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PREFACE

It gives us immense pleasure to present the proceedings of the International Conference on Materials and Mathematical Sciences (ICMMS – 2020) organized by the School of Advanced Sciences, comprises the Departments of Physics, Chemistry and Mathematics, Kalasalingam Academy of Research and Education, Krishnankoil during June 19 & 20, 2020.

As known, due to the massive potential of various materials, a diverse range of efforts has been directed towards collaborative research activities between institutions and industries including meeting between scientists / researchers and experts from dissimilar backgrounds, so that the sharing of knowledge and updates on latest progress in materials can be realized, in order to have their desired impact.

The International Conference on Materials and Mathematical Sciences (ICMMS-2020) aims to bring together foremost academic scientists, researchers, industrialists and post-graduate students to share their experiences and research results on all aspects of Materials. It also provides a leading interdisciplinary platform for researchers and educators to present and discuss the most recent innovations, trends, and concerns as well as practical challenges encountered and solutions adopted in the fields of Materials.

The proceedings book covers topics such as energy materials, nano and biomaterials, chemo and biosensors, semiconducting materials, catalytic materials, electro materials, mathematics for materialists, optical materials, crystal growth of advanced materials, materials for environmental applications, polymer and composite materials and organic & inorganic materials. Researchers working in these areas are invited to participate and deliver lectures highlighting recent advances in their field of research.

We express our sincere thanks to our Chancellor, Pro-Chancellor, Vice-Presidents, Vice-Chancellor, Registrar and Advisory Committee Members for their constant encouragement and support to organize this conference. We are grateful to all the keynote speakers and also authors of contributed papers for their participation in the conference and cooperation to bring out this book.

We thank all the members of the local advisory committee and all our colleagues in the School of Advanced Sciences and fellow colleagues in the other departments for their support and efforts in making the event successful.

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Nanostructured thin film sensors for toxic gas sensing applications: efficacy and advancements

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Abstract

Nanotechnology has enormous capabilities for development of multifunctional materials having specific characteristics which can be utilized to fabricate nanosensors for detection of poisonous gases and organic vapors. Thin film materials comprise of metal oxide semiconductors, conducting polymers, graphene based carbon nanotube materials which exhibit excellent morphological, physical and chemical properties due to which they qualify for novel gas sensing materials. The enhanced electrical conductance, large specific surface area, high aspect ratios, fast response, sensitivity and low maintenance along with high stability, chemical resistance and flexibility makes these materials the best option for being used as thin film gas sensors. These materials are embedded as thin films on substrates or electrodes and change in electrical conduction and/or flow of electrons causes the detection of gas molecules in the vicinity of the gas sensor. These materials are sometimes used as thin films in conjunction with field-effect transistor (FET) with specific electric field strength to observe the sensing current and detection of trace gases. The advantages of thin film gas sensors are manifold including detection of gases at very low concentration (traces), fast detection and reliable sensing for sensing gases such as nitrogen dioxide, hydrogen, and CO_2. Highly selective, stable and durable hybrid materials based chemi-resistor gas sensors are the upcoming future of gas sensing technology. The paper outlines and describes the upcoming gas sensing technologies for the near future applications.

Keywords: thin film gas sensors, metal oxide, conducting polymers, graphene, chemi-resistor

1. Introduction

The thin film gas sensors are utilized at ambient temperature, and these have many applications for sensing toxic gases and real-time gas monitoring of harmful gases [1,2]. These sensors have specific advantages such as high sensitivity, low energy consumption, cost effectiveness, low concentration based detection and flexibility of sensing. Different gases need to be detected and sensed in the industrial and domestic environments. The commonly sensed gases include CO, CH_4, NO, NH_4, SO_2, NO_2, CO_2, volatile organic compounds (VOC) and other hydrocarbons [3–6]. Apart from these certain hazardous gases such as hydrogen sulphide, ammonia, methane, benzene, ethanol, toluene, acetone, hydrogen and methanol are prevalent in industrial environment and from vehicular exhausts. Out of these, hydrogen and methane tend to be explosive if subjected to open air, and other gases such as NO_2, methane and toluene, are very dangerous for humans and the biosphere, even if they exist in very low concentrations in the atmosphere [7]. These toxic gases are harmful to human health when they are present in the atmosphere in more than permissible concentrations [5]. The gas sensing applications depend upon type of application such as detection of a single analyte (gas) or detection of multiple analytes (gases) during the same time of sensing; this feature of gas sensors is usually described by the selectivity of the thin film gas sensor which is defined as the capability of the gas sensor to detect what is required to be sensed over what is not required to be sensed. The variability exhibited by the gas sensing techniques is based upon physical, structural and chemical phenomenon. The changes in physical and/or chemical parameters can be measured and target gas can be identified. Different sensing techniques offers their own merits and demerits, due to which no single solution for different end uses exist.

Thin film technology in gas sensing area is getting enormous attention across the globe due to its greater applications and advantages over other technologies [8]. Utilization of thin film technologies involve fabrication, embedding the films on the substrate and/or condensation of target substances having thickness of few nanometers up to several microns onto the substrate material and their transportation. The material films with a thickness of a few nanometers to 10 μm are described as thin-films which bear different properties as compared to the bulk materials. Hence development of thin film gas sensors characterized with high sensitivity, less

energy input, high selectivity, stability, significant limit of detection (LOD), fast response and in situ and online monitoring features is very essential. Different types of gas sensors including resistive, optical, ultrasonic, acoustic wave, thermoelectric and electrochemical sensors have been fabricated [9]. The resistive gas sensor (RSG) happens to be the most commonly employed gas sensor, which is simple, cost effective and easy to fabricate and has wide applications [3]. The transduction mechanism of a RGS banks upon the change of the resistance in the sensing material's surface after adsorption and subsequent reaction along with target gas to be detected. The thickness of sensing layer decides the parameters like sensitivity, chemical stability and selectivity of the gas sensor. Hence, the materials employed for sensing and their respective structures are very critical for fabricating the gas sensor. As compared with carbon materials and organic semiconductors, semiconductor metal oxide based nanomaterials generally have higher selectivity, fast response, higher sensitivity, speed, stability, reversibility and cost-effectiveness along with easy fabrication.

2.1 Materials for gas sensors

Nanostructured thin film gas sensors utilize nanomaterials such as metal oxide semiconductors, conduction polymers, reduced graphene oxides, carbon nanotubes and quantum dots etc. [10,11]. A nanomaterial based gas sensor constitutes a sensing material embedded or fixed on a substrate/electrode e.g. metal oxide sensor. As the gas concentration in the vicinity of the sensor increases the chemical reaction or adsorption occurs and signals are produced which can be amplified and recorded. Different types of transducer units, such as chemi-resistive surface acoustic waves (CRSAW), optical, metal oxide semiconductor FET, piezoelectric, and quartz crystal microbalance and are generally employed [10,12]. Metal oxide semiconductor based thin film gas sensors possess many merits e.g. enhanced selectivity, high sensitivity, high speed of response, cost effective, less maintenance and the capability to sense gases at low concentration [2]. In conducting polymers type gas sensors, the polymer materials are embedded on the substrate surface forming a thin film.

In carbon nanotubes (CNT) bases gas sensors, by presence of oxygen group at sensor surface, sensing activity of the CNT based sensor increases. Other sensors materials employed are graphene oxide based sensors, these sensors are used to sense hydrogen, methane and NO_2. The nanomaterial-based gas sensors are highly efficient and can effectively sense LPG, methane, alcohols, ethane, propane, hydrogen, CO_2 and CO concentrations ranging from 200 to 10000 ppm. Hence by fabricating nanomaterial based gas sensors and connecting them to the user interfaces such as smart phones/PCs, alarms can be generated and preventive action can be scheduled. Highly selective, stable and durable hybrid materials based chemi-resistor based gas sensors are the upcoming nanostructured gas sensors.

2.2 Chemireistive Gas sensors

Chemiresistive gas sensors are based on the principle that they detect changes in electrical resistance of sensing material as the surrounding atmosphere is affected by the toxic or harmful gases. A potential difference is applied across thin sensor film, and measuring output signal obtained is used as required change detected. Another important variable here is the value dissipation factor which changes with frequency, and also the indicated peak position gets shifted as the thin film gas sensor is subjected to environmental gases. The obtained shift is specifically aimed for specific gas and is utilized to sense the same gas [4]. The thin film gas sensors exhibit wide applications in environmental pollutants control, air quality arena, national security, and industrial processing. Volatile organic compounds are also very harmful and need to be sensed using the gas sensors. Some of the VOCs include acetone, methylene chloride, phenol, benzene etc. having very high concentration levels. Apart from this there is increased focus on utility of chemiresistive gas sensors in health e.g. disease biomarkers and other health problems [13]. The existing VOCs in the industrial environment at very low concentrations can be detected by the chemiresistive gas sensors.

2.3 Gas sensing mechanisms

The mechanism of sensing for semiconductor metal oxide (SMO) thin chemiresistive sensors is commonly dependent upon variance in resistance when the gas sensor faces directly the incoming gas. There are some chemical interactions among the oxygen ions and the gas molecules at sensor surface. The conductance of n-type SMO nanomaterial sensor depends upon on the electron charge carriers. When the n-type SMO nanomaterial sensors are subjected to open air, the oxygen molecules get absorbed on their surfaces. The electrons are extracted by oxygen molecules from within the conduction band of sensing material layer, thus giving the chance for negatively charged ions to be formed e.g. O_2^- , O^- and O^{2-} at various sensing temperatures. With the downfall of e^- charge density, the electron depletion layer deposits on SMO nanomaterials and thus giving rise to a potential barrier. Hence conductivity of thin film sensing material (SMO) decreases, which gives rise to increased resistance. Chemical stability and electronic sensitivity of the SMO

nanomaterials is increased by addition of noble metals on sensing surface give rise to manifold enhancement in sensing properties of gas sensor materials. Another strategy is to go for surface modification of the thin film material and introduction of defects at surface of the sensor material and interface which remarkably increases their efficiency. Sometimes heterojunctions are added and vacancies are introduced which greatly improve the sensing efficiency of SMO nanomaterials sensing surface. Introduction of carbon or organic nanomaterials on surface of SMO nanomaterials greatly enhance their conductivity and increase the sensitivity at ambient temperatures [5].

2.4 Gas response and sensitivity

The most vital and required characteristic for a gas sensor is its response towards the destination gas. The response of thin film gas sensor made from semiconductor metal oxide nanostructure can be defined in different ways. One way to define response of thin film gas sensor is to determine resistance of gas present in air to target gas (Res_a/Res_g) where Res_a and Res_g depict the resistance possessed by gas sensor in the atmosphere and that in observed gas environment. The ratio Res_a/Res_g is employed to calculate sensitivity of n-type semiconductor sensor in reducing environment and for p-type sensor in oxidizing environment, e.g. NO_2 etc. The inverse of the ratio (Res_g/Res_a) is taken in the case when n-type metal oxide is used in oxidizing environment or p-type sensor in reducing environment. Hence to determine sensitivity of a thin film sensor, its resistance when exposed to air (Res_a) and in destination gas (Res_g) needs to continuously being monitored and measured [3].

2.5 Selectivity

The important parameter for a gas sensor is the selectivity. This parameter showcases the capability of sensor to differentiate between the specific destination gas and other interfering gases present in the sensing environment. The sensitivity is defined as the ratio of the monitored sensitivity to sensor signal sensitivity of interfering gases (i.e. stimulus). The selectivity exhibited by gas sensor is required to be more than 1. The higher selectivity means a greater response of the gas sensor towards the destined gas as compared to gas sensor response towards the interfering gases. Generally, the gas sensor surfaces are sensitive towards multiple gases and show cross-sensitivity. Therefore, achieving higher selectivity for the gas sensors becomes very difficult, due to which the applications of gas sensors tend to become limited [3]. The generally applied strategies for enhancing the selectivity of gas sensors are (i) utilization of noble-metal catalysts to increase the functionality of the gas sensors [14], (ii) control of sensing temperature, (iii) making heterojunctions and use of additives for enhancing selectivity (iv) employing different filters (v) addition of carbon nanoparticles, fibres and metal oxides.

3. Fabrication of thin film gas sensors

3.1. Metal oxide based gas sensor

A gas sensor usually converts concentration of target or harmful gas into the standard electrical signals by employing some physical or chemical effects [6]. For a semiconductor metal oxide sensor, the property of electrical conductivity possessed by sensor material gets altered, upon exposed of sensor surface to target gas [15]. The nanostructure based metal oxide thin films produce highly sensitive and selective sensing surface due to enhanced surface area and active sites and specific structure. There is increased adsorption of different gas molecules on the sensing surface. The adsorbed species provide the increased sensing capability for gas sensor. Response time of metal oxide sensor happens to be shorter than conventional microstructure gas sensors i.e. response is very quick. The sensor schematic is shown in Fig.1 below:

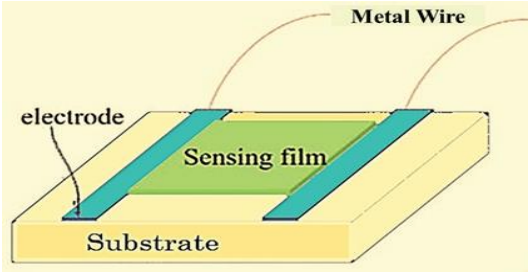

Figure 1. Metal oxide based gas sensors [16]

3.2 Conducting polymer based chemiresistor

Another type of thin film gas sensors is conducting polymer type. This sensor (chemiresistor) simply utilizes a thin film of a conducting polymer type material such as polypyrrole, polyaniline and polythiophene. The chemiresistor sensors are used to sense different analytes such as amines, alcohols, aromatic compounds, medicine, ionic species, organic vapor and gases [17]. The thin film gas sensors employing conducting polymers consist of a thin film deposited on a substrate. The physical structure of the gas sensor can consist of either thin film with two electrodes as shown in Figure 2 or employ a field-effect transistor having controlled electric strength to monitor the sensing current

through the gas sensor (Figure 3). The sensitivity of the conducting polymer constituted thin film sensor primarily lies upon sensing surface area of physical sensor and upon thickness of the sensing material film. The schematic of the gas sensor is shown in Figure 3 as below:

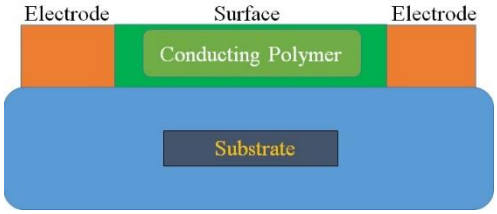

Figure 2. Conducting polymer based chemiresistor

3.3 Conducting polymer based thin film transistor and diode gas sensor

Transistors and diodes exhibit or provide extra parameters for the current signal measurements as compared to chemiresistor polymer and possess very good detection capability and increased sensitization due to the signal amplification of transistor devices [4]. The conducting polymers happen to be simpler than the transistors. Depending upon the semiconductor material and its surface properties, the conducting polymer based thin film transistor gas sensors works on the principle that upon applying the potential difference across the sensor and then measuring the output current signals, the sensor measures the concentration of the gas. Output amperage gets altered as conducting polymer film gets across the given analyte as shown in Figure 3. Conducting polymer thin film sensors are classified according to the fact that current flows through the sensor or does not [4].

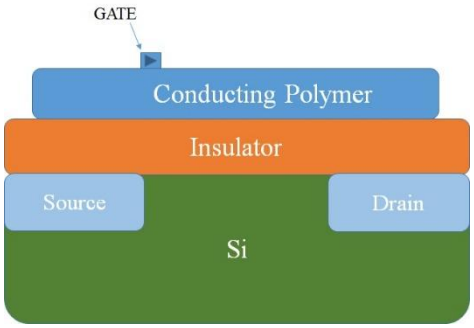

Figure 3. Conducting polymer based thin film transistor (TFT) with active polymer layer

3.4 Carbon nanotubes based gas sensor

It was reported by the researchers that 1-Dimensional (1-D) carbon nano tube (CNT) and 2-D graphene based CNTs can efficiently detect the presence of harmful gases at low concentrations at ambient temperatures [11,16,18]. CNTs possess characteristics such as high sensitivity, good absorption efficiency, flexible and strong physical structures and have large applications in gas sensing field. The CNTs are composed of hexagonal networks of the carbon atoms, CNTs measure about 1nm in diameter and possess 1 to 100 mm lengthwise. Single-walled carbon nano tubes possess single layer of graphene cylindrical sheets as compared to multi-walled carbon nano tubes which can possess up to 50 layers. Physical CNTs possess stable structure under large electric fields and are known to be the best field emitters. The adsorption of gas species at sensor surface changes electrical conductivity property of gas sensor which is detected. Mechanism of the CNT based gas sensor using Single-walled carbon nanotube (SWCNT) and single stranded DNA (SS-DNA) is shown in Figure. 4.

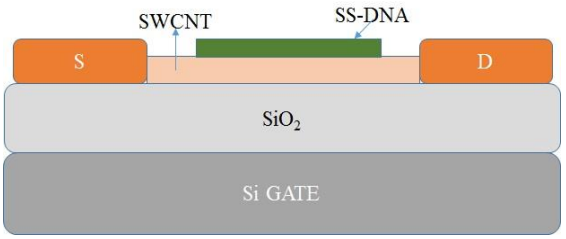

Figure 4. Carbon nano tube (CNT) based gas sensors

4. Conclusion

The paper summarizes the latest technologies utilized in fabrication of thin film sensors and their characteristic features. Various types of thin film gas sensors depending upon starting (sensor) material like metal oxide semiconductors, polymers, and graphene based nanotubes and their applications in detecting toxic and industrial gases such as NO_2, CH_4, NO, NH_3, SO_2, H_2, CO_2 etc. have been discussed. The materials used for making thin films e.g. polymers, CNTs etc., transducer types e.g. resistors and diodes and other details of assembly of gas sensors and working principles of different types of thin film gas sensors have been explained. The mechanisms of different gas sensors have been explained with suitable illustrations. The parameters affecting the performance of thin film gas sensors such as sensitivity, selectivity, speed of response and how to increase the functionality of gas sensors have been discussed in length. Hence this paper provides useful knowledge towards the thin film gas sensing technologies and their applications. The in-depth research on advent of novel gas-sensors is going on and commercial sensors needs to be developed at low cost

and with improved functionalities to provide safety and security to residential and industrial establishments.

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Structural and electronic property investigations of 10,10'-(3-bromo-5-methyl-4-oxo piperidine-2,6-diyl)-bis-(anthracene-9-carbaldehyde) by DFTmethod

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ABSTRACT

The target molecule has best binding energy of -11.4 Kcal/mol with 2B7N protein of *H.Pylori* which causes peptic ulcerto human beings. The theoretical studies of the target molecule were carried out by using Gaussian 16W and viewed by Gauss view 06 software. Bond length, bond angle and dihedral angle of optimized geometry was performed by DFT method with B3LYP/6-311++G(d,p) basis set. The charge transfer and electronic properties of the target molecule were explained by the basis of highest occupied molecular orbital and lowest unoccupied molecular orbital. In addition to that, molecular electrostatic potential, Mulliken population and Fukui function analysis were calculated and discussed for predicting the reactive site. NBO analysis was used to study the charge delocalization and stability of molecule. The calculated hyper polarisability of the target molecule was found to be 20 times greater than that of standard reference NLO material Urea. So the title compound possesses considerable NLO properties. NCI and shaded surface map with projection effect of electron localization function also studied by Multiwfn 3.7 software.

Keywords: DFT, ESP, HOMO-LUMO, Mulliken population analysis, NBO, NLO, Fukui, NCI.

1. INTRODUCTION

Piperidine and its derivatives are most widely used in the field of pharmacological industry due to their large number of biological activities. Numerous piperidine based derivatives have been reported as antimicrobial, anti viral and anti fungal, herbicidal, antitubercular, insecticidal, fungicidal, anti inflammatory, bactericidal, anticancer, antihistaminic, hypotensive, CNS stimulant, nerve activities and anti depressant [1]. In last decade thousands of piperidine compounds have been mentioned in clinical and preclinical studies and it leads to the development of new drugs [2]. In recent years 2,6-diphenyl piperidone and their substituted compounds have been studied by the researchers due to the potent analgesic character [3]. This high degree of biological activity of the piperidine compounds attracts us to do the present work. More than forty thousand piperidine-4-one compounds were virtually drawn by chemsketch and docked with 2B7N protein of *H.pylori* with PyRx software and viewed by Pymol. The target compound is having higher binding affinity (-11.4 Kcal/mol) with better inhibitor activity against 2B7N protein.

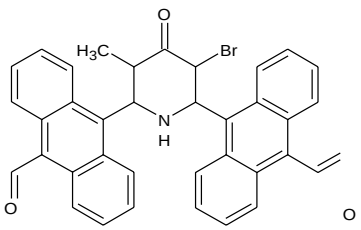
2. COMPUTATIONAL METHOD

In this present investigation, computational based (Density Functional Theory) theoretical studies have been employed for the target compound. The computational quantum chemical calculations were performed by Gaussian 16W program package [4] with DFT method and Becke3- Lee-Yang-Parr (B3LYP) [5] with standard 6-311++G(d,p) basis set was opted. The molecule was completely converged and fully optimized. Imaginary frequency calculations also performed and no negative frequencies are seen. The optimized geometrical parameters like bond length, bond angle and dihedral angle are calculated. The HOMO-LUMO analysis has been carried out and the energy gap explains the charge transfer takes place within the molecule. Using HOMO-LUMO values the electronegativity, chemical potential, chemical hardness, softness, ionization potential, electron affinity, electrophilicity index, electron donating capability, electron accepting capability have been determined. The reactive sites of thecompound have been predicted by electrostatic potential map and Fukui function. The Mulliken population analysis, natural population analysis and NLO also performed by DFT with B3LYP/6-311++G(d,p) basis set. Using Multiwfn 3.7 software the NCI and shaded surface map with projection effect of electron localization function also studied.

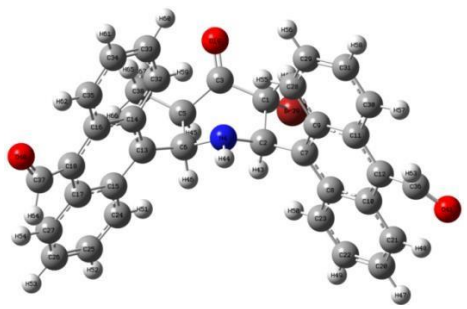
3. RESULTS AND DISCUSSION

Molecular Geometry

The optimized molecular structure for the target molecule along with numbering of atoms generated by Gaussian 16W software and viewed by Gauss view 6 program. The 2D and 3D representations of optimized structure are shown in Figure 1(a,b). The target molecule consists of 67 atoms, 308 electrons, singlet and it is a neutral molecule.



a). 2D structure



b). 3D structure representation

Figure 1. 2D and 3D representation of optimized structure for target molecule by B3LYP/6-311++G(d,p) basis set

The Table 1 shows the list of atoms of the target molecule. From the Table 1 carbons 1, 2, 3, 5, 6 are present in piperidine ring and the other carbons are present in anthracene ring.

