was first discovered by the English doctor James Parkinson, and its performance is remarkable among mature researchers [3].

In the last many years, some work has been devoted to planning answers to help PD analyze. To this end, a main framework that relies on machine learning programs has been used, which shows promising results. Several researchers have studied machine learning techniques to estimate the accuracy of the classifier and other effective indicators to detect patients with Parkinson's disease regarding the rationality of anti-acoustic estimation, Little et al. [4] proposed that it is better to mix unconventional measures with conventional harmonics to achieve the motion ratio, which can easily isolate the solid phase individual from the PWP. The part support vector machine considers the four characteristics of the harmonic to noise ratio, repetitive cycle density entropy, trend fluctuation analysis and pitch cycle entropy,

This article is part of the topical collection "Computational Biology and Biomedical Informatics" guest edited by Dhruba Kr Bhattacharyya, Sushmita Mitra and Jugal Kr Kalita.

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IOP Publishing

J. Phys. D: Appl. Phys. 54 (2021) 275502 (10pp)

Journal of Physics D: Applied Physics

https://doi.org/10.1088/1361-6463/abf959

Effects of 10 MeV Al^{4+} ions irradiation on fluorine-doped tin oxide substrates for photovoltaic device applications

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Received 27 December 2020, revised 29 March 2021
Accepted for publication 19 April 2021
Published 4 May 2021

Abstract

The effects of 10 MeV Al^{4+} ions irradiation on structural, surface morphological, optical and electrical properties of fluorine-doped tin oxide (FTO) substrates are presented for solar cell applications. The ions irradiation changes the surface morphology, average roughness, interface width, roughness exponent, and several other fractal parameters of the FTO surfaces. The UV–visible transmittance measurement shows an enhancement of transmittance in the ions irradiated substrates up to 95%. The electrical properties such as mobility, work-function, sheet resistance, and resistivity are also modified due to ions irradiation. In order to have functional applications of these ions irradiated substrates, we fabricated organic solar cells on these ions irradiated and pristine FTO substrates. The device performances are significantly improved for the case of ions irradiated FTO substrate in comparison to the pristine one. Thus, better device performance due to effective changes in physical properties suggests that the ions irradiated FTO substrates can be used as better electrodes for organic and hybrid photovoltaic device applications.

Supplementary material for this article is available online

Keywords: FTO substrates, ion irradiation, work-function, surface morphology, photovoltaic devices

(Some figures may appear in colour only in the online journal)

1. Introduction

Transparent conducting oxides (TCOs) are one of the primary materials for the fabrication of solar cells, light emitting diodes and gas sensing applications. TCOs like indium-doped tin oxide (ITO) and fluorine-doped tin oxide (FTO) are generally used for the fabrication of optoelectronic devices as a primary photo-anode [1–3]. Among the various TCOs, FTO coated on a glass substrate has better thermal and chemical stability, which makes FTO as a promising candidate for device application [4, 5]. The surface roughness, higher transmittance, and suitable work function are the key characteristics for TCOs which affect the overall device performance [6]. To improve the device performance, various efforts have been

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ISSN - 2348-2397
UGC CARE LISTED JOURNAL
GIS
Shodh Sarita
January-March, 2021
Vol. 8, Issue 29
Page Nos. 51-55
AN INTERNATIONAL BILINGUAL PEER REVIEWED REFEREED RESEARCH JOURNAL

MANAGEMENT OF SUBSTANCE USE DISORDER IN AN ADOPTED YOUNG WOMAN : A CASE STUDY

Jyotsna Gulati*
Annu Tyagi**

ABSTRACT

Objective : To study the factors and management of factors responsible for substance use disorder in an adopted female. **Method :** Both official and informal evaluations were conducted. On an informal level, a detail clinical interview was done, a mental status examination was performed, and a subjective rating of symptoms was obtained; on a formal level, drug screening questionnaire, cope inventory, perceived stress scale was performed. For the purpose of management and rapport building psycho-education, cost-benefit analysis, relaxation techniques, Supportive psychotherapy, addiction cycle, written ventilation, assertiveness training, anger management, stress management, coping skills, and relapse prevention strategies were employed. **Results :** The overall outcome of process was improvement in the desirable behavior with the rate of 50% improvement. On further exploration environmental factors were elicited which was initiating and maintain the substance seeking behavior **Conclusion :** Overall improvement was seen in the desirable behavior, but for holistic improvement and sustained recovery modifications in the environment factors was required.

Keywords : Substance use disorder, Stress, Coping Mechanisms, Environmental Factor

Introduction

Addiction is a serious condition defined by compulsive or difficult-to-control substance seeking and use, despite adverse effects. Most people make the decision to use drugs voluntarily at first, but chronic drug use can cause brain changes that test an addict's self-control and make it difficult to resist strong drug cravings.

The transition from adolescence into adulthood is a particularly formative period for a number of behaviors. In the case of substance use, both initial experimentation and continued use are thought to be due to both genetic and environmental influences.

Family, friends, as well as economic position and general quality of life, all are crucial part of a person's environment. Peer pressure, sexual and physical abuse, early drug exposure, stress, and parental supervision can all have a significant impact on a person's chance of drug use and addiction.

According to Yoon et al., adopted children have higher rate of substance use disorder associated with genetic and environmental factors.

There have been very few studies in relation to environmental influences on substance use disorder. There has not been any large scale study in India whereas, the role of genetics on substance use is well documented.

This case will focus on the environmental factors precipitating and perpetuating substance use disorder in a young female. This case is likely to provide more information and insight on environmental factors.

So, we are presenting a case study of a young girl from Nagaland having opioid dependence where adoption and poor family support are acting as precipitating and perpetuating factors.

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