Table 1. list of the optimized target molecule

1	2	3	4	5	6	7	8	9	10
C	C	C	N	C	C	C	C	C	C
11	12	13	14	15	16	17	18	19	20
C	C	C	C	C	C	C	C	C	C
21	22	23	24	25	26	27	28	29	30
C	C	C	C	C	C	C	C	C	C
31	32	33	34	35	36	37	38	39	40
C	C	C	C	C	C	C	C	Br	O
41	42	43	44	45	46	47	48	49	50
O	H	H	H	H	H	H	H	H	H
51	52	53	54	55	56	57	58	59	60
H	H	H	H	H	H	H	H	H	H
61	62	63	64	65	66	67			
H	H	H	H	H	H	H			

The distance between the nuclei of two bonded atom in amolecule is called as bond length. The bond length of optimized target molecule is given in Table 2.

Table 2. The bond distance of optimized target molecule by B3LYP/6-311++G(d,p) basis set

Atom set	Bond distance (A°)	Atom set	Bond distance (A°)
C1 - C2	1.5499	C18 - C37	1.4853
C1 - C3	1.5333	C20 - C21	1.3665
C1- Br39	1.9923	C20 - C22	1.4152
C1 - H42	1.0849	C20 - H47	1.0841
C2 - N4	1.4768	C21 - H48	1.078
C2 - C7	1.5275	C22 - C23	1.3659
C2 - H43	1.0908	C22 - H49	1.0841
C3 - C5	1.5274	C23 - H50	1.0788
C3 - O19	1.2079	C24 - C25	1.3669
N4 - C6	1.477	C24 - H51	1.0803
N4 - H44	1.0152	C25 - C26	1.4155
C5 - C6	1.587	C25 - H52	1.0839
C5 - C38	1.5283	C26 - C27	1.3669
C5 - H45	1.098	C26 - H53	1.0839
C6 - C13	1.5298	C27 - H54	1.0804
C6 - H46	1.0927	C28 - C29	1.3662
C7 - C8	1.4198	C28 - H55	1.0775
C7 - C9	1.4177	C29 - C31	1.4159
C8 - C10	1.4502	C29 - H56	1.0838
C8 - C23	1.4353	C30 - C31	1.3666
C9 - C11	1.4446	C30 - H57	1.0804
C9 - C28	1.4349	C31 - H58	1.084
C10 - C12	1.4172	C32 - C33	1.366
C10 - C21	1.4314	C32 - H59	1.076
C11 - C12	1.4176	C33 - C34	1.4161
C11 - C30	1.4328	C33 - H60	1.0841
C12 - C36	1.487	C34 - C35	1.3677
C13 - C14	1.4157	C34 - H61	1.0843
C13 - C15	1.4192	C35 - H62	1.0781
C14 - C16	1.4487	C36 - O41	1.2149
C14 - C32	1.4326	C36 - H63	1.1044
C15 - C17	1.4456	C37 - O40	1.2154
C15 - C24	1.4349	C37 - H64	1.1046
C16 - C18	1.4181	C38 - H65	1.0899
C16 - C35	1.4308	C38 - H66	1.0918
C17 - C18	1.4187	C38 - H67	1.0914
C17 - C27	1.4323		

From the Table 2, it is clear that, the longest bond is obtained from C1- Br39 with bond length 1.9923 Å, the highest value is due to the presence of the electron withdrawing nature of bromine. The C - C bond length in the piperidine ring lay in the range of 1.5274 Å to 1.587 Å respectively.

The bond length of N4 - C6 and C2 - N4 are found to be 1.477 Å and 1.4768 Å respectively. The C - H bond length in the anthracene ring lay in the range between 1.076 Å to 1.0843 Å. The bond distances of piperidone are having good agreement with previous literature [3]

Table 3. The bond angle of optimized target molecule by B3LYP/6-311++G(d,p) basis set

Atom set	Bond angle (°)	Atom set	Bond angle (°)
C2 - C1 - C3	111.093	C16 - C18 - C17	119.8446
C2 - C1 - Br39	111.4651	C16 - C18 - C37	122.1643
C2 - C1 - H42	113.6687	C17 - C18 - C37	117.9036
C3 - C1- Br39	107.5438	C21 - C20 - C22	120.2126
C3 - C1- H42	108.7547	C21 - C20 - H47	119.8369
Br39 - C1- H42	103.9135	C22 - C20 - H47	119.9463
C1 - C2 - N4	105.1075	C10 - C21 - C20	121.5932
C1- C2 - C7	114.76	C10 - C21 - H48	118.4339
C1 - C2 - 43H	106.8215	C20 - C21 - H48	119.9536
N4 - C2 - C7	113.292	C20 - C22 - C23	120.2299
N4 - C2 - H43	108.3922	C20 - C22 - H49	120.0232
C7 - C2 - H43	108.1339	C23 - C22 - H49	119.7459
C1 - C3 - C5	115.8012	C8 - C23 - C22	122.1893
C1 - C3 - C19	120.3825	C8 - C23 - H50	120.2279
C5 - C3 - C19	123.8153	C22 - C23 - H50	117.5663
C2 - N4 - C6	110.2882	C15 - C24 - C25	122.1943
C2 - N4 - H44	110.8485	C15 - C24 - H51	119.9929
C6 - N4 - H44	110.5978	C25 - C24 - H51	117.7625
C3 - C5 - C6	109.4322	C24 - C25 - C26	120.0771
C3 - C5 - C38	112.3921	C24 - C25 - H52	119.9487
C3 - C5 - C45	104.066	C26 - C25 - H52	119.9604
C6 - C5 - C38	116.5635	C25 - C26 - C27	120.0436
C6 - C5 - H45	105.5904	C25 - C26 - H53	119.9682
C38 - C5 - H45	107.8015	C27 - C26 - H53	119.9689
N4 - C6 - C5	108.7772	C17 - C27 - C26	121.9856
N4 - C6 - C13	111.8095	C17 - C27 - H54	119.6984
N4 - C6 - H46	107.1696	C26 - C27 - H54	118.2642
C5 - C6 - C13	116.7693	C9 - C28 - C29	121.974
C5 - C6 - H46	105.6447	C9 - C28 - H55	119.0454
C13 - C6 - H46	106.0452	C29 - C28 - H55	118.964
C2 - C7 - C8	119.487	C28 - C29 - C31	120.1631
C2 - C7 - C9	120.5125	C28 - C29 - H56	119.8748
C8 - C7 - C9	120.0002	C31 - C29 - H56	119.9595
C7 - C8 - C10	120.0004	C11 - C30 - C31	121.8637
C7 - C8 - C23	122.8305	C11 - C30 - H57	119.7505
C10 - C8 - C23	117.1687	C31 - C30 - H57	118.3584
C7 - C9 - C11	119.9262	C29 - C31 - C30	120.0815
C7 - C9 - C28	122.3811	C29 - C31 - H58	119.9886
C11 - C9 - C28	117.6862	C30 - C31 - H58	119.9289
C8 - C10 - C12	119.6932	C14 - C32 - C33	121.8163
C8 - C10 - C21	118.5677	C14 - C32 - H59	119.0817
C12 - C10 - C21	121.7304	C33 - C32 - H59	119.0979
C9 - C11 - C12	120.0399	C32 - C33 - C34	120.1464
C9 - C11 - C30	118.098	C32 - C33 - H60	119.8364
C12 - C11 - C30	121.8333	C34 - C33 - H60	120.0166
C10 - C12 - C11	120.1513	C33 - C34 - C35	120.4945
C10 - C12 - C36	121.9775	C33 - C34 - H61	119.8301
C11 - C12 - C36	117.7571	C35 - C34 - H61	119.6692
C6 - C13 - C14	122.2716	C16 - C35 - C34	121.3477
C6 - C13 - C15	118.1541	C16 - C35 - H62	118.4449
C14 - C13 - C15	119.5563	C34 - C35 - H62	120.1724
C13 - C14 - C16	120.2897	C12 - C36 - O41	127.2465
C13 - C14 - C32	121.9187	C12 - C36 - H63	114.1306
C16 - C14 - C32	117.7809	O41 - C36 - H63	118.5947
C13 - C15 - C17	119.8569	C18 - C37 - O40	127.446
C13 - C15 - C24	122.5776	C18 - C37 - H64	114.0168
C17 - C15 - C24	117.5457	O40 - C37 - H64	118.4972
C14 - C16 - C18	119.5408	C5 - C38 - H65	111.8548
C14 - C16 - C35	118.3499	C5 - C38 - H66	110.6985
C18 - C16 - C35	122.1038	C5 - C38 - H67	109.8223
C15 - C17 - C18	120.0227	H65 - C38 - H66	108.4832
C15 - C17 - C27	118.1486	H65 - C38 - H67	107.5593
C18 - C17 - C27	121.7912	H66 - C38 - H67	108.3037

Bond angle is the formation of angle between the three adjacent atoms in a molecule. The bond angle for the optimized target molecule is listed in Table 3. From the Table 3, it is clear that, the largest bond angle is seen in C12 - C36 - O41 with an angle of 127.2465° and the shortest bond angle is observed in Br39 - C1 - H42 with an angle of 103.9135°. The angles between C1 - C2 - N4 and C2 - N4 - C6 are 105.1075° and 110.2882° respectively. The N - C - C angles for N4 - C2- C7, N4 - C6 - C5 and N4 - C6 - C13 are 113.292°, 108.7772° and 111.8095° respectively. N - C - C bond angles are longer than C - C - N and C - N - C bond angles. The bond angles are in good manner.

Table 4. The dihedral angle of optimized target molecule by B3LYP/6-311++G(d,p) basis set

Atom set	dihedral angle (°)	Conformation
C3 - C1 - 2C - N4	-26.9714	SC
C3 - C1 - C2 - C7	-152.1095	AP
C3 - C1 - C2 - H43	88.0553	SP
Br39 - C1 - C2 - C4	-146.8942	AC
Br39 - C1 - C2 - C7	87.9677	SP
Br39 - C1 - C2 - H43	-31.8675	SP
H42 - C1 - C2 - C4	96.0757	AC
H42 - C1 - C2 - C7	-29.0623	SC
H42 - C1 - C2 - H43	-148.8975	AC
C2 - C1 - C3 - C5	-34.2906	SP
C2 - C1 - C3 - C19	145.3719	AC
Br39 - C1 - C3 - C5	87.9376	SP
Br39 - C1 - C3 - C19	-92.4	AC
H42 - C1 - C3 - C5	-160.1202	AP
H42 - C1 - C3 - C19	19.5423	SC
C1 - C2 - N4 - C6	77.6344	SP
C1 - C2 - C4 - H44	-159.5362	AP
C7 - C2 - C4 - C6	-156.3133	AP
C7 - C2 - C4 - H44	-33.4839	SP
H4 - C2 -C4 - C6	-36.2974	SP
H43 - C2 - C4 - H44	86.532	SP
C1 - C2 - C7 - C8	-113.5562	AC
C1 - C2 - C7 - C9	66.2371	SP
C4 - C2 - C7 - C8	125.7108	AC
C4 - C2 - C7 - C9	-54.4959	SP
H43 - C2 -C7 -C8	5.5478	SC
H43 - C2 -C7 - C9	-174.6589	AP
C1 - C3 - C5 - C6	51.676	SP
C1 - C3 - C5 - C38	-177.1594	AP
C1 - C3 - C5 - H45	-60.7936	SP
C19 - C3 - C5 - C6	-127.9736	AC
C19 - C3 - C5 - C38	3.191	SC

C19 - C3 - C5 - H45	119.5569	AC	C8 - C10 - C21 - H48	179.7174	AP
C2 - C4 - C6 - C5	-59.1449	SP	C12 - C10 - C21 - C20	-179.7533	AP
C2 - N4 - C6 - C13	170.4309	AP	C12 - C10 - C21 -H48	-1.3544	SC
C2 - C4 - C6 - H46	54.631	SP	C9 - C11 - C12 - C10	4.8395	SC
H44 - C4 - C6 - C5	177.8791	AP	C9 - C11 - C12 - C36	-171.3545	AP
H44 - C4 - C6 - C13	47.4549	SP	C30 - C11 - C12 -C10	-173.1733	AP
H44 - C4 - C6 - H46	-68.3449	SP	C30 - C11 - C12 -C36	10.6327	SC
C3 - C5 - C6 - C4	-5.316	SC	C9 - C11 - C30 - C31	2.9446	SC
C3 - C5 - C6 - C13	122.3472	AC	C9 - C11 - C30 -H57	-175.1169	AP
C3 - C5 - C6 - H46	-120.0877	AC	C12 - C11 - C30 - C31	-179.0055	AP
C38 - C5 - C6 - C4	-134.2194	AP	C12 - C11 - C30 - H57	2.933	SC
C38 - C5 - C6 - C13	-6.5561	SC	C10 - C12 - C36 - O41	26.7813	SC
C38 - C5 - C6 - H46	111.0089	AC	C10 - C12 - C36 - H63	-151.2406	AP
H45 - C5 - C6 - C4	106.1531	AC	C11 - C12 - C36 - O41	-157.0986	AP
H45 - C5 - C6 - C13	-126.1837	AC	C11 - C12 - C36 - H63	24.8795	SC
H45 - C5 - C6 - H46	-8.6186	SC	C6 - C13 - C14 - C16	-170.2847	AP
C3 - C5 - C38 - H65	-61.287	SP	C6 - C13 - C14 - C32	10.9322	SC
C3 - C5 - C38 - H66	177.6026	AP	C15 - C13 - C14 - C16	8.1446	SC
C3 - C5 - C38 - H67	58.0603	SP	C15 - C13 - C14 - C32	-170.6385	AP
C6 - C5 - C38 - H65	66.1781	SP	C6 - C13 - C15 - C17	170.2997	AP
C6 - C5 - C38 - H66	-54.9323	SP	C6 - C13 - C15 - C24	-11.3591	SC
C6 - C5 - C38 - H67	-174.4746	AP	C14 - C13 - C15 - C17	-8.194	SC
H45 - C5 - C38 -H65	-175.3895	AP	C14 - C13 - C15 - C24	170.1472	AP
H45 - C5 - C38 -H66	63.5001	SP	C13 - C14 - C16 - C18	-0.4852	SC
H45 - C5 - C38 -H67	-56.0422	SP	C13 - C14 - C16 - C35	178.6777	AP
C4 - C6 - C13 - C14	46.0994	SP	C32 - C14 - C16 - C18	178.3473	AP
C4 - C6 - C13 - C15	-132.3509	AC	C32 - C14 - C16 - C35	-2.4898	SC
C5 - C6 - C13 - C14	-80.0711	SP	C13 - C14 - C32 - C33	179.4541	AP
C5 - C6 - C13 - C15	101.4786	AC	C13 - C14 - C32 - H59	0.1952	SC
H46 - C6 - C13 -C14	162.5826	AC	C16 - C14 - C32 - C33	0.6418	SC
H46 - C6 - C13 - C15	-15.8677	SC	C16 - C14 - C32 - H59	-178.6171	AP
C2 - C7 - C8 - C10	-177.2147	AP	C13 - C15 - C17 - C18	0.6133	SC
C2 - C7 - C8 - C23	2.5493	SC	C13 - C15 - C17 - C27	178.4262	AP
C9 - C7 - C8 - C10	2.9909	SC	C24 - C15 - C17 - C18	-177.8102	AP
C9 - C7 - C8 - C23	-177.2451	AP	C24 - C15 - C17 - C27	0.0026	SC
C2 - C7 - C9 - C11	179.5235	AP	C13 - C15 - C24 - C25	-178.8082	AP
C2 - C7 - C9 - C28	-1.4209	SC	C13 - C15 - C24 - H51	-1.4473	SC
C8 - C7 - C9 - C11	-0.6842	SC	C17 - C15 - C24 - C25	-0.4307	SC
C8 - C7 - C9 - C28	178.3713	AP	C17 - C15 - C24 - H51	176.9302	AP
C7 - C8 - C10 - C12	-1.4096	SC	C14 - C16 - C18 - C17	-7.1268	SC
C7 - C8 - C10 - C21	177.5411	AP	C14 - C16 - C18 - C37	169.3996	AP
C23 - C8 - C10 -C12	178.8133	AP	C35 - C16 - C18 - C17	173.7429	AP
C23 - C8 - C10 -C21	-2.2361	SC	C35 - C16 - C18 - C37	-9.7307	SC
C7 - C8 - C23 - C22	-178.1666	AP	C14 - C16 - C35 - C34	2.3475	SC
C7 - C8 - C23 - H50	3.3424	SC	C14 - C16 - C35 - H62	-179.8022	AP
C10 - C8 - C23 -C22	1.6037	SC	C18 - C16 - C35 - C34	-178.5123	AP
C10 - C8 - C23 -H50	-176.8873	AP	C18 - C16 - C35 - H62	-0.662	SC
C7 - C9 - C11 - C12	-3.2479	SC	C15 - C17 - C18 - C16	7.0765	SC
C7 - C9 - C11 - C30	174.8383	AP	C15 - C17 - C18 - C37	-169.5964	AP
C28 - C9 - C11 -C12	177.6528	AP	C27 - C17 - C18 - C16	-170.6546	AP
C28 - C9 - C11 -C30	-4.261	SC	C27 - C17 - C18 - C37	12.6725	SC
C7 - C9 - C28 - C29	-176.2964	AP	C15 - C17 - C27 - C26	0.6189	SC
C7 - C9 - C28 - H55	5.2013	SC	C15 - C17 - C27 - H54	-176.7188	AP
C11 - C9 - C28 -C29	2.7793	SC	C18 - C17 - C27 - C26	178.3909	AP
C11 - C9 - C28 -H55	-175.723	AP	C18 - C17 - C27 - H54	1.0532	SC
C8 - C10 - C12 -C11	-2.5223	SC	C16 - C18 - C37 - O40	24.0673	SC
C8 - C10 - C12 -C36	173.5069	AP	C16 - C18 - C37 - H64	-153.5747	AP
C21 - C10 - C12 -C11	178.5612	AP	C17 - C18 - C37 - O40	-159.3419	AP
C21 - C10 - C12 -C36	-5.4096	SC	C17 - C18 - C37 - H64	23.0161	SC
C8 - C10 - C21 - C20	1.3185	SC	C22 - C20 - C21 - C10	0.3683	SC

C22 - C20 - C21 - H48	-178.0067	AP
H47 - C20 - C21 - C10	179.6308	AP
H47 - C20 - C21 - H48	1.2558	SC
C21 - C20 - C22 - C23	-1.0817	SC
C21 - C20 - C22 - H49	178.5465	AP
H47 - C20 - C22 - C23	179.6566	AP
H47 - C20 - C22 - H49	-0.7152	SC
C20 - C22 - C23 - C8	0.0504	SC
C20 - C22 - C23 - H50	178.5796	AP
H49 - C22 - C23 - C8	-179.5788	AP
H49 - C22 - C23 - H50	-1.0497	SC
C15 - C24 - C25 - C26	0.2563	SC
C15 - C24 - C25 - H52	178.8994	AP
H51 - C24 - C25 - C26	-177.1608	AP
H51 - C24 - C25 - H52	1.4823	SC
C24 - C25 - C26 - C27	0.3724	SC
C24 - C25 - C26 - H53	178.7734	AP
H52 - C25 - C26 - C27	-178.2705	AP
H52 - C25 - C26 - H53	0.1305	SC
C25 - C26 - C27 - C17	-0.8157	SC
C25 - C26 - C27 - H54	176.5587	AP
H53 - C26 - C27 - C17	-179.2167	AP
H53 - C26 - C27 - H54	-1.8422	SC
C9 - C28 - C29 - C31	0.2532	SC
C9 - C28 - C29 - H56	179.6696	AP
H55 - C28 - C29 - C31	178.7566	AP
H55 - C28 - C29 - H56	-1.8269	SC
C28 - C29 - C31 - C30	-1.7565	SC
C28 - C29 - C31 - H58	177.8793	AP
H56 - C29 - C31 - C30	178.8275	AP
H56 - C29 - C31 - H58	-1.5366	SC
C11 - C30 - C31 - C29	0.0988	SC
C11 - C30 - C31 - H58	-179.5372	AP
H57 - C30 - C31 - C29	178.1864	AP
H57 - C30 - C31 - H58	-1.4497	SC
C14 - C32 - C33 - C34	1.4592	SC
C14 - C32 - C33 - H60	-178.2699	AP
H59 - C32 - C33 - C34	-179.2821	AP
H59 - C32 - C33 - H60	0.9888	SC
C32 - C33 - C34 - C35	-1.6777	SC
C32 - C33 - C34 - H61	179.2359	AP
H60 - C33 - C34 - C35	178.051	AP
H60 - C33 - C34 - H61	-1.0355	SC
C33 - C34 - C35 - C16	-0.2691	SC
C33 - C34 - C35 - H62	-178.0827	AP
H61 - C34 - C35 - C16	178.8188	AP
H61 - C34 - C35 - H62	1.0052	SC

The dihedral angle is the angle between planes through two sets of three atoms, having two atoms in common. The dihedral angles for the optimized target molecule aretabulated in Table 4. From the Table 4, it is clear that, the synperiplanar (SP), antiperiplanar (AP), synclinal (SC) and anticlinal (AC) conformations are present in the target molecule. The dihedral angles between the atoms are found to be good.

Mulliken's charge distribution

The electronic population of each atom for the optimized title compound is obtained by Mulliken atomic charge method by DFT/ B3LYP using 6-311++G(d,p) method. Mulliken Population Analysis (MPA) explains the net charge and charge distribution in the molecule. It plays an important role in the application of quantum chemical calculation to molecular system [6]. It explains atomic charges, electronic structure, dipole moment, and polarisability of the molecule and it elucidates lot of properties of molecular structure [7]. The total atomic charge of the target molecule obtained from MPA with DFT method B3LYP using 6-311++G(d,p) basis set werelisted in Table 5.

Table 5. Mulliken's charge distribution for target molecule

Atom no		Mulliken charge (a.u.)	Atom no		Mulliken charge (a.u.)
1	C	-0.607135	35	C	-0.543420
2	C	-0.031399	36	C	-0.397798
3	C	-0.555771	37	C	-0.306511
4	N	-0.016725	38	C	-0.681139
5	C	-0.091285	39	Br	-0.045339
6	C	-0.270907	40	O	-0.208923
7	C	0.494328	41	O	-0.201946
8	C	0.742754	42	H	0.342764
9	C	0.451510	43	H	-0.099295
10	C	0.964932	44	H	0.269018
11	C	0.605332	45	H	0.261810
12	C	0.679872	46	H	0.085709
13	C	0.315728	47	H	0.177830
14	C	-0.069273	48	H	0.182247
15	C	0.372558	49	H	0.179234
16	C	0.820191	50	H	0.061434
17	C	0.297895	51	H	0.129489
18	C	0.501539	52	H	0.181199
19	O	-0.086928	53	H	0.176339
20	C	-0.416518	54	H	0.142697
21	C	-0.585442	55	H	-0.082313
22	C	-0.309682	56	H	0.193164
23	C	-0.678083	57	H	0.133813
24	C	-0.359080	58	H	0.180157
25	C	-0.352630	59	H	0.059660
26	C	-0.493883	60	H	0.193524
27	C	-0.290540	61	H	0.175706
28	C	-0.348748	62	H	0.205142
29	C	-0.264503	63	H	0.087321
30	C	-0.697089	64	H	0.086500
31	C	-0.386848	65	H	0.186296
32	C	-0.197426	66	H	0.140476
33	C	-0.037484	67	H	0.173828
34	C	-0.537933			

From the Table 5, the charge distribution of the target molecule shows that the carbon atom attached with hydrogen atom is having negative charge and other carbons are having positive charge [8]. C14 shows very low negative value due to the delocalization of electrons. The maximum positive charge is obtained from C10 carbon when compared with all the other carbon. The nitrogen, bromine and all the three oxygen shows negative charges which are donor atoms [9]. The order is O40 > O41 > O19 > Br39 > N4. The atoms O40 and O41

are having more negative charges when compared to O19, because it is present in piperidine (alicyclic) ring and O40, O41 are present in anthracene ring (aromatic). H43 and H55 unusually show very low negative values due to the asymmetric distribution of electrons in chemical bonds [10]. All the other hydrogen atoms show positive charge. H42 shows more positive value because it is attached with carbon atom which bears electronegative bromine atom. The bar diagram of Mulliken charge distribution is presented in the Figure 2.

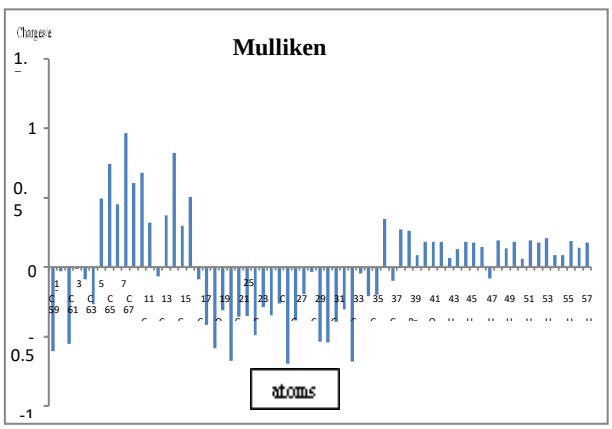


Figure 2. The Mulliken atomic charge distribution of target molecule

Molecular Electrostatic Potential

The molecular electrostatic potential (MEP) is generally located in the space around the molecule. The MEP is the useful way to illustrate the charge distributions of a molecule. It is also used to visualize various charged region of a molecule [11]. The charge distribution explains how the molecules interact with another molecule. It is used to understand the sites of nucleophilic attack and electrophilic reaction for the study of biological recognition process and hydrogen bonding interactions [3].

The MEP for the title compound is calculated by B3LYP/6-311++G(d,p) method and shown in Figure 3. From the Figure 3, the different colours represent the different values of electrostatic potential of the compound. Simultaneously, it displays molecular size and shape of the target molecule. It is very useful to analyze the molecular structure with its physiochemical property respectively [12-14]. The most electronegative potential is present in the red region and most electropositive potential present in the blue region. The potential increases from red to blue, the order is given as red < orange < yellow < green < blue.

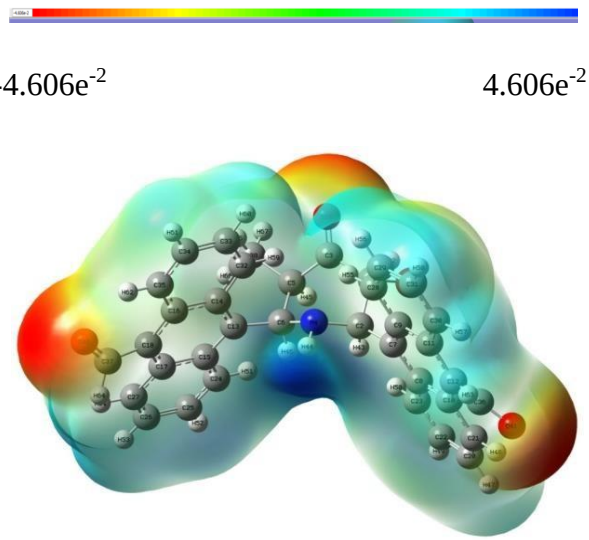
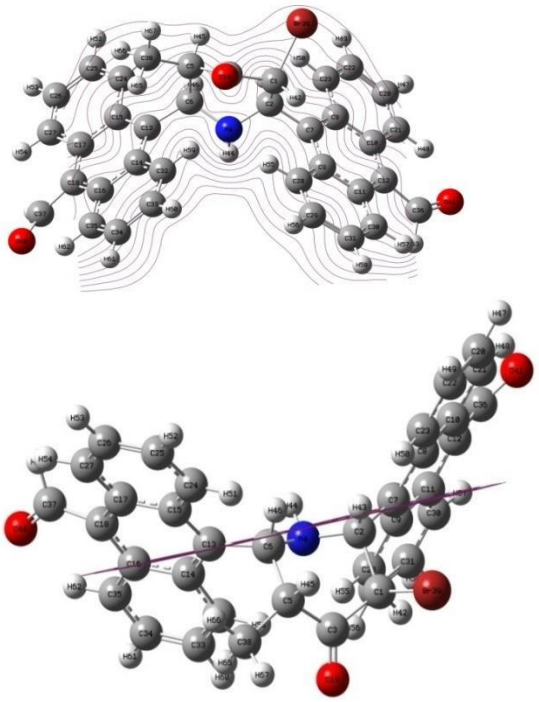


Figure 3. Electrostatic potential of target molecule

The colour code of this map lies in the range between $-4.606e^{-2}$ to $4.606e^{-2}$. In the target compound, blue colour represents the strongest attraction, red colour represents the strongest repulsion; and the green colour signifies the neutral electrostatic potential and the yellow colour indicates repulsion [15].

From the Figure 3, the target compound has several possible sites for electrophilic reactivity. The maximum negative electrostatic potential regions are mainly localized over the oxygen atoms and the positive electrostatic potential sites are on hydrogen atoms and nitrogen atom, which prefers nucleophilic attack. It indicates the strongest attraction. The contour diagram of the target molecule is given in Figure 4. It confirms the different positive and negative potential sites of the molecule in accordance with the total electron density surface [11,16].

From the Figure 4, carbonyl group and bromine occupy below the plane and the aldehyde group occupies above the plane. The contour diagram divides both the aromatic rings.



HOMO-LUMO energy of target molecule

The highest occupied molecular orbital (HOMO) andlowest unoccupied molecular orbital (LUMO) energies are very important parameters for quantum chemical calculations. We can determine the way the molecule interacts with other species hence they are called the Frontier orbitals. HOMO, it can be considered as the outer most orbital containing electrons. It tends to give these electrons and it can act as an electron donor. On the other hand, LUMO is showing low energy and low elec- tronic density [17]. It tends to accept electrons [18]. Therefore the HOMO and LUMO is directly related to ionization potential and electron affinity respectively. The energy difference between the HOMO and LUMO orbital is called energy gap and it is important for the stability of the compound [19].

The HOMO and LUMO energies for the target mole- cule are calculated as -6.0866 eV and -3.0618 eV respectively. The energy gap between the two orbitals is calculated as 3.0248 eV. The lower HOMO LUMO en- ergy gap is responsible for the bioactive property of the compounds and explains the fact that eventual charge transfer interaction is taking place within the mole- cule [20,21]. The HOMO and LUMO orbitals for the target molecule are shown in Figure 5. From the Figure 5, the HOMO is appeared on the whole of aromatic rings and some parts in the centre six membered ring, whereas LUMO is developed on the whole of the aromatic rings and on more atoms of the centre six membered ring.

Global chemical reactivity

The physical parameters like chemical hardness, softness, electronegativity, chemical potential and electrophilicity index serve as global reactivity parameters by using DFT for the title molecule using B3LYP/6-311++G(d,p) method, HOMO and LUMO energies, energy gap, electronegativity, chemical potential, chemical hardness, softness, electrophilic- ity index [22] were also calculated and listed in Table 6.

Ionization potential (I)

It characterizes the susceptibility of the molecules towards attack by electrophiles. Hard nucleophiles having low HOMO energy and hard electrophiles having high LUMO energy [3,23]. It is directly related to the energy of E_{HOMO} and defined as, $\boldsymbol{I = -E_{HOMO}}$.

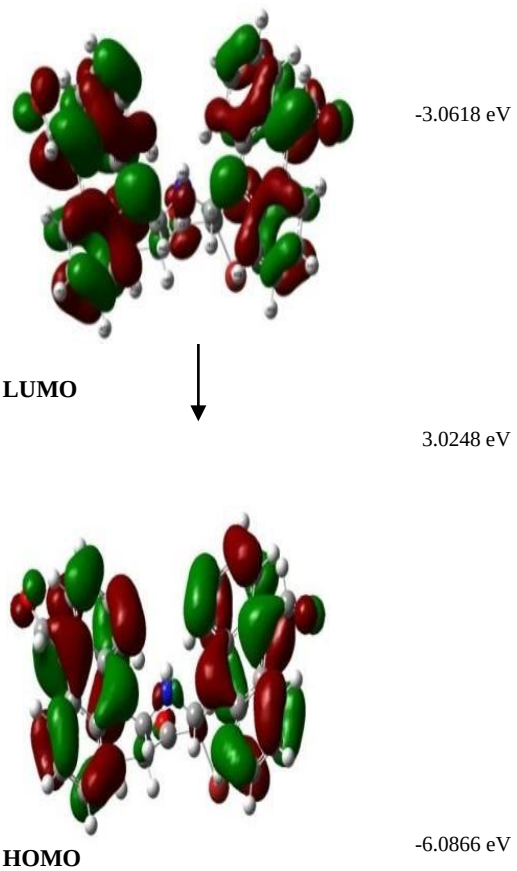


Figure 5. The Homo and Lumo orbitals for thetarget molecule

Electron affinity (A)

The energy of LUMO is directly related to the electron affinity and characterizes the susceptibility of the molecule towards attack by nucleophile. The electron affinity is defined as, $\boldsymbol{A = -E_{LUMO}}$.

Electro negativity (χ)

Electonegativity is a measure of the power of an atom or group of atoms to attract electrons towards it. Mulliken finds the electronegativity is the average of ionization potential and electron affinity and calculatedby, $\chi = \frac{I+A}{2}$.

Chemical potential (μ)

Chemical potential is the first derivative of the energy with respect to the 'n' number of electrons. The chemical potential is related to the escaping tendency of an electron from equilibrium [24,25]. Therefore chemical potential is the negative of electronegativity and calculated as, $\boldsymbol{\mu = -\frac{I+A}{2}}$.

Chemical hardness (η)

The energy gap between the HOMO and LUMO of the molecule is directly related to its hardness. A larger en- ergy gap suggests that is a harder molecule. It is related to polarizability of the molecular system [26,27] and defined by, $\eta = \frac{I-A}{2}$.

Chemical softness (S)

It is a measure of the capacity of an atom or group of atoms to receive electrons. It is a reciprocal of the hardness. Smaller the HOMO-LUMO energy gap implies the molecule is soft and S is defined by, $\boldsymbol{s = \frac{1}{\eta}}$.

Electrophilicity index (ω)

The electrophilicity index represents the stabilization energy of the system when it gets saturated by electron coming from the surrounding [5,28-30]. It is related to electronic chemical potential and chemical hardness. It defined as, $= \frac{\mu^2}{2\eta}$.

This electrophilicity index measures the susceptibility of chemical species to accept electrons, low ω value indicates the presence of good nucleophile and high ω value indicates the presence of good electrophiles [31].

Electron accepting capability

The electron accepting power have been defined [31,32] as, $\omega^+ = \frac{(I+3A)^2}{16(I-A)}$.

The larger ω^+ value represents better capability of accepting charge.

Electron donating capability

The electron donating power have been defined [31,32] as, $\omega^- = \frac{(3I+A)^2}{16(I-A)}$.

The smaller ω^- value corresponds the electron donatingcapability of a system.

Net electrophilicity

In order to compare electron donating (ω^+) and electron accepting capability ($^-$) the net electrophilicity have been proposed [33] as,

$$\Delta m^{\pm} = m^+ - (-m^-) = m^+ + m^-$$

That is the electron accepting power relative to the electron donating power.

Global softness

The global softness is defined [34] as the reciprocal of chemical hardness.

$$\sigma = \frac{1}{2\eta}$$

Table 6. Calculated quantum chemical parameters of target molecule

S.No	Quantum chemical parameters
1.	HOMO
2.	LUMO
3.	Energy gap
4.	Ionization potential (I)
5.	Electron affinity (A)
6.	Electro negativity (χ)
7.	Chemical potential (μ)
8.	Chemical hardness (η)
9.	Chemical softness (S)
10.	Electrophilicity index (ω)

From the Table 6, the energy gap of the molecule is found to be 3.0248 eV. It clearly indicates the molecule is very stable.

3.6. NLO studies

The interaction between incident electromagnetic fieldsin various media (NLO materials) to give new field that altered in phase, amplitude, frequency are other propagation characteristics from the incident fields [35]. NLO studies are very important in current research, because it provides the key function of optical modulation, optical memory, optical switching,frequency shifting and optical logic due to its wide applications in the area of signal processing, optical inter connection, data storage technology,

tele-communications and laser technology [36]. The relationships among molecular structure, photo current generation and NLO properties are investigated by polarisability and hyper polarisability [18].

Using DFT B3LYP/6-311++G(d,p) basis set method, the first order hyper polarisability and its related properties like dipole moment, polarisability and vector component are calculated for the target molecule based on the finite field approach. The first order hyper polarisability is calculated for the title compound by taking into account of Kleinmen symmetry relations and square norm of the Cartesian expression for the β tensor [37]. The first order hyper polarisability is a third rank tensor described by 3x3x3 matrix. The 27 components of 3 dimensional matrixes can be reduced to ten components due to the Kleinmen symmetry [38]. The output from Gaussian 16W provides ten component of the matrix as β_{xxx}, β_{xyy}, β_{xzz}, β_{yyy}, β_{xxy} β_{yzz}, β_{zzz}, β_{xxz}, β_{yyz}, β_{xyz} and they are given in Table 7.

The β component is defined as the coefficients in the Taylor series expansion of the energy in the external electric field. When the external electric field is weak and homogeneous, this expansion becomes,

$$E = E^{0} - \mu_{\alpha}F_{\alpha} - \frac{1}{2}\alpha_{\alpha\beta}F_{\alpha}F_{\beta} - \frac{1}{6}\beta_{\alpha\beta\gamma}F_{\alpha}F_{\beta}F_{\gamma} + \ldots\ldots\ldots$$

Where, E^0 is the energy of the unperturbed molecules. F_α is the field at the origin. μ_α, $\alpha_{\alpha\beta}$ are the components of dipole moment and polarisability. $\beta_{\alpha\beta\gamma}$ is the component of hyper polarisability

The total static dipole moment μ, the mean polarisability α_0, the first order hyper polarisability β_0 and the vector component β_{vec} [18] using x,y,z components are defined as follows,

Dipole moment $\mu_{Tot} = [\mu_x^2 + \mu_y^2 + \mu_z^2]^{1/2}$

Mean Polarizability $\alpha_{Tot} = \frac{\alpha_{xx}+\alpha_{yy}+\alpha_{zz}}{3}$

First order hyper polarisability

$$\beta_{Tot} = [\beta_x^2 + \beta_y^2 + \beta_z^2]^{\frac{1}{2}}$$

Vector component

$$\beta_{vec} = \frac{3}{5}[\beta_x^2 + \beta_y^2 + \beta_z^2]^{\frac{1}{2}}$$

Where,

$$\beta_x^2 = (\beta_{xxx} + \beta_{xyy} + \beta_{xzz})^2$$

$$\beta_y^2 = (\beta_{yyy} + \beta_{xxy} + \beta_{yzz})^2$$

$$\beta_z^2$$

The first order hyper polarisability β is associated with the intramolecular charge transfer (ICT), resulting from the electron cloud movement through the π conjugated framework from electron donor to acceptor groups. The electron cloud is capable of interacting with an external electric field and thereby altering the dipole moment and the first order hyper polarisability. The μ_{Tot}, α_{Tot} and β_{Tot} values are obtained from Gaussian 16W frequency job output file.

Table 7. The mean polarizability, Dipole moment and First order hyper polarisability and Vector component of target molecule

Parameters	Charge (a.u.)	Parameters	Charge (a.u.)
μ_x	-1.1228	β_{xxx}	338.943
μ_y	-2.3291	β_{xyy}	100.668
μ_z	1.8306	β_{xzz}	179.605
α_{xx}	533.499	β_{yyy}	108.468
α_{yy}	378.637	β_{xxy}	428.064
α_{zz}	574.043	β_{yyz}	-51.0943
α_{xy}	-37.2258	β_{zzz}	135.279
α_{xz}	33.0483	β_{xxz}	-235.080
α_{yz}	-23.8212	β_{yzz}	40.2090
		B_{xyz}	-146.361
μ_{Tot}	3.16807 Debye		
α_{Tot}	$73.4172426 \times 10^{-24}$ e.s.u		

The results are presented in Table 7 and the atomic unitsare converted to electro static units. (Conversion factor for α, 1a.u = 0.1482×10^{-24} e.s.u.; for β, 1a.u = 8.6393×10^{-33}e.s.u.) [39]. From the Table 7, the value of mean polarisability is $73.4172426 \times 10^{-24}$ e.s.u. and the Dipole moment is 3.16807 Debye. The dipole moment and first hyper polarisability of the title compound is greater than that of urea. μ and β of urea are 1.3732 Debye and 0.3728×10^{-30} e.s.u. obtained by DFT B3LYP/6-311++G(d,p) method and basis set. Urea is one of the prototypical molecules used in the study of the NLO properties of molecular system. Therefore, it is used frequently as a threshold value for comparative purpose.

hyper polarisability value for the title compound is $7.425747576x10^{-30}$ e.s.u. It is 20 times higher than that of urea. Higher the values of molecular polarisability, hyper polarisability and dipole moment are important for more active NLO properties. So the title compound possesses considerable NLO properties.

The dipole moment value gives an idea about the ionic character of a molecule. Larger the value of dipole moment more will be the ionic character. It helps to predict the shape of the molecule. Polarisability and hyper polarisability are widely used in drug design. Polarisability is used in QSPR [40] (qualitative structure property relationship) and QSAR (qualitative structure activity relationship).

3.7. NBO analysis

NBO analysis is a very effective method for predicting the inter and intra molecular bonding and interaction between donor and acceptor molecular system [41-43]. Itis also used to investigate the charge transfer or conjugative interaction in molecular systems. NBO analysis of the target molecule has been performed by DFT method with hybrid function B3LYP/6-311++G(d,p) level of theory. It is used to elucidate the delocalization of electron within the molecule. The hyper conjugative interaction energy was calculated from the second order perturbation approach.

$$(2) = \mathbb{E} \quad q \quad = (i,)^2 \quad \frac{}{i \quad E_i - E_J}$$

Where, q_i → donor orbital occupancy; E_i-E_j → diagonal element, and F(i,j) → off diagonal NBO Fock matrix elements.

The electron donor and electron acceptor orbital and the interacting stabilization energy of the target molecule are selectively shown in Table 8. The more intensive interaction take place between the electron donor to electron acceptors having larger E(2) value [44]. These more tendency of more electron donor to electron acceptor leads to the greater extent of conjugation in the whole system [45].

From the Table 8, the largest stabilization energy shows that σ C26 - H53→ σ* C37 - O40 antibonding orbital having highest E2 value 76351.14 Kcal/mol.

From this Table 8, the NBO analysis revealed that π* C34 - C35 → σ* C38 - H66, σ C23 - H50 → σ* C38 - H66, σ C25 - C26 → π* C34 - C35, σ C25 - C26 → σ* C38 - H66 and σ C26 - H53 → σ* C38 - H67 interaction gives a strong stabilization energy of the title compound by 30385.91, 24919.29, 23513.94, 22479.71 and 17546.37 Kcal/mol respectively. There are many double bonds present in the molecule which also enhances the stability of the molecule.

Table 8. Second order perturbation theory analysis of Fock matrix in NBO basis

Donor (i)	Acceptor (j)	E(2) kcal/mol	E(j)-E(i) a.u.	F(i,j) a.u.
σ C13 - C14	π* C36 - O41	13237.15	1.22	3.666
σ C14 - C32	σ* C15 - C24	15907.00	0.05	0.790
π C16 - C18	σ* C35 - H62	12780.99	0.28	1.887
σ C22 - C23	π* C36 - O41	11327.98	0.96	3.019
σ C23 - H50	σ* C38 - H66	24919.29	1.93	6.219
σ C23 - H50	σ* C32 - H59	16696.30	3.81	7.128
σ C23 - H50	π* C34 - C35	10630.30	1.60	3.869
σ C25 - C26	π* C34 - C35	23513.94	3.23	8.174
σ C25 - C26	σ* C38 - H66	22479.71	3.56	8.016
σ C25 - C26	σ* C32 - H59	13703.68	5.43	7.713
σ C26 - H53	σ* C37 - O40	76351.14	18.58	33.755
σ C26 - H53	σ* C38 - H67	17546.37	33.23	21.636
σ C26 - H53	σ* C38 - H66	12410.67	37.46	19.318
σ C26 - H53	π* C34 - C35	11372.65	37.14	19.281
CR (1) C12	σ* C38 - H67	22054.05	1.34	4.852
CR (1) C13	σ* C38 - H67	13905.40	11.394	11.69
CR (1) C17	σ* C38 - H67	17379.41	5.03	8.355
CR (1) C35	σ* C38 - H67	18146.48	2.70	6.259
CR (1) C38	σ* C38 - H66	10418.94	4.16	5.884
CR (2) Br39	π* C37 - O40	25727.59	0.08	1.316
LP (1)O 19	σ* C36 - H63	1463.80	0.03	0.179

3.8. Fukui function

Fukui Function or Frontier Function (FF) is a functionwhich explains the electron density in a Frontier orbital as a result a little variation in the total number of electrons [46]. Kolandaivel et al., [47] has introduced the atomic descriptor to find out the local reactive sites in a molecule

Table 9. Fukui function analysis of target molecule

Atoms	MPA				NPA			
	f^+	f^-	f^o	$\Delta f(r)$	f^+	f^-	f^o	$\Delta f(r)$
1 C	-0.608083	-0.600215	-0.607135	-0.00787	-0.595525	-0.377219	-0.492898	-0.21831
2 C	-0.127091	0.058163	-0.031398	-0.18525	0.928079	0.961742	1.001839	-0.03366
3 C	-0.517382	-0.599464	-0.555771	0.082082	0.555190	0.439504	0.487423	0.115686
4 N	-0.020615	0.001320	-0.016725	-0.02194	-1.064823	-0.886774	-0.976377	-0.17805
5 C	-0.128301	-0.058056	-0.091285	-0.07025	0.159164	0.260088	0.217275	-0.10092
6 C	-0.251728	-0.295955	-0.270907	0.044227	0.629788	0.536506	0.607028	0.093282
7 C	0.500230	0.470893	0.494328	0.029337	-0.516658	-0.706236	-0.681095	0.189578
8 C	0.741251	0.743915	0.742754	-0.00266	0.160001	0.232957	0.244936	-0.07296
9 C	0.447761	0.456240	0.451510	-0.00848	0.442016	0.501311	0.510308	-0.05929
10 C	0.970275	0.948891	0.964931	0.021384	0.145156	0.171194	0.163472	-0.02604
11 C	0.592983	0.612099	0.605331	-0.01912	-0.072027	-0.072660	-0.071958	0.000633
12 C	0.698603	0.667895	0.679872	0.030708	-0.127426	-0.251156	-0.203077	0.12373
13 C	0.332925	0.285058	0.315728	0.047867	-0.446793	-0.573198	-0.559024	0.126405
14 C	-0.065686	-0.079208	-0.069272	0.013522	0.259987	0.314157	0.320556	-0.05417
15 C	0.361038	0.381549	0.372558	-0.02051	0.289462	0.339945	0.349210	-0.05048
16 C	0.810026	0.818851	0.820191	-0.00882	0.093515	0.158985	0.138170	-0.06547
17 C	0.293460	0.307618	0.297895	-0.01416	0.034695	0.072459	0.050860	-0.03776
18 C	0.519665	0.491656	0.501539	0.028009	-0.179291	-0.379529	-0.290060	0.200238
19 O	-0.065602	-0.113853	-0.086928	0.048251	-0.448836	-0.493721	-0.465590	0.044885
20 C	-0.397930	-0.437112	-0.416518	0.039182	-0.107676	-0.222583	-0.161380	0.114907
21 C	-0.558024	-0.592596	-0.585442	0.034572	-0.165398	-0.210064	-0.213816	0.044666
22 C	-0.289568	-0.335633	-0.309682	0.046065	-0.078569	-0.103426	-0.078907	0.024857
23 C	-0.651349	-0.680185	-0.678083	0.028836	-0.167521	-0.255561	-0.253585	0.08804
24 C	-0.327439	-0.381123	-0.359080	0.053684	-0.274035	-0.313136	-0.321616	0.039101
25 C	-0.328419	-0.377414	-0.352630	0.048995	-0.015968	-0.092394	-0.043790	0.076426
26 C	-0.483634	-0.518304	-0.493883	0.03467	-0.132846	-0.208815	-0.167807	0.075969
27 C	-0.258039	-0.310780	-0.290540	0.052741	-0.146199	-0.194424	-0.180884	0.048225
28 C	-0.332293	-0.356934	-0.348748	0.024641	-0.312753	-0.368979	-0.374127	0.056226
29 C	-0.227383	-0.294556	-0.264503	0.067173	-0.044663	-0.091567	-0.055846	0.046904
30 C	-0.668171	-0.711290	-0.697089	0.043119	-0.141666	-0.178951	-0.175551	0.037285
31 C	-0.376219	-0.404020	-0.386848	0.027801	-0.100354	-0.179563	-0.138203	0.079209
32 C	-0.197050	-0.188828	-0.197426	-0.00822	-0.117161	-0.242622	-0.215279	0.125461
33 C	-0.016194	-0.061829	-0.037484	0.045635	-0.155722	-0.153666	-0.144331	-0.00206
34 C	-0.530756	-0.553614	-0.537933	0.022858	-0.084127	-0.181039	-0.122377	0.096912
35 C	-0.512001	-0.549253	-0.543420	0.037252	-0.174929	-0.255311	-0.248131	0.080382
36 C	-0.375080	-0.435887	-0.397798	0.060807	0.488210	0.505853	0.520146	-0.01764
37 C	-0.280402	-0.348392	-0.306512	0.06799	0.509959	0.572360	0.561340	-0.0624
38 C	-0.665545	-0.690203	-0.681139	0.024658	-0.463212	-0.403730	-0.439098	-0.05948
39 Br	0.013828	-0.109803	-0.045339	0.123631	-0.012123	-0.158679	-0.079844	0.146556
40 O	-0.170599	-0.262415	-0.208923	0.091816	-0.445096	-0.588827	-0.512653	0.143731
41 O	-0.163617	-0.254343	-0.201946	0.090726	-0.434650	-0.562431	-0.495424	0.127781
42 H	0.345972	0.337020	0.342764	0.008952	0.241471	0.165401	0.205367	0.07607
43 H	-0.059320	-0.142145	-0.099295	0.082825	-0.104014	-0.145453	-0.142562	0.041439
44 H	0.268901	0.264846	0.269018	0.004055	0.371084	0.317806	0.347639	0.053278
45 H	0.269823	0.252876	0.261810	0.016947	-0.032641	-0.070161	-0.054862	0.03752
46 H	0.074865	0.097220	0.085709	-0.02236	-0.052991	-0.054044	-0.055057	0.001053
47 H	0.212425	0.145327	0.177830	0.067098	0.158709	0.132069	0.145149	0.02664
48 H	0.199465	0.172239	0.182247	0.027226	0.189223	0.185016	0.190216	0.004207
49 H	0.209772	0.151710	0.179234	0.058062	0.148128	0.109843	0.126740	0.038285
50 H	0.076481	0.052280	0.061435	0.024201	0.120616	0.132135	0.134252	-0.01152
51 H	0.154142	0.105651	0.129489	0.048491	0.146703	0.131216	0.142368	0.015487
52 H	0.210939	0.151927	0.181199	0.059012	0.134775	.105480	0.119080	0.029295
53 H	0.209436	0.142766	0.176339	0.06667	0.156364	0.123081	0.140125	0.033283
54 H	0.167869	0.121737	0.142697	0.046132	0.170228	0.143150	0.156464	0.027078
55 H	-0.088940	-0.082154	-0.082313	-0.00679	0.199150	0.198060	0.201805	0.00109
56 H	0.216350	0.172763	0.193164	0.043587	0.134982	0.110763	0.120516	0.024219
57 H	0.160770	0.112017	0.133813	0.048753	0.175973	0.147567	0.162190	0.028406
58 H	0.212378	0.149101	0.180157	0.063277	0.147105	0.114054	0.131088	0.033051
59 H	0.077887	0.054650	0.059660	0.023237	0.141165	0.167071	0.158986	-0.02591
60 H	0.219762	0.169663	0.193524	0.050099	0.167185	0.127675	0.145096	0.03951
61 H	0.209530	0.143223	0.175706	0.066307	0.152893	0.121509	0.136131	0.031384
62 H	0.223182	0.194129	0.205142	0.029053	0.201197	0.210319	0.210257	-0.00912
63 H	0.108230	0.059875	0.087321	0.048355	-0.012515	-0.049701	-0.032567	0.037186
64 H	0.109088	0.056445	0.086500	0.052643	-0.014139	-0.061308	-0.037928	0.047169
65 H	0.188277	0.180649	0.186296	0.007628	0.120762	0.097300	0.110662	0.023462
66 H	0.142396	0.138458	0.140476	0.003938	0.122879	0.086203	0.107106	0.036676
67 H	0.192475	0.154845	0.173828	0.03763	0.146531	0.094148	0.121907	0.052383

The individual atomic charges calculated by natural population analysis (NPA) and Mulliken population analysis (MPA), have been used to carry out the Fukui function of the target molecule [11]

The Fukui function is defined as,

$$u(\vec{r}) = \left(\frac{\partial \rho / \partial N}{\delta \mu / \delta u}\right)_{(\vec{r})}$$

The following equations are used to calculate the Fukui function.

For nucleophilic attack

$$f^{+}(\vec{r}) = q_r(N+1) - q_r(N)$$

For electrophilic attack

$$f^{-}(\vec{r}) = q_r(N) - q_r(N-1)$$

For radical attack

$$f^{0}(\vec{r}) = \frac{[q_r(N+1) - q_r(N-1)]}{2}$$

Where, q_r is the atomic charge (evaluated from the MPA, electrostatic derived charge, etc) at the r^{th} atomic site is the neutral (N), anionic (N+1) and cationic (N-1) chemical species.

Table 9 shows the f^{+}, f^{-}, f^{0} values for the title molecule by MPA and NPA gross charge at DFT theory with the basis set B3LYP/6-311G++(d,p). It has been found that for MAP schemes of cationic, anionic and neutral molecules. 10C has a higher value. From the Table 9, theMPA schemes predicts the reactivity order for nucleophilic attack is 10C > 16C > 8C > 12C >11C > 18C > 7C > 9C > 15C > 42 H > 13C. The

order of electrophilic attack for all f^{+}, f^{-}, f^{0} species for MPA analysis is 30C > 38C > 23C > 1C. For f^{+} is 33C > 39Br, for f^{-} is 4N and f^{0} is 2C and 4N respectively.

From MPA calculation, the highest possibility of electrophilic attack is possible at 30C and for nucleophilic attack is possible at 10C. The 10C has higher magnitude (-0.970275 a.u.) than the 30C (-0.068171 a.u.). The molecule exerts nucleophilic attack. Parr and Yang [5,45,48] showed that sites in chemical species with the biggest values of Fukui function shows high reactivity of corresponding attack.

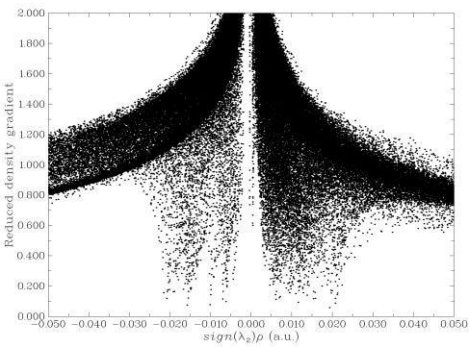
NCI analysis

Non Covalent Interaction (RDG) analysis helps us to know the interaction seen within a molecule. RDG is calculated as,

$$RDG(r) = \frac{1}{2(3A^2)^{\frac{1}{3}}} \frac{|\nabla(r)|}{(r)^{\frac{4}{3}}}$$

$(\lambda_2)\rho$ (a.u.) is plotted against reduced density gradient (a.u.), for the title molecule and reproduced in

Figure 6 (a)



6(a). NCI interaction

6(b). Isosurface

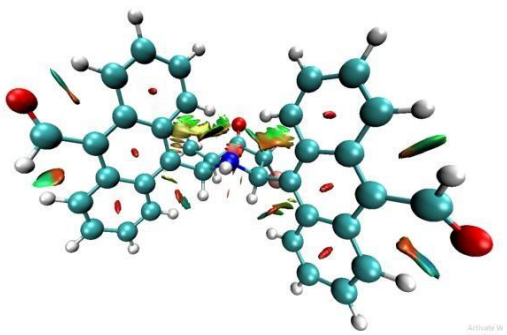


Figure 6. (a) & (b) NCI interaction and Isosurface of the title molecule

From the Figure 6 (a) we can see that, there is a strong electrostatic attraction seen between the aromatic rings and centre six membered ring system. Also it is seen that around the centre six membered ring there are some attractive forces like Van der Waals force appeared side by side. The spike near -0.020 to +0.010 a.u. explains the presence of Van der Waals Force and spike near +0.020 conforms the presence of steric effect [49].

The NCI interaction of the title molecule is viewed by VMD 1.9.3 software and shown in Figure 6(b). It gives more clear interaction inaccordance Multiwfn3.7 software.

According to the Figure 6(b) green circle show Van der Waals force. Green and light brown mapped colour rep- esents the low electron density region. The red colour

circle represents strong steric interaction. All the aro-

matic ring exert strong steric interaction since there are red colour mapped circle

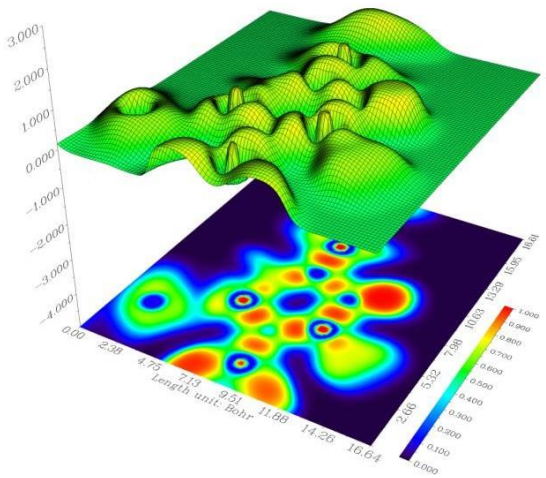


Figure 7. Shaded surface map with projection of LOL of target molecule

The shaded surface map with projection for the target molecule was investigated and shown in Figure 7. The region around both aldehyde in both aromatic ring experience low electron density region. The region between the two aromatic rings and nitrogen in centered six membered ring shows that the area is having low electron density. The centered six membered ring also having strong steric effect due to the development of red coloured map [50]. A Van der Waals force is developed between bromine and aromatic ring. The area between CH_3 and C=O also having electron low density area.

CONCLUSION

In the present study, the title compound 10,10ˈ-(3-bromo-5-methyl-4-oxo piperidine-2,6-diyl)- bis-(anthracene-9-carbaldehyde), is theoretically optimized using B3LYP with standard 6-311++G(d,p)basis set. The charge distribution of the molecule was calculated by Mulliken Population Analysis. The molecular electrostatic potential map showed that negative potential region on oxygen atom and positive region on nitrogen and hydrogen atom. The HOMO - LUMO energy gap indicates that the charge transfer takes place within the molecule. Using HOMO-LUMO values the ionization potential, electron affinity, electronegativity, chemical hardness, softness, electrophilicity index and electron accepting and donating capability are calculated semi quantitatively. The NBO calculation explains the stabilization, delocalization and hyperconjugation interaction of the molecule. Larger the E(2) value confirms the title compound it highly stable. Using Fukui Function the nucleophilic electrophilic sites within the molecule is predicted. The title compound has larger value of hyper polarizability. It suggests that, this compound can beused as NLO material. NCI interaction study confirms the presence of Van der Waals force of attraction and steric effect. The shaded surface map predicts the area of electron depletion.

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Vibrational Analysis of Sodium Ion Conducting Polymer Blend Electrolytes

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1. INTRODUCTION

Recently, many researchers are working on bio based polymer electrolytes for energy storage device and its electrochemical application such as battery, supercapacitor, sensor, fuel cells etc. Polymer blend plays a vital role to develop the electrolyte membrane and its properties[1]. Biopolymers are produced from living organisms which are easily degradable, biocompatible, non-toxic and sustainable. It is generally extracted from biomass, bio based monomers and microorganism/bacteria [2]. Nowadays polysaccharides are important material for preparing electrolyte because of it repeat units of saccharide. Chitosan, cellulose, pectin, starch are examples of polysaccharides which are extracted directly by the biomass[3].

Pectin is a natural polymer consists of D-galacturonic acid of polysaccharide which may abundance in nature, low cost and easily renewable polymers. Major source of pectin derived from cell wall of the plants such as apple, citrus peels like orange, lemon and other materials. Galacturonic acid contains 70-80 % carboxyl esterified with methanol and partially esterified with Homogalacturonan (HG) link can be extended as Rhamnogalacturonan I&II [4, 5]. Pectin is soluble in water and organic solvent that can be expected to blend other polymers easily. Polymer-polymer interaction has great attention on many research because of blend makes to improve the conductivity value in the electrolyte [5]. On that synthetic polymer is a good blend material like PVA (Poly vinyl alcohol), PEO (Poly ethylene oxide), PVP (Poly vinyl pyrrolidon) which can maintain the structural stability and thermal properties [6]. PVA is a biodegradable synthetic polymer, water soluble, biocompatibility and non-toxic. It is able to blend easily and structural stability is too good when compared to other polymers. Sodium nitrate ($NaNO_3$) salt is used as a dopant for further improvement of properties[7, 8]. For example: Manjuladevi et.al reported that pectin doped with lithium ions has good ionic conductivity[9]. Plenty of blend polymers are reported like chitosan blend PVA doped with NH_4I were reported by M.H. Buraidah et.al[10]. M. Vahini et.al reported pectin doped sodium nitrate [11]. In our study, we discuss about Pectin:PVA based polymer blend electrolytes.

2. EXPERIMENTAL METHODS

MATERIAL

Pectin, Sodium nitrate($NaNO_3$)and PVA with average molecular weight (44.05g/mole) are purchased from sigma Aldrich. Distilled water is used as solvent throughout the work.

PREPARATION METHODS

Distinct molecular weight percentage of Pectin-PVA doped $NaNO_3$ certain concentration like (100:0:4, 75:25:4, 50:50:4, 25:75:4 and 0:100:4) ratio are taken to prepare electrolytes by using solution casting technique. Pectin and PVA are dissolved in 20ml of deionized water separately. Sodium nitrate salt was dissolved in 10ml of water. The mixture was continuously stirring to obtain a uniform solution. Solution were poured it into the petri dish and kept oven at 70^{o}c for 15 hours. After drying the electrolyte

membrane were peeled out from the petri dish and further the film are used for characterization of FTIR.

ELECTROLYTECHARACTERIZATION

FTIR SPECTROSCOPY

Fourier transform infrared spectroscopy are analysed by using Shimadzu IR affinity-1 spectrometer to observe the complex formation and vibrational modes. The vibrational excitation is achieved when the broad band source of radiation in infrared generally 400-4000 cm^{-1} wavenumbers are used. It can provide information about the presence of chemical compounds and interaction of polymers and salt[15]. Generally, spectrum consists of wavenumber and transmittance for the polymer sample.

3. RESULT AND DISCUSSION

FTIR ANALYSIS

The FTIR spectroscopy of vibrational modes has been observed from the following film of pectin:PVA blend doped with $NaNO_3$ salt [12]. Mainly it explains the hydroxyl group, carbonyl group which combine carboxylic acid of the different samples and composition are listed in *table.1*.

INTERACTION BETWEEN PECTIN-$NaNO_3$

The electrolyte (100:0:4) pure pectin doped with 4% of sodium nitrate are observed using FTIR spectrum. The hydroxyl band of pectin is observed at 3286 cm^{-1} but addition of salt it is shifting to 3356 cm^{-1} [13]. The band at 1737 cm^{-1} is due to C=O stretching vibration of carboxylic group of pectin, is shifted to 1733 cm^{-1}. The presence of pectin was observed at 1009 cm^{-1} due to CH-O-CH stretching vibration[11].

BLEND INTERACTION WITH SALT

Polymer blend of Pectin-PVA doped with $NaNO_3$ salt at composition of (75:25:4, 50:50:4, 25:75:4) are observed by the spectrum. The hydroxyl group of OH bond at 3329 cm^{-1}, 3338 cm^{-1} and 3320 cm^{-1} are observed. C-H stretching is appeared at 2928 cm^{-1} in the bend composition[14]. The carboxylic group reveals the peak at 1733 cm^{-1}, 1741 cm^{-1} and 1724 cm^{-1}. The C-O-C stretching vibration band at 1233cm^{-1}, 1224cm^{-1}, 1241cm^{-1} are shifted due to addition of salt [16]. In blend polymer, CH-O-CH stretching vibration reveals the presence of pectin has been observed at 1009cm^{-1}, 1009$cm^{-1}$and 1018cm^{-1}[11]. Most of the bands originate at 822cm^{-1}, 840cm^{-1}, 831cm^{-1} it denotes the presence of PVA. The stretching of CH_2 rocking vibration appears when the PVA is added[17]. The new peaks are observed in the film is 626 cm^{-1} in various composition and it shows the nitro compound of addition of salt [19].

Table.1 FTIR analysis of Pectin:PVA polymer electrolytes

100:0:4	75:25:4	50:50:4	25:75:4	0:100:4	Vibrational band
3356	3329	3338	3320	3347	O-H stretching
2928	2928	2928	2928	2928	C-H stretching
1733	1733	1741	1724	1715	C=O stretching
1224	1233	1224	1241	1250	C-O-C stretching
1009	1009	1009	1018	-	CH-O-CH
-	822	840	831	849	CH_2 rocking
626	626	626	626	-	NO_2 stretching

INTERACTION BETWEEN PVA:$NaNO_3$

The interaction of PVA – $NaNO_3$ shows the hydroxyl group of OH band at 3347 cm^{-1} because addition of salt and it is shifted. The bands at 2928cm^{-1} and 1715cm^{-1} indicates the C-H stretching and C=O stretching of carboxylic group shifted due to dopant of salt[18]. The band at 849 cm^{-1} reveals the presence of PVA and also CH_2 rocking vibration

in the spectrum [20]. The FTIR graph is given in *figure.1*

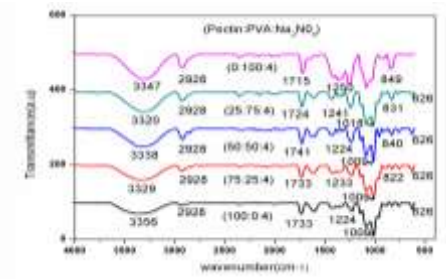

Figure.1 FTIR spectrum of Pectin:PVA:$NaNO_3$ polymer electrolytes

4. CONCLUSION

The biopolymer electrolytes based on Pectin:PVA doped with fixed weight percentage of sodium nitrate salt are prepared by solution casting technique. The FTIR characterization explains the complex formation and vibrational modes of electrolytes. The interaction of polymer and salt shows the presence of hydroxyl group and carbonyl group. The strong interaction between polymers and salt are confiremd. Thus we can apply the prepared electrolytes for electrochemical applications.

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Analysis of silver dispersed poly (aniline-co-3-bromoaniline) nanostructured composites for electro active applications

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Abstract:

A new series of nanostructured poly(aniline-co-m-bromoaniline) copolymer has been synthesized by chemical oxidative insitu polymerization method using dodecylbenzenesulphonic (DBSA) acid as soft template. These polymers possess unique electrical and magnetic properties leading to wide range of industrial applications such as sensors, rechargeable batteries, electromagnetic shielding and solar cells etc. The synthesized polymer composites were subjected to various characterization techniques such as UV-visible spectroscopy, FT-IR spectroscopy. The copolymer samples were found to be soluble in common organic solvents like DMSO, NMP, THF and DMF. The UV-visible spectra show the $\pi - \pi^*$ transition and the n-π^* transition. FT-IR spectra confirmed the formation of the benzenoid ring and quinoid ring of the copolymer system. The electrical conductivity study indicates the increase in conductivity of 3-bromoaniline monomer feed ratio.

Keywords: aniline, 3-bromoaniline, Silver nanoparticle in-situ polymerization, Surfactant, Conductivity.

1. Introduction

Polyaniline is most widely studied among the conducting polymers due to its processability, environmental stability and its adjustable electro optical properties [1,2].. PANI is an electro active polymer due its excellent electrifying effect, photovoltaic and dielectric properties [3,4,5,6]. Due to its environmental stability, PANI is widely used in applications such as Light emitting devices (LEDs), solar cells, nano-electronics, light weight batteries, sensors and electro chromic devices [7]. Conversely the applications of PANI are limited due to its poor solubility in common organic solvents and processability. The poor solubility produces some complexity in the film formation, which is the main requirement for device fabrication [8]. Dodecyl benzene sulfonic acid (DBSA) was fond to be best example for improving solubility and electrical conductivity [9] due to its long chain of alkyl group and act as doping agent. Several research works was done to improve the solubility of PANI, substitution in alkyl chain, derivatives of PANI and copolymers have been synthesized [10]. The lateral substituent present in the polymer chain reduces the stiffness of the polymer chain and improves the solubility characteristics. This substituent group present in the polymer backbone decreases in stiffens of the polymer chain and results more salvation tendency [11]. Also it decreases the overlap of p-electron, nitrogen lone pairs and leads to decreases in the conductivity [12]. Substituted PANI can be prepared by chemical or electrochemical polymerization of aniline with ring substituted derivatives [13]. Also doping of PANI with suitable dopant like protonic acid, sulfonic acid is the another way to improve the processability [14,15]. Therefore copolymerization reaction of aniline with different monomers was found to improve the processability [16].

Several studies has been reported to prepare PANI dispersion; polymerization of aniline in micelle [17,18], emulsion [19,20] and reversed microemulsion [21] as a polymerization medium.

Halogen substituted aniline copolymers such as fluorine [22], chlorine [23], iodine [24] and bromine [25] groups in polymer chain have been examined well. It has been reported that the presence of electronegative group such as fluorine and chlorine decreases the electrical conductivity [26,27]. The halogen substituted aniline copolymers depicts significant electrical conductivity and superior solubility [28-30]

Silver (Ag) nanoparticles are of current significance due to its unique electrical, thermal, catalytic, optical properties, sensing characteristics that are suited for applications including biomolecule detection, immunoassays, surface Plasmon optics, data storage, Photonics and photography [31,32].

Roy et al. reported on the chemical synthesis of homopolymer and a copolymer based on o-bromoaniline and aniline in the presence of methane sulfonic acid in an aqueous solution [33]. However, only a few reports on copolymerization of aniline and bromine substituted aniline at meta position were studied [34]. Here, we report the synthesis of oxidative copolymers of aniline and m-bromoaniline monomers at various concentrations in presence of DBSA and ammonium persulphate as oxidant.

2. Experimental Techniques:

Synthesis of silver nanoparticals

The silver nanoparticles are prepared by the following procedure [35]. 0.01 M of DBSA dissolved in 90 ml of distilled water. Then aniline 0.019 M is added to the mixture slowly, and stirred vigorously to form a transparent solution. AgNO3 solution of 0.019 M was added to the above solution drop wise. Then the solution is allowed to stir for 15 min and then heated up to 90^{o} C. After by adding 0.137 M of NaOH solution into the mixture, the formation of silver nanoparticles was triggered and heated further for an hour with constant stirring. The synthesized silver nanoparticles DBSA coated colloids were cooled down without any further treatment.

In-Situ Chemical synthesis of Silver dispersed DBSA doped poly(An-co-3-BA) copolymers:

The silver dispersed DBSA doped poly(An-co-3-BA) nanocomposites were prepared as follows. Aqueous micellar dispersion was prepared first by introducing DBSA in distilled water (80 ml) under slow stirring. Then 0.05 M each of aniline monomer and 3-bromoaniline were added to the solution. Then 10 ml 1M HCl aqueous solution was slowly added into the reaction mixture and continuously stirred to form a homogeneous solution. Then 1 mL of metal nanoparticles was added. Finally 0.1M of APS solution was added drop wise to initiate the polymerization. The reaction mixture was stirred continuously for 12 hr in an ice-cold water bath. As the polymerization proceeded, the colour of the solution changed from colourless to yellow, brown and finally to green, confirming the formation of copolymer composites. The synthesis route of silver dispersed DBSA doped poly (aniline-co-3-bromoaniline) copolymer composite is shown in the reaction Fig.1.

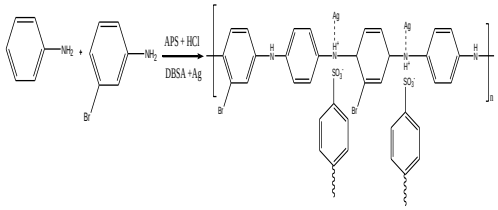

Fig.1. Synthesis route of Ag dispersed poly (aniline-co-3-bromoaniline) copolymer

3. Result and Discussion

UV- Visible Spectroscopy:

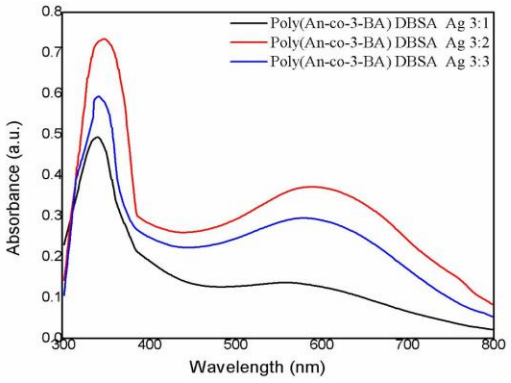

Fig.2 UV-Vis spectra of DBSA doped Ag dispersed poly(An-co-3-BA) copolymer

Figure 2 shows the optical absorption spectra of surfactant aided Ag embedded poly (An-co-3-BA) copolymers. It exhibits the peak at 338 nm is attributed to the π-π* transition of benzenoid ring [36]. It is related to the extent of conjugation between phenyl rings along the polymer chains. Another peak at 554 nm is due to charge transfer from HOMO of benzenoid to LUMO of quinoid ring [37]. A blue shift observed is due to the dispersion of silver nanoparticles, shifts the n-π* transition from 590 nm to 554nm. This is due to the strong interaction between the DBSA dopant molecules and the polymer composite [38]

Table 1 Optical Absorption Peak Values of Surfactant Aided Poly (An-co-3-BA) and Ag Embedded Copolymers

Sl.No.	Electronic Transition	Wavelength (nm)		
		3:1	3:2	3:3
1	π-π* transition	338	344	340
2	n– π* transition	554	590	576

FTIR analysis

Figure 3 shows the FT-IR spectra of surfactant aided silver embedded poly (An-co-3-BA) nanocomposites. The spectra of the synthesized nanocomposite reveals characteristics bands at 3221, 3050, 2932,1569, 1488, 1289, 1142, 1036, 807 and 545 cm^{-1}. The peaks at 3221 cm^{-1} and 3050 cm^{-1} are attributed to the N-H stretching of amine. The formation of benzenoid and quinoid rings in the copolymer is confirmed from the peaks at 1569 and 1488 cm^{-1}. The peak at 1569 cm^{-1} is due to C=C bond of quinoid ring, whereas the peak at 1488 cm^{-1} arises due to vibration of C=C associated with the benzenoid ring. The peak at 1305 cm^{-1} is related with the C-N stretching in a secondary aromatic amine. The appearance of broad band at 1142 cm^{-1} is attributed with C-H stretching vibration in the N=Q=N. This confirms electrical conductivity of copolymer due to the electron delocalization. The peak at 807 cm^{-1} is due to the C-H out plane bending and the peak at 545 cm^{-1} is due to the C-N-C bending. Finally the band observed around 2932 cm^{-1} depicts the DBSA dopant plays a very important role in the formation of conducting nanocomposites and acts as a dopant [40].

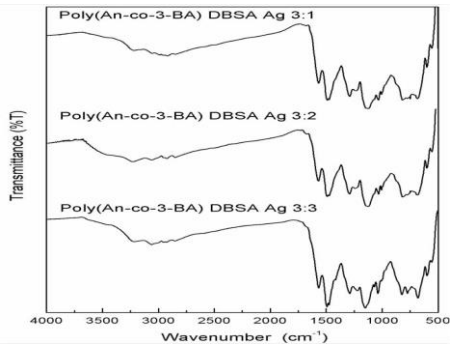

Fig3. FTIR spectrum of Ag dispersed DBSA doped Poly(An-co-3-BA) copolymer

Electrical conductivity

The Ag dispersed poly (An-co-3-BA) nanocomposites depicts the higher electrical conductivity. This may be due to the Ag nanoparticles enhances the delocalization. The increased channeling character of Ag nanoparticles enhances the mobility of the charge carriers along the polymer backbone [41]. The interaction nano-scale Ag nanoparticle improves the fast charge transfer. The electrical conductivity values are decreased with the increased bromoaniline concentration which controls the charge transfer and also increased steric hindrance of the side chain and decreased conjugation.

Copolymer composition	Conductivity (S/cm)
Polyaniline	1.98×10^{-2}
Poly (An-co-3-BA) DBSA	1.98×10^{-9}
Poly (An-co-3-BA) DBSA Ag 3:1	1.13×10^{-5}
Poly (An-co-3-BA) DBSA Ag 3:2	1.17×10^{-6}
Poly (An-co-3-BA) DBSA Ag 3:3	5.16×10^{-8}

Table 2 Electrical Conductivity Values of Ag dispersed DBSA doped Poly (An-co-3-BA) copolymer

4. Conclusion:

The nanocomposites were synthesized using chemical oxidative polymerization method. The UV-Visible spectrum shows the π-π* and n-π* electronic transition between the energy levels. TheUV visible and FTIR spectrum confirms functional groups present in the synthesized copolymer. Since the copolymer is highly soluble, this copolymer can be used in the fabrication of flexible electronic devices.

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The Microencapsulated Phase Change Material (PCM) Used in Mitigating Urban Heat Island to Improve the Energy Performance in Building

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In the mitigating urban heat island (UHI) the Micro Encapsulated Phase Change Material (MEPCM) are used. This helps to reduce the indoor temperature and the major effects of reduce the indoor temperature by using of MEPCM. The study wants to illustrate that the Phase Change Material (PCM) application is helpful for surface temperature supervision and enhancing indoor thermal performance by passive cooling. Suitable PCMs will maintain comfort room temperature at the summer by reducing the inner temperature and increasing the temperature in the winter. PCM implantation in the buildings will be achieved by basic methods of PCM incorporation which are macro encapsulation and micro encapsulation. Encapsulation of PCM is essential to increase the latent heat of fusion of the material. Amongst variety of PCMs, fatty acids, Paraffin and Fatty acid esters are produced as (MEPCM) by several manufacturing companies on the commercial scale. PCM application in the Inter Building Environment, which is a PCM embedded building envelope, reduces the negative impact on energy usage and reasonable progress of annual Heating Ventilation and Air Conditioning (HVAC) energy consumption.

Keywords: Urban Heat Island (UHI), Phase Change Material (PCM), paraffin wax, cool roof, thermal comfort.

An Efficient Construction of Biopertinent *bis*-Pyrazole Decorated Heterocycles through C=C Formation using Sodium Hydroxide in Aqueous PEG-400

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Biopertinent *bis*-pyrazole decorated heterocycles have efficiently been constructed through carbon-carbon double bond formation using catalytic amount of sodium hydroxide in aqueous PEG-400. The reactions were culminated with good to excellent yields in short reaction time irrespective of the nature of the reactants. The reaction media is environmentally benign as PEG-400 is a stable, non-volatile, non-toxic, low flammable and biodegradable one. The PEG-400 could be reused without appreciable loss in the yield.

Fredholm and K-Hyponormal Weighted Translation Operators On $L^2(\mu)$

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In this paper we characterize the Fredholm weighted translation operators on non atomic measure space. Also the characterization of invertible weighted translation operator on $L^2(\mu)$ is also given.

Ion transport and dielectric relaxation studies of Li_2SO_4-Li_2O-P_2O_5-V_2O_5 glasses

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Lithium ion conducting glasses have attracted considerable importance because of their possible applications in solid state batteries and electrochemical devices. In this work we report Li^+ ion transport properties of xLi_2SO_4-$30Li_2O$-$(70-x)[0.70P_2O_5:0.30V_2O_5]$ (x=5, 10, 15, 20 and 25 mol%) glasses. Glasses are fabricated using melt quenching technique and their amorphous nature is confirmed by XRD studies. Conductivity measurements are carried out in the frequency range of 100 Hz - 11 MHz over and a temperature range of 313 K to 463 K. Impedance plots exhibit good semicircles and reveals the domination of ionic conductivity. D.C conductivities (σ_{dc}) extracted from impedance plots follow Arrhenius behavior and d.c activation energies (E_{dc}) are estimated from regression analysis. Activation energies (E_{dc}) decreases and d.c conductivities (σ_{dc}) increases with the addition of Li_2SO_4 content. The impedance and modulus spectroscopic plots (Z″ and M″ versus frequency) reveals that the relaxation mechanism of Li^+ ions in the investigated glasses is due to localized movement of charge carriers (short range), temperature dependent and of non-Debye type.

Key words: Ion conductivity, activation energies, impedance spectroscopy, relaxation

Synthesis and Characterization of Polymeric Olive Oil Grafted Methyl Methacrylate or Styrene

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Synthesis of wholly natural polymeric olive oil containing peroxide groups have been reported. Peroxidation, epoxidation and/or perepoxidation reactions of olive oil, either under air or under oxygen flow at room temperature, resulted in polymeric peroxides, Polymeric Olive Oil-air and Polymeric Olive Oil-ofl, containing 1.3 and 3.5 wt.-% of peroxide, with molecular weights of 2100 and 3780 Da, respectively. Polymeric Olive Oil air contained cross-linked film up to 46.1 wt.-percent after a reaction time of 60 d, associated with a waxy, soluble part (Polymeric Olive Oil-air-s) that was isolated with chloroform extraction. Polymeric Olive Oil-ofl was obtained as a waxy, viscous liquid without any cross-linked part at the end of 24 d under visible irradiation and oxygen flow. Polymeric peroxides, Polymeric Olive Oil-air-s and Polymeric Olive Oil ofl initiated the free radical polymerization of both methyl methacrylate (MMA) and styrene (S) to give PMMA-graft Polymeric Olive Oil and PS-graft-Polymeric Olive Oil graft copolymers in high yields with Mw varyingfrom37to470kDa.The polymers obtained were characterized by FT-IR, 1H NMR, TGA, DSC and GPC techniques. Cross-linked polymers were also studied by means of swelling measurements. PMMA-graft-Polymeric Olive Oil graft copolymer film samples were also used in cell-culture studies. Fibroblast cells were well adhered and proliferated on the copolymer film surfaces, which is important in tissue engineering.

Inventory Control in Retrial Service Facility System with Two Types of Customers – SMDP

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In this article, we concentrate on problem of optimally controlling the ordering inventory in retrial service facility system. The arrival of customers (priority and non - priority) to the system is assumed as two independent Poisson streams and service times are assumed to follow an exponential distribution. For the given values of maximum inventory, maximum waiting space, reorder level and lead times, we determine the optimal ordering policy at various instants of time. The system is formulated as a Semi-Markov Decision Process (SMDP) and the optimum inventory control policy to be employed is found using linear programming method. Numerical examples are provided to illustrate the model.

One- pot Hydrothermal Synthesis and Characterisation of WS2 quantum dot and WO3 nanorods

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We report simple, green hydrothermal route for the synthesis of both WS2 quantum dot and WO3 nanorods in same pot. L-cystine serves as source of sulfur and reducing agent as well. Using such biomolecules and minimizing the synthesis process of hybrid quantum dots emit blue and green light in shorter wavelength. The crystallinity, optical, morphological and scattering properties are studied by using X- ray diffraction, UV absorption spectroscopy, Field Emission Scanning Electron Microscopy, High functional materials is of great advantage in both economical and environmental view. The as prepared WS2 quantum dots have average size of ~5nm with emission maximum at 427nm and WO3 nanorods are 200-400nm in range with emission maximum at 367nm. WS2 Resolution Transmission Spectroscopy and Raman spectroscopy. These materials would be potential candidates for bioimaging, sensing, electrodes and energy applications.

Application of tin-oxide nanostructures for LED assisted photo-mineralization of organic pollutant in water

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The present work illustrated the photocatalytic degradation of an organic dye by using SnO_2 catalyst under LED irradiation. The work systematically evaluated the as-synthesized material for its morphology, the electronic band level, elemental composition, and the zeta potential. Further, the demonstration of photodegradation of a model pollutant, methylene blue was carried out to determine the efficiency of SnO_2. The maximum degradation obtained was ~83% corresponding to 30mg of catalyst within 90 minutes. Also, the kinetics and possible mechanism involved in the photocatalysis is illustrated. The present work emphasize on the ease of catalyst synthesis, the energy efficient photon source, and overall performance of SnO_2 to achieve maximum degradation of the dye. Finally, the catalyst has its importance in practical applications like water and wastewater treatment wherein, dyes could be eliminated with ease.

Weighted dom-chromatic number of some classes of Type-II weighted caterpillar graphs

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Let $G = (V, E)$ be a graph. A set D of vertices is a dominating set of G if every vertex in D is adjacent to at least one member of D. A dom-chromatic set D is a subset of V which is a dominating set and $\chi(\langle D \rangle) = \chi(G)$. A Weighted tree, (T, w) a tree together with a positive weight function on the vertex set $w: V(T) \longrightarrow R^+$. The weighted domination number $\gamma_w(T)$ of (T, w) is the minimum weight $w(D) = \sum_{v \in D} w(v)$ of a dominating set D of T. The weighted dom-chromatic number $\gamma_{wch}(T)$ of (T, w) is the minimum weight $w(D) = \sum_{v \in D} w(v)$ of a dom-chromatic set D of T. A caterpillar is a graph which can be obtained from the path on n vertices by appending x_i pendent verices to the i^{th} vertex of the path, P_n. The caterpillar with parameters $n, x_1, x_2, \ldots, x_n$ will be denoted as $P_n(x_1, x_2, \ldots, x_n)$. In this paper, we obtain the weighted dom-chromatic number of some classes of Type-II weighted caterpillar graphs.

Study of electronic properties of $CdTe_2$

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Transitional metal dichalcogenides have emerged as a family of crystals with great interest due to their intriguing properties and fundamental applications in technological field. We have used the full potential-linearized augmented plane wave (FP-LAPW) method to predict the electronic properties of $CdTe_2$. The density of states and energy bands of these materials suggest non-magnetic semiconducting nature of $CdTe_2$, with an energy band gap of 0.71 eV, that has been enhanced 0.95 eV, which is close to the experimental report of 1.08 eV by employing mBJ functional. The analysis of the energy band structure reveals the presence of energy bands mainly formed by Cd-4*d* and Te-5*p* states, where the valence region and conduction region are predominated by Te-5*p* electronic states. The dispersion of conduction bands around Γ is fairly flat giving rise to effective absorption coefficients of the material. Hence narrow band gap coupled with high absorptions coefficients, $CdTe_2$ can be regarded as an efficient absorber of the solar spectrum.

Elucidation of photocatalysis and antibacterial activity studies of Gold nanoparticles using *Abrus precatorius* seed

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Recently, nanotechnology plays a very important role for the production of nanomaterials. Various methods can be used to synthesis nanoparticles. But the production of nanoparticles using plant extract is a very simple, rapid, low cost and eco-friendly method. In the present study, gold nanoparticles (AuNPs) were rapidly synthesized using seed extract of *Abrus precatorius*. The synthesized nanoparticles were systematically characterized by using UV-Visible, FTIR, XRD, EDAX, SEM analysis. The formation of gold nanoparticles was priliminary identified by the change of colour of the solution from yellow to purple within 5 minutes and shows surface plasmon peak around 540-580nm. The average size of the synthesized gold nanoparticles is found to be 10-20 nm and have spherical shape. The gold nanoparticles are used to photocatalytic degradation of methylene blue with the efficiency of above 95%. Besides, the antibacterial activity study was performed against the *Listeria monocyte, Klabsiellapheumonia, Haemophilous influenza, Serratiamarcesers and Vibrio cholera* bacterial pathogens.

External Direct Product and Internal Direct Product of Picture Fuzzy Graphs

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In this work we introduce the external and internal direct product $G_1 \otimes G_2$ and $G_1 \odot G_2$ of of two picture fuzzy graphs G_1 and G_2 are defined. It is proved that when two picture fuzzy graphs are effective then their external and internal direct product are effective. The degree of vertex in the external and internal direct product $G_1 \otimes G_2$ and $G_1 \odot G_2$ of two picture fuzzy graph is obtained and it is proved that internal direct product of two complete picture fuzzy graph is complete.

Automated Detection of White Blood Cell Cancer using Segmentation and Classification Algorithm

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The main objective of this project is to detecting and the blood cell cancer cells in microscopic blood sample images. Blood circulatory system is one of the most important systems in human ‘s body. The function of this system is to transport blood throughout the body. This system consists of blood vessels which are arteries, veins, and capillaries, heart that act as pumping system, and blood that act as the medium for the system. Blood transportation is very important in order to supply oxygen to our body, carries carbon dioxide for gaseous exchange, minerals, nutrients, and ensure healthiness.

Keywords: CT Image, Segmentation, Classification and preprocessing.

Synthesis of Cerium Oxide Nanoparticles and its Corrosion Behaviour –A Review

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Cerium oxide nanoparticles have recently become a significant material in many applications such as photocatalyst, corrosion inhibitor, and biological applications, etc., This review article is focussed on the behaviour of CeO_2 nanoparticles on the corrosion properties. The corrosion resistance hybrid-film based on CeO_2 nanoparticles becomes a more powerful inhibitor than hazardous chromate-based protective materials. Based on results available in the literature, this article is summarizing, the corrosion resistance of CeO_2 on different substrate and Tafel polarization and electrochemical impedance spectroscopy techniques revealed an effective barrier against the acidic medium and aqueous medium. Research-based on the CeO_2 composite coating, incorporation with metal, metal oxide or graphene etc., has been investigated that shows the effect in grain size, cracking, pore size, microstructure, and microhardness towards the corrosion inhibition. One of the most important is cerium oxide nanoparticles on coatings decrease current densities and increase the potential, thereby decrease the corrosion rate. This review article discusses about the synthesis of CeO_2 nanoparticles through various methods and the corrosion resistance of CeO_2 composite coatings in details.

Coprime Irregular Graphs from Hexagonal Snakes

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A k-edge-weighting of a graph G = (V,E) is a map φ: E(G) → {1,2,3,...k}, where k is a positive integer. Denote $\mathbf{S_{\varphi}}(v)$ is the sum of edge-weights presenting on the edges incident at the vertex v under the edge-weighting φ. A k- edge-weighting of G is coprime irregular edge-weighting of G if gcd ($\mathbf{S_{\varphi}}(u)$, $\mathbf{S_{\varphi}}(v)$) = 1 for every pair of adjacent vertices u and v in G. A graph G is coprime irregular if G admits a coprime irregular edge-weighting. In this paper, we discuss about coprime irregular edge-weighting for hexagonal snakes and corona of hexagonal snakes.

Theoretical investigation on solitary transmission of neuronal signals: A He's semi inverse approach

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An investigation of solitary transmission of neuronal signals is intended in this paper through the establishment of solitary wave solutions for the improved Heimburg Jackson model governing the propagation of mechanical wave in biomembranes. The computation of soliton solutions is established out employing He's semi inverse variational principle. The essential role of nonlinearity and dispersive effects in the solitonic propagation is correlated to the role of compressibility, elasticity and inertia over the neuronal signal transmission in the unilamellar DPPC vesicles at T = 45^{o}. The investigation reveals that He's semi inverse method is a direct and effective algebraic method to study the experimental features of the nerve pulse in the bio membranes.

Keywords: Soliton, Neural network, Semi inverse.

Degree - Based Topological Indices of Graphene Structure

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The theory of chemical reaction networks is a branch of mathematics that aims to mimic real-world behavior. This area of research has drawn the attention of many researchers, primarily due to its biological and empirical chemistry applications. Because of the fascinating problems that emerge from the mathematical structures involved, it has kindled the interest of pure mathematicians. In this paper, we estimate a few topological indices based on the neighborhood degree and obtain results based on both sum and products of indices such as SK index, SK1 index, SK2 index, Modified Randic index and Inverse Sum Index for the Graphene structure. We also present their 3D representations using MATLAB

Half-metallicity in equiatomic quaternary Heusler alloy PdFeCrAl: A first principle study

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The first principle method has been implemented in determining the half-metallicity of a new class of equiatomic quaternary Heusler PdFeCrAl and its befitting possibility in the spintronic applications. The structural optimization leaves the material stabilized in LiMgPdSn type structure of *F-43m* space group with lattice constant of 5.94 Å. The analysis of the formation energy and the dynamical stability further supports the possibility of synthesis in laboratory for further study. The studied material is 100 % spin-polarized near the Fermi energy level, with a half metallic gap of 0.08 eV in the minority spin channel and a metallic type for the majority spin channel. The magnetic profile of the material shows its ferromagnetic nature with a magnetic moment of 2.99 μ_B per formula unit which is in compliance with the Slater Pauling rule of MT = Z_T – 24. In overall, the 100% spin-polarized half-metallic ferromagnetic nature of this material is predicted that may be suitable for effective spintronic applications.

NBO, NLO, NCI, Fukui function and other parameter analysis of Amifampridine by DFT

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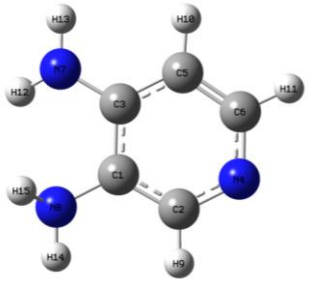
Amifampridine (3,4-Diaminopyridine [3,4DAP]) is used to treat a number of rare muscle diseases. So this molecule was investigated by DFT/B3LYP/6-31 G basis set with the help of Gaussian 16W software. Gaussview 06 is used to view the molecules. The bond angle, bond distance and dihedral angles are having good correlation with the reported pyridine molecule. The ESP explains about the electron rich and electron poor sites in the molecule. Mulliken population analysis and Frontier Orbital energy gap are determined. NBO studies explains the reason for the stability of the molecule. The NLO studies reports that the molecule is 12 times greater then the urea molecule. Fukui function analysis explains the choice of electrophilic attack in the molecule. The NCI interaction also studied by Multiwfn 3.7 software. This molecule is having Van der Waals interaction and steric effects. The shaded surface map with projection effect of electron localisation function clearly indicates that the presence of electron depletion area on 5 carbon atoms and 3 nitrogen atoms.



Optimized structure of Amifampridine molecule

Remarks on fuzzy binary soft set and its characters

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Fuzzy set theory plays a vital role in the field of engineering, computer science, medical field, communication and all other sciences. Soft set theory is an generalization of fuzzy set theory. Soft set theory was introduced by Molodtsov in the year 1999. In 2016 Ahu Acikgoz and Nihal Tas introduced the concept of binary soft set theory on two initial universal set. In this paper we introduced "Fuzzy binary soft set" and its basic operations with needed examples. Also we have studied some results.

Study of electronic properties of $PrFe_4Sb_{12}$

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The electronic properties of the filled skutterudite $PrFe_4Sb_{12}$ have been investigated in the BCC structure by employing the density functional theory using the full potential-linearized augmented plane wave (FP-LAPW) technique. The optimized lattice constant (9.207Å) corresponding to the lowest energy for the system in the cubic phase is obtained. The electronic energy band structure of the sample alloy has been explored along the high symmetry direction of Brillouin Zone. A careful analysis of the energy band structure reveals the degenerate and parabolic type of bands. Moreover, the conduction region displays the flat band like feature due to *f*-state electrons of Pr atom whereas the valence band in minority spin channel is found to be mainly populated by the Fe-*d* electrons. We found that both the spin channel displays the energy bandgap like feature above the Fermi energy level (E_F). The close analysis of energy band structure suggests the semimetallic behaviour of the alloy with enhanced concentration of bands at E_F that may push them for possible applications in thermoelectric devices that requires further investigation.

The Vertex Signal Number of a Graph

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For two vertices u and v in a connected graph G, the signal distance $d_{SD}(u,v)$ from u to v is deined by $d_{SD}(u,v)=\min_S\{d(u,v)+\sum_{w\in V(G)}(\deg w - 2)+(\deg u - 1)+(\deg v - 1)\}$, where S is a path connecting u and v, d(u,v) is the length of the path S and in the sum $\sum_{w\in V(G)}$runs over all the internal vertices between u and v in the path S. A path between the vertices u and v of length $d_{SD}(u,v)$ is called a u – v geosig path. A set $S\subseteq V$ is called a signal set, if every vertex y in G lies on a geosig path joining a pair of vertices of S. The signal number *sn(G)* is the minimum order of a signal set of a graph G. Let u be a vertex of a connected graph G. A set S of vertices of G is an u-signal set if each vertex x of G lies on an u – v geosig path in G for some element v in S. The minimum cardinality of an u-signal set of G is defined as u-signal number of G and denoted by $sn_u(G)$ or

simply sn_u. An *u*-signal set of cardinality $sn_u(G)$ is called a sn_u-set of G. In this paper, we initiate a study on the Vertex signal number of a graph G.

Fabrication of a Bio-Inspired Self-Healing Metal Matrix Composite- A Review

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The concept of self-healing is inspired from the Natural materials such as bone and trees, that all are capable of self-repair its damages. Recently, there has been a huge interest in materials that can self-heal, as this property can potentially increase materials life, reduce replacement costs, and improve product safety and reliability. After the Stone Age, it was the discovery of metals that has dramatically changed the human evolution. Over the time people started using alloys like brass, bronze, gold etc. in their day-to-day life. Today materials have become an integral part of industrial development. Higher strength along with longer useful life has been a primary pre-requisite of the materials for industrial applications. This has challenged the material scientists to think beyond the boundaries of conventional materials and develop new generation materials with better characteristic properties. As a result of which various smart materials are come into existence like, self-healing, self-lubricating, Self-cleaning. Out of the various developments, self-healing composites have emerged as most influencing materials inspired by the biological concept of self-healing in living things. This paper highlights, from Engineering perspective, the various fabrications methods propelling research in self-healing materials especially in metals and current areas of practical applications.

Key words: Self-Healing metals, bio mimics. Self-lubricating, Self-cleaning

A Study of Fluorescence Behaviour of Rhodamine Rose and Cresyl Blue Dyes

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Fluorescent dyes are widely used in the, textile, polymer, printing, biological and medicinal fields. The dye effluent from textile industries causes serious water and land pollution. The concentration of dye in the effluent can be determined using absorption and emission spectral studies which are helpful for dye effluent treatment studies. The present deals with the study of fluorescent behaviour Cresyl Blue and Rhodamine Rose dyes. These dyes have significantapplications in textile, biological and medicinal fields. The fluorescent behaviour of the dyes was studied in water and ethanol solvents and in presence of quenchers *viz.* KI and Benzophenone and also in polar binary solvents. From the present study it may be concluded that Rhodamine Rose shows excellent fluorescent behaviour than Cresyl Blue in polar solvents.

Existence of Solution to a model for COVID-19outbreak in Wuhan, China with governmental action

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A mathematical model of the coronavirus disease (COVID-19) in Wuhan, Chinawith governmental action which has been solved by using Homotopy perturbation method and found its approximate analytical solution. The initial conditions are formulated based on `COVID-19 coronavirus pandemic' data of China. The solution of the model is exhibitedby graphs and the effects of governmental action upon COVID-19 pandemic is discussed.

Studies on Porphyrin derivatives as a potential anode material for LIBs and NIBs

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Because of the interesting properties in electronic applications, such as high carrier mobility, superior mechanical flexibility etc, 2D materials have ignited great research since the discovery of graphene. In general, 2D materials are also believed to be promising candidates for the anode in metal-ion batteries. This is because of their advantages such as large surface-to-volume ratio. Further, the specific capacity of graphite is ~372 mAh/g, which is too low for the limited intercalation sites for Li in the graphite. Thus, 2D materials are likely replacement to graphite for use as anode materials in Lithium-ion batteries (LIBs) and Sodium-ion batteries (NIBs). Hence, the search for new anode material for LIBs, which must have large capacity, high rate capability and long cycle life to replace the commercialized graphite, is essential. Recently, porphyrin based metal organic framework is studied for Li-S batteries. Hence, in the present study porphyrin base and its derivatives are investigated to explore its potential application as anode material for LIBs and NIBs. Alkali metal ions / atoms such as Li, Na adsorption on porphyrin base and its derivatives are studied using M06-2X functional. The structural and energy parameters are calculated for the above systems and are discussed with the available experimental and previous theoretical results.

Nanostructured thin film sensors for toxic gas sensing applications: efficacy and advancements

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Nanotechnology has enormous capabilities for development of multifunctional materials having specific characteristics which can be utilized to fabricate nanosensors for detection of poisonous gases and organic vapors. Thin film materials comprise of metal oxide semiconductors, conducting polymers, graphene based carbon nanotube materials which exhibit excellent morphological, physical and chemical properties due to which they qualify for novel gas sensing materials. The electrical conductivity, high specific surface area, high aspect ratios, fast response, sensitivity and low maintenance along with high stability, chemical resistance and flexibility makes these materials the best option for being used as thin film gas sensors. These materials are embedded as thin films on substrates or electrodes and change in electrical conduction and/or flow of electrons causes the detection of gas molecules in the vicinity of the sensor. These materials are sometimes used as thin films in conjunction with field-effect transistor with controlled electric field to monitor sensing current and detection of trace gases. The advantages of thin film gas sensors and manifold including detection of gases at very low concentration (traces), fast detection and reliable sensing for sensing gases such as nitrogen dioxide, hydrogen, and CO_2. Highly selective, stable and durable hybrid materials based chemi-resistor gas sensors are the upcoming future of gas sensing technology. The paper outlines and describes the upcoming gas sensing technologies for the near future applications.

The Isolate Domination Number and Some Special Families of Graphs

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A set S of vertices in a graph G is a dominating set if each vertex of G that is not in S is adjacent to at least one vertex of S. The minimum cardinality among all dominating sets in G is called the domination number of G and denoted $\gamma(G)$. A dominating set S such that $< S >$ has at least one isolated vertex is called an isolate dominating set. The minimum cardinality of an isolate dominating set is called the isolate domination number and denoted by $\gamma_0(G)$. In this paper we study the isolate domination number values for some special families of graphs.

Structure, Stability, Reactivity and NLO property of Substituted Toluenesulfonamides

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Sulfonamides are well known for their significant biological activity such as antibacterial, insulin releasing, carbonic anhydrase inhibitory etc. Because of these significant biological activities, enormous amount of attention is given on sulfonamide and its derivatives. In order to explore new potential applications in sulfonamide derivatives, in the present investigation, we have studied the structure, stability, reactivity and NLO property of substituted sulfonamide. The substituted functional groups are –H, -CH_3, -OH, and –NH_2. Our calculations indicate that the structural parameters are significantly altered due to substitution of different functional groups. The reactivity of the sites and stability of the substituted sulfonamides are significantly changed. Further, the biological activity of the substituted sulfonamides is investigated. The optical activity of substituted sulfonamides are also studied and compared with the available experimental data. Further our calculated structural parameters and energy parameters are compared with the available experimental and theoretical data and discussed.

Anion Induced Fluorescence Quenching of Various Aromatic amino fluorophores

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Fluorescence quenching of Aromatic amino fluorophores [Such as 2-aminodiphenyl(2ADP), 4-aminodiphenyl (4ADP), 2-amino7-bromofluorine (2ABF), 2-aminodiphenylsulphone (2ADPS), 3,3′-diaminodiphenylsulphone (3DADPS), and 4,4′-diaminodiphenylsulphone (4DADPS),)] by inorganic anions [The inorganic anions used for quenching were the sodium salts of chloride (Cl^-), Br^-, SO_4^{2-} SO_3^{2-}, $S_2O_3^{2-}$, CO_3^{2-}, NO^{3-}, & HPO_4^{2-}] have been studied in 95% (v/v) water –ethanol mixture medium. 2ADP, 4ADP, 2ADPS and 3DADPS of the fluorescence quenching was observed with only one or two anions and so the quenching of these compounds is not discussed. The quenching was found to be dynamic in all systems. The plots of log kq values with singlet transition energy (E_s) of the fluorophore and with E_{CTTS} of the quencher are linear indicating the presence of electron transfer quenching mechanism. ΔG_{TH} values for charge transfer quenching have been determined for aminodiphenylsulphone.

Dominating Sets of Cell Graphs

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To comprehend the nature of cells in biological tissues, its biological structure have to be converted into a mathematical object called cell graph. A cell graph is a graph, whose vertices are cells or cell clusters of a tissue and edges between the vertices are defined by considering the biological foundations between the cells or the cell clusters. In this paper, we discuss some existing methods of constructing cell graphs and introduce some new methods of constructing cell graphs. Also, we study the dominating sets associated with the cell graphs.

Structure, Stability, Reactivity, NLO property and TDDFT studies in Toluenesulfonamide Derivatives

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Nitrogen-containing compounds have significant importance in pharma industry and they are novel bio-active compounds. In the last few decades, versatile catalytic procedures for carbon-nitrogen bond formation have been developed. The sulfonamides constitute an important class of compounds because the sulfonamide moiety is found in a large number of agrochemicals and pharmaceuticals. Further, sulfonamides have also been used as protecting groups, which can be readily removed. Due to this, enormous amount of experimental and theoretical studies are performed on sulfonamide derivatives. In order to get deeper insights as well as to explore new potential applications on these systems, in the present study, density functional theory calculations are performed. The structure, stability, reactivity, and NLO property of ortho, para and meta tolune sulfonamide are studied. Further, TDDFT studies are also performed on these systems. The obtained results are compared with the previous experimental and theoretical results and are discussed.

Analysis of silver dispersed poly (aniline-co-3-bromoaniline) nanostructured composites for electro active applications

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Nanostructured Conducting polymers possess unique electrical and magnetic properties leading to wide range of industrial applications such as sensors, rechargeable batteries, electromagnetic shielding and solar cells etc. Here we prepared a new series of silver dispersed nanostructured poly(aniline-co-m-bromoaniline) copolymer composites by chemical oxidative *in-situ* polymerization method using DBSA. The synthesized composites were subjected to various characterization techniques such as UV-visible spectroscopy, FT-IR spectroscopy, X-ray diffraction, scanning electron microscopy. The copolymer samples were found to be soluble in common organic solvents like DMSO, NMP, THF and DMF. The UV-visible spectra show the $\pi - \pi^*$ transition (340nm) and the n-π^* transition(576nm). FT-IR spectra confirmed the formation of the benzenoid ring and quinoid ring. XRD pattern confirms the amorphous nature of the polymer. SEM image reveals a large number smooth surfaced and agglomerated granular structure as shown in figure. Thermal analysis shows that the copolymer composite high thermal stability than the homopolymer polyaniline. The electrical conductivity value of the composites ranges from 1.13×10^{-5} to 5.16×10^{-8} S/cm.

Application of Divisor Degree Energy

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The divisor degree energy is defined as the sum of the absolute value of eigen values of divisor degree matrix. In this paper, we compare the divisor degree matrix and extended adjacency matrix of acyclic molecules. In addition to that, we also compare divisor degree energy with extended adjacency energy using correlation and regression, in which it is obtained from the chemical graph (hydrogen suppressed graph).

UV Spectroscopic Studies on Porphyrin and Toluenesulfonamide derivatives

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Skin cancer is a serious health issue around the world. Sunscreens can be used to prevent skin cancer. In the past few decades large number of studies was performed to identify better and safer sunscreens. Therefore, in the present study density functional theory studies are performed to identify potential UV filters. The systems we have selected are porphyrin and toluene sulfonamide derivatives. The reason for the selection of porphyrin and toluene sulfonamide is, they have significant biological activity. Our present study is to find out if the porphyrin and toluenesulfonamide and its derivatives are capable of absorbing harmful radiations in the UVB and UVA ranges. Our study could lead to the development of new UV filters. In DFT, TDDFT calculations are performed. All DFT/TD-DFT calculations were performed using Gaussian09W program package. The methodology employed in the present study could be useful for the determination of the UV spectra of porphyrin derivatives and sulfonamide derivatives and could be used as a tool for the development of novel UV filters.

A Fluorescent Chemosensor for Al^{3+} and HSO_3^- Detection

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Aluminum is found in its ionic form as Al (III) in many animals, natural waters, and plants. Besides, the aluminum ion is extensively utilized in different fields, including pharmaceuticals, food packaging, manufacturing industry and water cleansing. On the other hand, because of its wide use, aluminum ion can enter the human body directly through food and water. An extreme introduction of human body to Al^{3+} -ion prompts numerous risky diseases such as the progression of bone disease in children, encephalopathy, Alzheimer's disease, Meknes disorder and Parkinson's disease. Similarly, bisulfite is the one of the environmentally and biologically significant anions which attracted recent scientific researchers due to their simple bio accumulation in water body. Even though, bisulfite is known for food additive in beverages, anti-oxidation agent and preventing bacterial growth in several pharmaceutical products, the acceptable level of bisulfite to human body is margined between 0 to 0.7mg/Kg per day by World Health Organization (WHO). Therefore, to overcome these bio accumulation problems we report a simple and economic quinoline-naphthalene conjugate as fluorescent chemosensor for the selective fluorescence recognition of Al^{3+} and HSO_3^- -ions. The details of sensor development, characterization and fluorescent response will be presented.

Impact of Thermal Effect on the Propagation waves of Rotating Graphene Tubule

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The impact of thermal field on the propagation of waves of rotating graphene tubule is modelled using elastic shell theory. The scattered relation of rotating graphene tubule with thermal response is attained in consideration of centrifugal force and thermal force. The numerical value of non-dimensional phase velocities are computed and represented in the form of scattered curves for lower and higher modes of vibrations. In addition, scattered curves of graphene tubule at various thickness are plotted and is compared with the existing literature.

FTIR and FT-Raman Spectroscopic studies of Some Vegetable Oils and Chicken Oil

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Vegetable oils play very important role in human diet all over the world, even though the specific oil used in different parts are different. Many vegetable oils are used by the pharmaceutical, cosmetic or even biodiesel production industry. In recent years, use of spectroscopic techniques in general, and Raman spectroscopy in particular, in Food Chemistry has grown dramatically. Edible vegetable oils have been the subject of a number of applications of Raman spectroscopy, often in combination with chemometric methods. Advances in this field of analysis have been promoted by the availability of increasingly powerful Raman spectrometers and the development of fiber optic probes. Raman spectroscopy is very important practical tool for quickly identifying molecules and minerals, and is also has important scientific applications in studying molecular structure. In this paper we have used both kinds of applications. Here we applied the Raman spectroscopy to study the molecular structure of oils like Sesame oil, Mustard oil, Castor oil, Groundnut oil, Coconut oil, Neem oil and Chicken oil. We have also recorded the FTIR spectrum of the above oils and compared with the Raman spectrum of them. From all studies of IR and Raman spectrum, it is found that the functional groups found in oils are same in both studies. All the vegtable oils showed approximately same Raman shifts and IR absorption peaks, but Chicken oil showed more absoptional peaks. It reveals that Chicken oil contains few number of H_2O molecules as it does not react in Raman spectrum,but react in IR spectrum. All C-H bonds in oils are responsible for the peaks in Raman spectrum. All other vegetable oils have same peaks in Raman and it confirms that all

contains H_2O molecules in excess than Chicken oil. We feel that lesser no. of H_2O may be the reason of more peaks in Raman and high absoption in UV transmission. All oils contains same functional groups other than water groups.

Salicylaldehyde Based Fluorescent Chemosensor: Detection of Sr^{2+} Ion

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The alkaline earth metal, Strontium is a soft silver-white yellowish metallic element and is highly chemically reactive. While natural strontium (which is mostly isotope strontium-88) is stable, the synthetic strontium-90 is radioactive and its presence in bones can cause bone cancer, cancer of nearby tissues, and leukemia. It is one of the most dangerous components of nuclear fallout, as strontium is absorbed by the body in a similar manner to calcium. Natural stable strontium, on the other hand, is not hazardous to health. Strontium substitution for calcium in biomineralization during bone formation has been exploited in osteoporosis studies and in the development of osteoporosis medications. In contrast to its innumerable medical applications, most strontium compounds like strontium nitrate, owing to their high-water solubility, have been acknowledged as drinking water pollutants and cause detrimental effects on aquatic environment. Further, high uptake of strontium disrupts the bone development in children and its chromate salt is a renowned causative agent of lung cancer. Therefore, among various analytes, recognition of metal ions has attracted considerable attention from researchers these days because of their presence everywhere in the environment. Hence, a sensor for metal ions can be applicable in industrial processes, medical diagnosis and environmental inspection. Hereby we developed a salicylaldehyde based chemosensor that detects strontium (Sr^{2+}) ions accurately in DMSO:H_2O mixture at pH 7.4. The sensor development and its ion detection will be presented.

Analysis of steady-state behaviour of EC' catalytic mechanism at rotating disk electrode: Taylor series approach

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This paper deals with EC' reaction mechanism arises in rotating disk electrode. This mathematical model contains a system of reaction-convection-diffusion equations. Taylor series method is applied to find the analytical expression of concentration and current. The solutions allow us to obtain the current response for steady-state voltammetry, and it is useful for studying system behavior. The obtained results are compared with the

numerical simulation. An excellent agreement is observed between the Taylor's series of solutions obtained and simulation results. The effect of the parameters on concentration and current are discussed and presented graphically.

FTIR Study of Possible Contamination Edible Oils Due to Repeated Heating Effects

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Vegetable oils are major lipid sources of high nutritional calorific value for human diet. Especially, coconut oil, sunflower oil, mustard oil and groundnut oil are the functional oils used. The quality of edible oils is determined by its contents and parameters inherent in vegetable oils. Infrared spectroscopy is an ideal technique for quantitative analysis of vegetable oils as well as for determination of oil parameters. It is believed that repeated heating of edible oils cause degradation of the oil, and in turn, causes health problem for us. Especially in fast food centre etc., the same oil is repeatedly used until it becomes black in color and very thick. The bad effect of the food prepared in such oils to cause even deadly diseases like cancer. Here we make an attempt to study the possible contamination of edible oils due to heating, using FTIR studies of the same, before heating and after repeated heating.

A Fluoro/colorimetric chemosensor for Cu^{2+} ion sensing based on a Schiff base derivative

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The design and synthesis of chemosensors for the sensing of various metal ions has showed major interest in present days due to their imperative advantages in environmental and biological areas [1]. Among all metal cations, Cu has significant attention because of its paramagnetic nature. The American Medical Association suggests that the presence of Cu in a normal human body should be between 1.2–1.3 mg/day. The presence of Cu for the development of human growth is in the order of 0.1 mg/L respectively [2]. Copper has more connectivity to human in daily life, which makes it more dangerous for environment bodies. It will easily enter into drinking water through human daily life usages and makes it more pollutant and led to serious pollution in human, animals and as well as plants. Therefore, detecting and monitoring of Cu in water bodies gets more attention nowadays. Till date, detection of copper has been reported by various analytical techniques. However, it is still a challenging one to detect Copper via both by colorimetry and fluorimetry. Considering the attention in detection of Copper, we have designed Schiff

base fluorescence probes HTPI and TPI for the detection of Copper. The synthesized probes were successfully characterized and applied for the detection of Cu^{2+} ions in water samples. These details will be presented.

New Sort of Mappings Via $^{*}\delta$- Set in Topological Spaces

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In this paper, we shall introduce and study on some new type of generalized functions called *δ-continuous, *δ-irresolute, functions via the concept of *δ –sets. The purpose of this work is to explore properties and characterizations of these functions. Using the concept of *δ - open sets, we also introduce *δ –open mappings and investigate certain characterizations of this type of functions.

Alzheimer Disease Detection using Artificial Neural Network

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Earlier diagnosis of Alzheimer growth leads to save lots of precious human lives. It is necessary to develop some automated tool, in order to detect malignant state at the beginning stage itself. Many algorithms had been proposed earlier by many researchers in the past, but the accuracy of prediction is always a challenging task. In this work, an artificial neural network-based methodology is proposed to find the abnormal growth of Alzheimer. Higher probability of detection is taken as an objective to get an automated tool, with great accuracy. Manual interpretation always leads to misdiagnosis. A full-fledged Computer Tomography image set of lung of 10 different humans, with normal and malignant health states have been considered in this work. The Distinct textural features of the images provide an intra class variation in its nature, make a neural network, feasible for classification of the normal images, identifying away from the malignant ones. Optimal feature sets derived from Haralick Gray level co-occurrence Matrix and used as the dimension reduction way for feeding neural network. In this work, a binary Support Vector Machine Neural network has been proposed to identify the normal images out of all the images. The capability of the proposed neural network has been quantitatively computed using confusion matrix and found in terms of classification accuracy.

Keywords: Classification, Feature Extraction,Accuracy

Dual Mode Fluoro/Colorimetric Chemosensor for the Detection of Pb^{2+} & Fe^{2+} Ions

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Lead is one of the earliest metals discovered by the human race. Notably, the primary application for lead can be found in Lead–acid batteries. It can be used for pipelines, paints and still are used in some bullets. Over the years, greater awareness about the negative health effects of lead has resulted in many countries banning numerous lead products. Lead (II) ion contamination gets accumulated along the food chain and cause a serious threat to public health. Lead is a neurotoxin that accumulates in soft tissues and bones; it damages the nervous system. Iron (as Fe^{2+}) is a necessary trace element used by all known living organisms. Owing to distinctive electrochemical properties interconvertible multiple oxidation states, iron plays a significant role in varies physiologically important function such as respiration, oxygen transport, energy production and enzymatic reaction. This redox activity can also potentially produce cellular damage and death, and numerous diseases are related to iron overload resulting from dysfunction of the iron regulatory system. Schiff bases can be synthesized from an aliphatic or aromatic amine and a carbonyl compound. The term Schiff base is normally applied to the compounds when they are being used as ligands to form coordination complexes with metal ions. Such complexes naturally occur, but the majority of Schiff bases are synthesized at Labs. Thus, in view of reason, we herein report a simple naphthalene based Schiff base colorimetric and flurometric chemosensor for detection of Pb^{2+} and Fe^{2+} ions.

Lower bound associated with the computation of combinations in an optimal way

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Discrete mathematics is the cornerstone of Mathematics and it is the language of data science. Its importance has increased exponentially in recent decades. Discrete math especially combinatorics is the backbone of modern computer science. In the modern digital world fulfilling the huge memory requirements associated with data transfer has become a challenging task. We are continuously working to minimize those memory requirements.

Many researchers have contributed in finding out the values of combinations with minimal computations so as to reduce the memory allocation for storage. The computation of combinations in an optimal way has already been introduced by considering the remainders in successive divisions by a natural number. In this paper we have found a lower bound for that natural number and the program for its computation is also incorporated.

Integrated Performance of Flat Plate Collector and Shallow Solar Pond in Enhancing the Productive Yield of Glass Top Cover Pyramid Solar Still in Arid and Semi-Arid Regions

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In this paper, a new model for a glass top cover pyramid solar still had been developed to increase the productivity of the still by taking account the effect of all walls of the still on the amount of incident solar radiation on the water surface and each wall. Also, an attempt had been made to enhance the productivity of the pyramid solar still by connecting it with flat plate collector and shallow solar pond. Pyramid solar still of area 0.5625 m2 is designed using a single piece of mild steel and 3mm transparent glass is used as a top cover. Chemical adhesive are used to join the top cover, which suppress the insignificant outflow of heat through the gap in top cover. Thermal performance of glass cover pyramid solar still is carried out under three modes of study namely, with pyramid still alone, pyramid solar still coupled with flat plate collector and pyramid solar still coupled with shallow solar pond. The main advantage of the pyramid top cover solar still is that the maximum radiation can penetrate inside the basin from the top cover when compared to normal single slope solar still. The study incorporates the influence of different environmental and operational parameters on the still productivity. Environmental parameters include solar intensity, ambient temperature and wind speed. Operational parameters include inner and outer cover temperature, basin water temperature, basin air temperature and basin water depth.

Main objective of this present paper is to study the behavior of the still performance with and without flat plate collector and shallow solar pond by analysing the internal and external heat transfer modes and thermophysical properties such as dynamic viscosity, density, thermal conductivity, latent heat of evaporation and saturated vapour pressure for three modes of the pyramid solar still. The instantaneous efficiency, performance ratio and dimensionless parameters (Nusselt number (Nu) and Grashof number (Gr)) are also calculated for the pyramid solar stills under three modes of study.

Fig (1) Pyramid Solar Still

Fig (2) Pyramid Solar Still with Flat Plate Collector with insulation

Fig (3) Pyramid Solar Still with Shallow Solar Pond with insulation

Instantaneous distillate yield obtained is in the range of 0.01 Kg to 0.045 Kg, 0.013 Kg to 0.062 Kg and 0.014 Kg to 0.056 Kg for still performance alone and that combined with flat plate collector and shallow solar pond. The maximum distillate output observed is around 2.366 L/0.5625 m2/day, 3.1696 L/0.5625 m2/day and 3.532 L/0.5625 m2/day for pyramid slope solar still performance study individually and the study combined with flat plate collector and shallow solar pond. Average daily efficiency observed for pyramid slope solar still under three modes of study are around 21.60%, 6.92% and 7.39% respectively. Even though the efficiency is reduced in combined performance, distillate yield is increased to higher level. In general the still performance is reasonable with a good daily output including nocturnal output. The additions of sensible thermal storage units were capable of enhancing the productivity with heat retention causing continued evaporation.

Comparing the performance ratio values, the maximum value obtained for still combined with shallow solar pond 11.3 %. Similarly the performance ratio for still with and without flat plate collector is around 8.66 % and 7.25% respectively. Saturation vapour pressure is predicted in the range of 4842 to 11889 Pa, 5050 Pa to 14114 Pa and 5121 pa to 13281 Pa for still under three modes of study. The difference in saturated vapour pressure is very less at higher temperature compared to the warm up period. So it suggests that the latent heat value has started or starts to increase and at the same time saturation vapour pressure starts to decrease. Latent heat value is observed in the range of 2416722 to 2375960 kg−1, 2414936 to 2367475 kg−1 and 2414341 to 2370510 kg−1 for still performance under three modes namely.

The thermal conductivity of water is analyzed for three modes of study and it is observed in the range of 26.89x10-3 Wm-2°C-1 to 28.19x10-3 Wm-2°C-1, 26.95x10-3 Wm-2°C-1 to 28.46x10-3 Wm-2°C-1 and 26.97x10-3 Wm-2°C-1 to 28.33x10-3 Wm-2°C-1. The dynamic viscosity of water is predicted in the range of 18.68x10-6 Nsm-2 to 19.46x10-6 Nsm-2, 18.71x10-6 Nsm-2 to 19.62x10-6 Nsm-2 and 18.73x10-6 Nsm-2 to 19.49x10-6 Nsm-2 for still without, with flat plate collector and shallow solar pond. Thermal conductivity and dynamic viscosity increase with respect to time and posses almost the same trend. The density of water is predicted for the still and it is observed as 11.52x10-1 kgm-3 to 10.94x10-1 kgm-3, 11.52x10-1 kgm-3 to 10.83x10-1 kgm-3 and 11.51x10-1 kgm-3 to 10.87x10-1 kgm-3 for still performance under three modes of study. It concludes that the density decreases with respect to increase in water temperature and it starts to increase with the decrease in water temperature.

Tabulation : 1 : Internal and external heat transfer values :

	Qci (W/m2)	**Qri (W/m2)**	**Qei (W/m2)**	**Qce (W/m2)**	**Qre (W/m2)**	**Qbe (W/m2)**
Pyramid solar still	17.22	51.52	127.47	37.11	78.93	4.65
Pyramid solar still coupled with flat plate collector	23.41	64.96	247.16	41.43	84.09	5.81
Pyramid solar still coupled with shallow solar pond	24.22	72.83	223.74	43.27	86.14	6.26

The performance of the pyramid top cover solar still is analyzed individually and study coupled with flat plate collector and shallow solar pond. The effect of water temperature in the still causes the increase in distillate yield. The combined performance results confirmed that even smaller surface area of the top cover in the still can also produce more distillate yield. The saturation vapour pressure and latent heat also plays a major hole in production of distillate yield. In general the still performance is reasonable with a good daily output including nocturnal output. The additions of sensible heat absorbing materials were capable of enhancing the productivity with heat retention causing continued evaporation.

Keywords : *Solar Still, Water Collection, Efficiency, Temperature, Heat Transfer*

Schiff Base Fluorophores: Detection of Copper by Fluorescence Quenching

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Currently, there is a lot of demand for fluorescence probes to efficiently detect transition and post-transition metals owing to their high toxicity and crucial role in biological systems. Among the essential heavy metals, Cu in the human body plays vital role in many physiological activities, including the smooth functioning of the liver and kidneys. Cu can also play as an enzyme cofactor and these enzymes have combined with Cu in order to play their respective catalytic function. Cu is essential for the cell, at the same time, produce a series of hazards as an element. The inference of Cu ions in the living things becomes a mandatory test for determining the health status. There are many analytical practices used to detect metal ions, such as inductively coupled plasma mass spectrometry, electro-chemical sensors, atomic absorption and emission spectrometer, and X-ray fluorescence spectroscopy. Since, most of the traditional methods are costly because they usually require sophisticated instrumentation and complex sample preprocessor. So fluorescent sensing technique is one of the convenient methods as these types of chemosensors have widespread applications in many areas, the advantages include simplicity, reducing time consumption, low detections limits and also they could be applicable for real-time monitoring of analytes in physiological conditions. Here we synthesized Schiff base molecules, HNBI and NBI, which are utilized for the fluorescent detection of metal ions.

Some stronger form of g*s closed sets in topological spaces

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In this paper, we introduce and study some stronger forms of *g*s* –continuous functions namely, strongly *g*s*-continuous, perfectly *g*s*-continuous and completely *g*s* -continuous functions in topological spaces. Further we introduce the concepts of strongly *g*s*-closed and strongly *g*s*-open maps and obtain some of their properties.

Estimation of Optical Properties of Thin Films using Envelope Method from Single Transmittance Method

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There are several optical parameters of interest useful for better understanding of a material particularly for solar cells and LED devices. These parameters are most often estimated using some experiments and spectroscopy indirectly. In a solar cell, the only important value is the optical gap which facilitates you to send the wavelength for favourable absorption and photo electric conversion. But in a light-emitting diode, however, applying a bias that corresponds to the optical gap is not enough. You have to apply a bias corresponding to the actual electronic gap, because you first have to inject electrons and holes into the system before they recombine to emit a photon. Hence estimation of electronic gaps, optical gap, the urbecks energy and refractive and extinction coefficients are important for semiconducting materials. In few optical devices the values of dieletctric constants, optical conductivity are essential. Envelop is a region of a series of curves encompassing a set of curves. In this work from a single transmittance measurement by applying the mathematics of envelop many optical parameters are estimated and reported. The estimated constants for various materials are found to be consistent with those estimated by other methods. The details are discussed.

Keywords: Thinfilm, Optical properties, Dielectric responses, LED, Solar cells

Graphene Oxide based Organic Nanocomposites as Fluorescent Chemosensors For Metal Ion Detection

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Due to their facile preparation and easy modification, pheneylenediamine belonging to simple aromatic diamines, are widely used in dye industry, energy storage, biological and chemical sensing. Graphene nanocomposites are of great interest due to

their exceptional optical, electrical and mechanical properties. In addition to possessing unique properties, grapheneoxide also shows great effect on fluorescence by either enhancing or quenching fluorescence signal. In this work, we have designed a novel nano hybrid structures, Graphene oxide-*para*phenylenediamine (GO-PPD) nanocomposite of two different molar ratios, 1:1 and 1:5. The composites are characterized by SEM, EDAX, XRD, UV Visible and Fluorescence spectroscopy which validates the successful synthesis of nanocomposites. The nanocomposites are utilized for detection of biologically and environmentally important metal ions. The synthesis and fluorescent details along with the detection of metal ions will be presented.

3-Equitable Intersection Labeling of Graphs

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In this paper, we define a new concept called 3-equitable intersection labeling and we check the 3-equitable intersection labeling for some standard graphs. It is proved the existence of 3-equitable intersection graphs. Also, it is proved some graphs such as star graph, complete bipartite graphs are not 3-equitable intersection labeling.

Synthesis of transition metal (Co) doped and rare earth (Nd) co-doped CuO nanostructure via a facile sol–gel method for spintronics applications

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In this work, the Nd doped Co:CuO nanocrystalline system was prepared via simple and low cost sol–gel method. The structural, optical, electrical and magnetic properties of the prepared nanopowders were investigated by XRD, UV-visible, Hall Effect and VSM, respectively. XRD spectra reveal the structure of prepared CuO nanoparticles as

monoclinic phase. It confirms that the introduction of Co and Nd ions does not alter the CuO crystal lattice. From SEM images, it is found that the grains are monoclinic in shape for all the prepared samples. Elemental mapping and EDAX studies confirm the presence of Cu, O, Co and Nd elements in Nd co-doped Co:CuO nanostructure. The band gap value of the synthesized pristine CuO nanostructures is 1.79 eV and the value decreases slightly on doping of Co and Nd elements. The PL spectra support our discussion that the crystallite size decreased with the addition of Co and Nd elements as arrived by XRD. Electrical studies show that the conductivity of the prepared samples considerably increases with increasing temperature. VSM study shows that all the samples have ferromagnetic behavior at room temperature. The maximum saturation magnetization value is ~0.074 emu/g for 3 wt%, Nd co-doped Co:CuO.

Utilization of Naphthalene Scaffolds as Chemosensors for the Specific Recognition of Aluminium ions

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Over the years, many analytical methods have been developed for the detection of various analytes including metal ions. Among them, the fluorescence spectroscopy is a powerful tool to sense the ions, due to its simplicity, high detection limit and applications in bio-imaging. Aluminium is the first abundant metal element in the earth's crust and has been widespread applied in water purification, food additives, clinical drugs, packing materials. It can easily enter human body through food, water and drugs. According to World Health Organization report, the average daily intake of aluminium is about 3-10 mg/day. Excessive intake of Al^{3+} ions and the accumulation in human body may lead to severe diseases such as Alzheimer's disease, Parkinson's disease etc. Aluminium in its ionic form (Al) has the ability to react with biological species by changing or defeating their function, leading to harmful effects. Out of various methods available for the detection of Al ions the spectrofluorometry is extensively used due to its high sensitivity. Due to this, detection of Al metal ions has attained a high significance in fluorescence chemosensing. Naphthalene based ligands create an environment similar to the biological systems usually by coordinating through oxygen and nitrogen atoms. They offers a number of attractive structural features such as the degree of rigidity, conjugated π-system and a NH unit that participates in hydrogen bonding and may be a site for protonation–deprotonation. Here, we designed and synthesized naphthalene based fluorescent probes **OHN** and **OHHN** for specific recognition of aluminium (III) metal ions.

On Faintly f-Continuous Functions in Topological Spaces

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In this paper, a new class of functions called faintly f-continuous functions has been defined and studied in topological spaces. Relationships among this new class of functions and GO-Connected spaces and GO-Compact spaces are investigated. Also, the relationship between faintly f-continuous functions and graphs are investigated.

Effect of molar concentrations change in structural and optical studies of CdO thin films using sol-gel dip coating

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Cadmium oxide (CdO) thin films were deposited on glass substrates using sol-gel dip coating technique. CdO thin films deposited using various concentration of cadmium acetate solution such as 0.3M and 0.4 M. X-ray diffraction studies revealed that the films are polycrystalline in nature with cubic structure. The average crystalline sizes difference from 2 to 4 nm. Optical studies expose that the films prepared from solution of 0.3M and 0.4M concentration have less transparency. Photoluminescence spectra of the CdO thin films recorded at room temperature under excitation wavelength of 290 nm. The emission peak is centered at 408 nm. Photoluminescence studies exposed that the optical quality of emission peaks which could be related to effective number of charge carriers resulting in the electrical conductivity of the films.

Environmentally Benign Method for the Synthesis of copper Oxide Nanoparticles using the Leaf Extract of Azadirachta Indica

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Chemical synthesis is a synthetic route of chemical reactions to obtain various desired products. This happens either by physical or chemical manipulations usually involving one or more reactions. Chemical synthesis is an effective method to generate the desired products in greater proportion at the same time the by-products obtained during these synthesis are unwanted and generate ill effects to the environment. Apart from that the chemicals and other reagents utilized for the synthesis are cost effective and are hazardous too. So in order to minimize the harmful effect to environment we havedeveloped a greener technique to synthesize the products we needed and this could be achieved via green method. In order to make the reaction effective mostly nano sized materials are preferred. As the nano sized materials have excellent electrical, magnetic, optical and mechanical

properties those are rapidly being developed for their use in numerous fields and they also create a great impact in the modern researches, nowadays the nanoparticles are utilized for the removal of pollutants generated in the environment. Nano technology is cost effective and is difficult to manufacture the products at desired nanosize and because of its small size it may cause problems when inhaled by humans soto minimize the risk coefficient, nanotechnology via a greener route is adopted for the synthesis of CuO nanoparticles. Green chemistry also called as sustainable energy focused on designing of the products and the process to reduce the environment and health hazards. This is an environmentally benign method to synthesize the products that are required. Here our work deals with the synthesis of CuO nanoparticles as it has numerous applications in various fields. The CuO nanoparticles are synthesized using the *Azadirachta Indica* leaf extract as a reducing agent and then characterized using XRD techniques to check their crystallinity and other factors.

α Generalized Closed Sets with Respect to an Ideal

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An ideal on a set X is a non empty collection of subsets of X with heredity property which is also closed under finite unions. The concept of generalized closed sets was introduced by Levine. Indeed ideals are very important tools in General Topology. It was the works of Newcomb[8], Rancin [9], Samuels [10] and Hamlet and Jankovic (see [1, 2, 3, 4, 5]) which motivated the research in applying topological ideals to generalize the most basic properties in General Topology. A nonempty collection I of subsets on a topological space (X, τ) is called a topological ideal [6] if it satisfies the following two conditions:

1. If $A \in I$ and $B \subset A$ implies $B \in I$ (heredity) 2. If $A \in I$ and $B \in I$, then $A \cup B \in I$ (finite additively) If A is a subset of a topological space (X, τ) , cl(A) and int(A) denote the closure of A and the interior of A, respectively. Let $A \subset B \subset X$. Then $cl_B(A)$ (resp. $int_B(A)$) denotes closure of A (resp. interior of A) with respect to B. Levine [7] introduced the concept of generalized closed sets. This notion has been studied extensively in recent years by many topologists. In this paper, we introduce and study the concept of αg-closed sets with respect to an ideal, which is the extension of the concept of g- closed sets.

Synthesis and characterization of Sodium cobalt (II) phosphate ($NaCoPO_4$) Cathode materials for energy storage application

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Energy storage plays an important role in the development of portable electronic devices, electric vehicles and large-scale electrical energy storage applications for renewable energy sources. Sodium-ion batteries (SIBs) have attracted the great attention recently, for these applications. They are considered to be one of the potential candidates to replace Lithium ion batteries (LIBs), due to its similar electrochemical properties. Sodium cobalt phosphate ($NaCoPO_4$) sample were successfully synthesized by sol-gel method. The thermogravimetric and differential thermal analysis (TG/DTA) cures of the material ($NaCoPO_4$) precursor, it is confirmed calcination temperature of 600°Cfor the prepared sample ($NaCoPO_4$). The structural properties analysis XRD pattern of the sample ($NaCoPO_4$) belongs to orthorhombic structure with space group Pnma. The presence of functional and vibrational groups of PO_4^{3-} polyanion types were ($NaCoPO_4$) identified using Fourier Transform and Infra-Red and Raman Spectroscopy. $NaCoPO_4$ was obtained non-uniform spherical like structure with porous morphology in Scanning Electron Microscopy. The presence elemental composites of the ($NaCoPO_4$) material from EDX and the chemical state can be obtained from X-ray photoelectron spectroscopy (XPS) measurement.

Thrust area: Energy, Sodium-ion batteries, Electrochemical, Sol-gel, Scanning Electron Microscope

Metal free catalyst for hydrogen evolution

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The evolution of photocatalytic hydrogen from water is a promising and sustainable approach for converting solar energy to chemical energy. Graphitic carbon nitride (g-C_3N_4) is an interesting candidate, but the activity of g-C_3N_4 is generally limited. In the present study, carbon nanodots is prepared from solid waste, by a simple efficient and cost-effective method. A hybrid nanocomposite structure is developed by incorporating carbon nanodots (CNDs) to the graphitic carbon nitride (g-C_3N_4) material. The nanocomposite is characterized by various techniques such as Fourier Transform – Infrared Spectroscopy (FT-IR), Powder X-ray Diffractometry (XRD), Scanning Electron Microscopy (SEM), Diffuse Reflectance Ultraviolet Spectroscopy (DRUV). Nanocomposite uses visible light for water splitting in the presence of sacrificial agent, triethanolamine. The photogenerated holes oxidize the sacrificial reagent, which enrich the electrons in a photocatalyst, allowing a swift delivery of photo-generated electrons and holes to the inner CND and outer g-C_3N_4 layers independently. Owing to electrostatic attraction, protons penetrate through g-C_3N_4 to bind with photo-generated electrons present in CND and to create hydrogen molecules. This resultindicates a high photocatalytic efficiency of CNDs / CN for the evolution of H_2.

Generalized Binary Closed Sets

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Let (X, Y, M) be a binary topological space. Let (A, B)$\in \wp(X)\times \wp(Y)$. Then (A, B) is called generalized binary closed if b-*cl*(A, B)$\subseteq$(U, V) whenever (A, B) $\subseteq$(U, V) and (U, V) is binary open in (X, Y, M). We discussed about the concepts of generalized binary closed sets, generalized binary open sets, Binary regular open sets, generalized binary regular open sets and generalized continuous functions. Also we introduce binary -$T_{1/2}$ spaces.

Influence of molar concentration changes in structural and optical studies of ZnO thin films by SILAR method

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Zinc Oxide thin films of two different molarities were deposited on the glass substrate by Successive Ionic Layer Adsorption and Reaction (SILAR) method. The effect of two different molarities of the deposited films was characterized by the structural, optical and morphological of the ZnO thin films were studied. The structural studies reveal that the deposited ZnO films polycrystalline nature with hexagonal structure. The optical studies carried out on the film shows higher morality of high transmittance and low absorption in nature. The morphological studies expose that smaller and bigger particles agglomerated randomly and found that there is no uniform shape.

Noble-metal free nanocomposite for hydrogen generation

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The generation of photo catalytic hydrogen through water splitting under light irradiation attracts considerable attention as a viable alternative for H_2 production. Carbon nitride (C_3N_4), a noble metal free photocatalyst, has emerged as an attractive material for photocatalytic hydrogen production. Massive techniques were introduced such as doping with metal, depositing with noble metals, sensitizing with organic colors and so on for photocatalytic hydrogen evolution. The present work deals with the synthesis of Cobalt oxide (CoO) nanoparticles on carbon nitride obtained from biomass to form (CoO/C_3N_4) nanocomposites and its application for hydrogen evolution. Complementary characterization techniques like X-ray diffraction (XRD), Fourier-Transform Infra-red spectroscopy(FTIR), Diffuse-reflectance UV-visible spectroscopy (DR-UV) were employed to understand the physical and chemical properties of the nanocomposites (Co_3O_4/C_3N_4) hybrid. The photocatalytic hydrogen evolution activity with an H_2 evolution is done with the sacrificial agent of triethanolamine (TEOA) and the photocatalytic H_2 evolution activity of (CoO/C_3N_4) composites is mainly ascribed to

effectively separate electron hole pairs and recombination reactions. The work creates new opportunities for the design of low-cost C_3N_4 based photocatalysts with high photocatalytic H_2 evolution activity from overall water splitting.

ss-Excellence in Graphs

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Let G be a simple graph with vertex set V (G) and edge set E(G). A subset S of V (G) is called a semi-strong set abbreviated as ss-set if $|N[v] \cap S| \leq 1$ for all v in V (G). This concept was introduced by E.Sampathkumar in the paper titled Semi-strong chromatic number of a graph. Any ss-set has hereditary property. That is, a subset of an ss-set is an ss-set. So, an ss-set is maximal iff for any $u \in V - S$, there exists v ∈V (G), $v \neq u$, such that v is adjacent with u and a vertex of S. Excellence is studied with respect to several parameters like domination. A vertex u is $\alpha-$good with respect to the parameter α if u belongs to a minimum (maximum)-set of G. A graph G is α -excellent if every vertex of G is α -good. A graph G is ss- excellent if every vertex of G is ss - good. ss - excellence and ss - just excellence are studied in this paper.

Thermal and Acoustical studies of Polyethylene glycol (PEG 10000)

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Ultrasonic and activation energy studies in polymeric solutions have drawn the attention of many researchers in the recent years. The extensive use of polymeric materials in technology has necessitated investigation of molecular interactions of polymers and solvent. In the present study, an attempt has been made to compute the activation energy and molecular interactions of binary mixtures of Polyethylene glycol (M.W : 10000) (PEG 10000) and toluene at different concentrations (1%, 3%, 5%, 7% and 9%) at different temperatures (303K, 308K, 313K, 318K) by determining relative viscosity, ultrasonic velocity and density. Various parameters like adiabatic compressibility, viscous relaxation time, inter molecular free length, free volume, internal pressure, etc are calculated at 303K and the results are discussed in the light of polymer-solvent interaction.

Key words: Activation energy, Adiabatic compressibility, Free volume, Internal pressure, Polyethylene glycol

Synthesis and structural characterization of substituted 1-oxacyclohex-2,5-dienes

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Multi-component reactions, occasionally also called as multi-component assembly processes (MCAPs) and an important sub-class of tandem reactions are nothing but chemical reactions performed with three or more components in a single-step wherein the resulting products must contain components from all the substrates utilized. In recent years, enormous interests have been exposed in the direction of the reactions under the category of multi-component in the domains of medicinal chemistry as well as organic synthesis. A diverse range of advantages associated with these methodologies includes atom economy, structural diversity, eco-friendliness, high selectivity, solvent-free strategies, and good yields. Specifically, synthesis of heterocyclic compounds utilizes multi-component reactions in larger ways. Subsequently, development of proficient and green reaction strategies which focus on target chemical entities is a vital noteworthy challenge in synthetic organic chemistry.Heterocyclic molecules resembling oxacyclohexadienesadd functional variety to the chemical entity and offer prolific area to learn their bio-activity. It is recognized that chemical entities possessing 1-oxacyclohexa-1,5-diene structural motif are one of the honored heterocyclic ones for the reason that many of their derivatives enjoy useful pharmacological profilesand a wide variety of biological properties, which include anticancer, anti-HIV, antimalarial, anti-inflammatory, antibacterial, antifungal, and antimalarial. In the present piece of research work, 1-oxacyclohexa-1,5-diene tethered with free amino and nitrile groups was synthesized from commercially available meta-bromobenzaldehyde, malononitrile and 2-(methacryloyloxy)ethyl 3-oxobutanoate by adopting a one-step three components synthetic methodology. The structure of the synthesized molecule has been established based on physical and spectroscopic methods including 2D NMR techniques.

Just β_o^{ee}-excellence in Graphs

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Let G= (V, E) be a simple graph. Let u in V(G). u is said tobe a β_o^{ee}-good vertex of G if u belongs to a β_o^{ee}-set of G. Otherwise, u is said to be a β_o^{ee}-bad vertex of G. G is said to be β_o^{ee}-excellent if every vertex of G is β_o^{ee}-good. A graph G is said to be just β_o^{ee}-excellent if every vertex in G belongs to exactly one β_o^{ee} -set of G. In this paper, a new concept called just β_o^{ee}-excellent introduced and a detailed study is made.

Mathematical and Experimental Investigation of Viscosity and Refractive index of Binary liquid Mixtures of Polypropylene glycol with Isopropyl Alcohol

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In the recent years a lot of importance is given to the behavior of mixed components rather than the single component system because of their widespread applications. In chemical process industries, materials are normally handled in fluid form and as a consequence, the physical, chemical and transport properties of fluids assume its importance. Thus, data on some of the properties associated with the liquids and liquid mixtures like ultrasonic velocity, viscosity and refractive index invention finds extensive application in solution theory models and molecular dynamics. The focus of the present investigation is to compute viscosity and refractive index of binary liquid mixtures of Polypropylene Glycol (M.W: 3000) (PPG 3000) and Isopropyl Alcohol at different concentrations (2%-20% in steps of 2%) at 303 K. The experimental viscosities are compared with theoretical methods like Grunberg-Nissan relation, Hind-Ubbelohde relation, Kendall and Monroe and Arrhenius relation. Similarly the experimental refractive index values are compared with theoretical methods like Lorentz-Lorentz relation, Newton relation, Heller relation and Arago-Biot relation. The average percentage error (APE) is determined to identify the most suited method that agrees with the experimental values.

Key words: Kendall and Monroe relation, Newton relation, Polypropylene glycol, Refractive index, Viscosity

A Brief Overview on Synthesis, Properties and Applications of Graphene

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Graphene, a single layer of sp2 carbon atoms in two-dimensional honey-comb, exhibit its extensive properties in various applications such as sensors, electronics, anti-corrosion and energy etc. Even though graphene has enormous applications, synthesis of graphene is not confined, it's still emerging. This review paper discuss about the recent progress in synthesis methods of graphene and its different fields of applications. A simple and effective method of Graphene has been developed, among them; chemical exfoliation method is one of the most promising methods to synthesize large quantities of graphene

layer. There are three different methods including Hummer's, Modified hummer's and Improved hummer's methods can produce nearly the same product, but the conditioning of reaction with reactants or time is different. Moreover, modified hummer's and improved hummer's can eliminate the release of toxic gases and minimize the byproduct over hummer's. Chemical exfoliation method involves three process i) oxidation ii) exfoliation iii) reduction. A wide variety of reducing agent were used such as sodium borohydride, hydrazine, lithium aluminum hydride, saccharides, proteins, and ascorbic acid etc., with the exception of all chemical agents, sodium acetate trihydrate is used since it is less toxic. Fourier transform infra-red spectroscopy, X-ray diffraction, scanning electron microscope and Raman spectroscopy analysis used to characterize the graphene layer. The results obtained from characterization techniques reveal the crystalline structure, purity of the graphene layer.

On the Integral Solutions of Diophantine Equations

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In this presentation, we find all the solutions of the Diophantine equations $\frac{\alpha}{\eta}+\frac{\beta}{\zeta}=\frac{\gamma}{\delta}$ and $\frac{\alpha}{\eta}+\frac{\beta}{\zeta}=\frac{\gamma}{\theta}$, where $\alpha,\beta,\gamma,\delta$ are given positive integers, and η,ζ,θ are unknown positive integers occur many times for particular values of $\alpha,\beta,\gamma,\delta$.

Miscibility Studies of Blends of PEG / PS by Physical Methods

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Polymers play an important role in all types of industries. Many notable advances in the technology have followed the exploitation of properties offered by new polymeric materials like blends, composites, etc. Polymer blends are prepared by physical mixing of two or more polymers. Blending of polymer is one of the simplest methods to obtain a variety of chemical and physical properties from the constituent polymers at molecular level. Usage of blended polymer is the most effective way to produce new multipurpose materials. Recently, researchers have paid considerable attention in the study of polymer blends. In the present wok, Polyethylene Glycol (PEG 10000) is blended with polystyrene (PS 35000) in toluene. The miscibility nature of the poly blend is analyzed by density, viscosity, refractive index and ultrasonic velocity techniques at 303K. Furthermore the

compatibility nature of the blend is confirmed by additive rule.

Key words: Additive rule, Miscibility, Polymer blend, Polyethylene glycol, Polystyrene

Designing an astonishing structure of 3,4-thienothiophene and phenothiazine as a π-bridge dyes for dye sensitized solar cells

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We focusing to synthesis a D-p-p-A dyes (D=donor, A=accpetor) based on a 3,4-thienothiophene and phenothiazine p-bridge were synthesized for use in dye-sensitized solar cells (DSCs). The proaromatic building block 3,4-thienothiophene and phenothiazine is organizing the stability of dye excited-state oxidation potentials. This enhance the deeper absorption into the NIR region with relatively low molecular weight dyes. The impress of 3,4-thienothiophene and phenothiazine functionality is inquiring through a computational analysis of optimized bond lengths and nucleus independent chemical shifts (NICS) for both the ground- and excited-states. Introduce of indole based moieties are utilized for strong donor functionalities in the dye designs to raise both the ground- and excited-state oxidation potentials of the dyes and to avoid a necessary lowering of the TiO2 semiconductor conduction band (CB) to promote efficient dye–TiO2 electron injection. Solubility, aggregation, and TiO2 surface protection are addressed by examining an various alkyl chain in comparison on the 3,4-thienothiophene and phenothiazine bridge. Power conversion efficiencies of up to 7.8% are observed.

Difference between Two Cubes Equal to the Square of an Integer

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Many researchers have been devoted to finding the solutions (x,y,z) in the set of non-negative integers, of Diophantine equations of the type $a^3 + b^3 = c^2$, where the values $a, b,$ and c are integers. In this presentation, we will discuss the integral solution of the cubic Diophantine equation $x^3 - z^3 = y^2$, where $x, y, z \in \boldsymbol{Z}$.

A Study On Rheological, Optical, Electrical And Magnetic Properties Of Fe_2O_3 Nanofluids

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In recent years, applications of nanofluids have landed in advanced technologies in various fields. Water-based nanofluids of Fe_2O_3 synthesised using two step method are prepared in the concentration range from 0.2% to2.0% (in steps of 0.2) and analysed in the present study. Rheological, optical, magnetic and electrical conductivity properties of Fe_2O_3 NF are analysed in this work. From the results, it is understood that the nanofluids follow Newtonian behaviour and the viscosity showed linear decrease with increase in concentration (from 0.2% to 0.6%). The refractive index of the nanofluid is found to be in range of 1.34 which is slightly higher than that of pure water. The magnetic susceptibility studies showed that the NF is paramagnetic and electrical conductivity values revealed that the NF is highly sensitive to the alternating current. The study on Fe_2O_3 NF have exploited strong applications in data storage devices and other electronic devices.

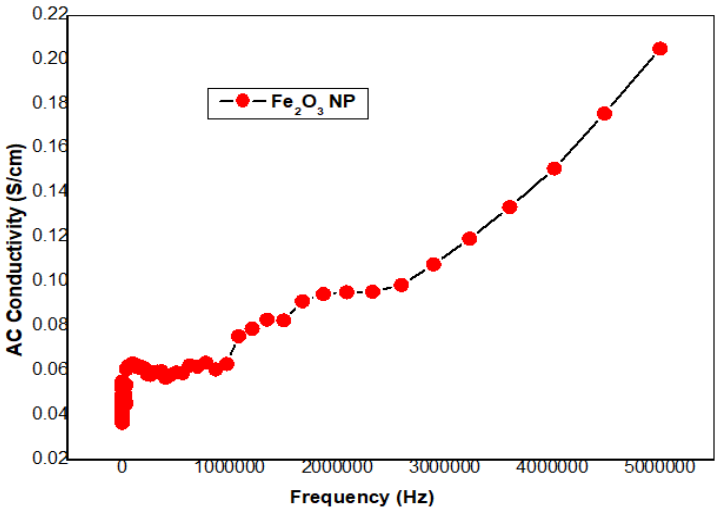

Fig 1. Variation of AC conductivity with frequency

Keywords: Conductivity, Nanofluid, Newtonian fluid, Paramagnetic, Susceptibility

Result on fixed point of generalized quasi contraction

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In 1980, Hegedus generalized quasi contraction map introduced by Ciric as follows: Let (X, d) be a metric space. A mapping $T: X \to X$ is said to be a generalized

quasi contraction, if sup $\{d(T^k x, T^l x) / k, l = 0,1,2, \dots\} = diam\{x, Tx, T^2 x, \dots\} < \infty$, for every $x \epsilon X$ and there exists a number $q \epsilon [0,1)$ such that $d(Tx, Ty) \leq q\ diam\{x, y, Tx, Ty, T^2 x, T^2 y, \dots\}$, for all $x, y \epsilon X$. He proved that on a complete metric space, generalized quasi contraction mapping has a fixed point. In this paper, we prove that Generalised quasi contraction has a fixed point on T-orbitally complete metric space. In a bounded metric space, this map generalizes the k-quasi contraction map introduced by Sujith, et al.

3-(10-Ethyl-10H-phenothiazin-3-yl)-2-(4-nitrophenyl) acrylonitrile: Synthesis and Density Functional Theory Studies

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Uncontrolled cell growth with greater spreading potential is coined as Cancer. Globally, cancer is the second most life threatening disease with an estimated death rate of 9.6 million in 2018 as per GLOBOCAN 2018 report.From the open literature it is inferred that lack of health awareness, poor life style, excess body mass index and physical, chemical as well as biological carcinogens cause cancer. Although there have been several drugs developed, still there is a need for developing new drugs in connection with the same. Phenothiazines are one among the most populous heterocyclic compounds that have been earning the interest of chemist since the discovery of methylene blue in 1883. Phenothiazine shows huge spectrum of applications including various biological activities. On the other hand, it may be noted that nitrile compounds are predominant in nature. They also find applications in fragrance,polymers, dyes and pharmaceutical industries. There are almost 30 nitrile drugs are in use. From the above deliberations it could be inferred that extensive application unveiled by phenothiazine and nitrile functionality has inspired us to hybridize both functionalities together in a single molecule. Hence, in the present piece of work we synthesized a representative molecule 3-(10-ethyl-10H-phenothiazin-3-yl)-2-(4-nitrophenyl)acrylonitrile by employing Knovenegal condensation as a key step. DFT-B3LYP theoretical studies of the molecule were executed by using 6-311++G(d,p) basis set. The suitable structure with related bonding characteristics and vibration frequencies for the molecule has been determined and the values obtained matches well with experimentally determined ones. Syntheses of its analogues along with computational and biological studies are under progress.

A Note on Exponential Diophantine equation

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Many researchers have been devoted to finding the solutions (x,y,z) in the set of non-negative integers, of Diophantine equations of the type $p^x + q^y = z^2$, where the values p and q are fixed. In this presentation, we will discuss the types of solutions say, one solution, finitely many solutions and no solution of the Diophantine equation $a^x + b^y = c^z$.

Fabrication of Ti_3C_2/g-C_3N_4@Ag Nanocomposite Modified Electrode for Sensor Applications

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MXenes are the recent advancements of emerging family of 2D layered materials produced by exfoliation of Selective MAX phases. The MAX phase corresponds to the general formula $M_{n+1}AX_n$. (M= represents transition metal, A stands for group 13, 14 elements and X is either C and N atoms). Mxene nanosheets have been extensively attracted in sensor applications. This paper deals with fabrication of Ti_3C_2/g-C_3N_4@Ag heterostructured nanocomposite for the ultra-sensitive detection of biologically relevant analytes. The nanocomposite is fabricated by pyrolysis of melamine, silver nitrate and titanium aluminium carbide precursors. The nanocomposite is characterized by Ultra-Visible spectroscopy (UV), Fourier Transform Spectroscopy (FT-IR), X- Ray Diffraction (XRD), Scanning Electron Microscope (SEM), Transmission Electron Microscope (TEM) and Raman Spectroscopy. The nanocomposite has potential application in electrochemical sensor due to its remarkable larger conductivity and high selectivity.

Ternary Exponential Diophantine Equation

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Numerous researches have been devoted to finding the solutions (x,y,z) in the set of non-negative integers of Diophantine equations of the type $p^x + q^y = z^2$, where the values p and q are fixed. In this presentation, we show that no more than two non-negative integral solutions (α, β, γ) of a Diophantine equation of the form $3^\alpha + 3^\beta = 6^\gamma, where\ \alpha, \beta, \gamma \in \boldsymbol{N} \cup \{0\}$.

Rheological behaviour of Magnetorheological Fluid: A Brief analysis

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Magnetorheological fluid is one unique and significant class of smart materials. This fluid has influence due the applied magnetic field and shows changes in its rheological properties. The reversible structural transformation objective of the fluid has crucial role in vibration damping properties notably in Mechanical and Automotive applications. This research work, reports the brief information about the rheological behaviour of the optimised and synthesised magnetorheological fluid. Silicon based carried fluid blended with similar lubricant and iron magnetic particles are used for fluid preparation. The fluid is optimised with specific ratio and differing the base materials used for fabrication. Basic rheological properties of the fabricated homogenous fluid are studied to know about its viscosity, shearing stress-strain and damping behaviour of the fluid. The obtained results are analysed and interpreted.

Keywords: Rheology; Viscosity; Damping; Magnetorheology; Shear force.

In-vitro Free Radical Scavenging Activity of Commiphoracaudata Engl. (Syn. Protiumcaudatum Wight &Arn.)

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Enhancing the shelf life of any product with natural extract from natural source is mostly easier and desirable in nature. Extracts with known and unknown bioactive compounds can also be exploited to inhibit the oxidation in human system. The present study, various solvent extracts of *Commiphora caudate* Engl.(Syn. Protiumcaudatum Wight &Arn.) have been assessed for their potential antioxidant activity by five methods selected which represents lipid peroxidation occurring in both foods as well as in biological system. They showed antioxidant activity both in ethanol and methanol extracts which were comparable to synthetic antioxidants such as TBHQ, BHA. Utilization of the extract may result in formulating better health care products which enhanced shelf life and little or no side effects.

On Arithmetic functions h and β

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We consider the arithmetic functions $f: \boldsymbol{N} \to \boldsymbol{R}$ *or* $\boldsymbol{C}$, where $\boldsymbol{N} = \{1,2,3,\cdots\}$. They explain arithmetic properties of numbers and are extensively used in the field of number theory. In this presentation, we define two arithmetic functions h & β and also obtain some of the results analog to well-known arithmetic functions.

Preparation and Characterization of Na^+ ion Conducting Biopolymer Electrolyte

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Bio-based solid polymer electrolytes (SPEs) based on I-Carrageenan with sodium iodide has been prepared by using solution casting technique. Both the concentrations of I-carrageenan and sodium iodide was varied. Distilled water was used as a solvent. AC impedance measurements were carried out in the frequency range of 42Hz to 1MHz. The same measurements were also carried out at different temperature for all the prepared samples. Maximum ionic conductivity 2.3293×10^{-4} Scm^{-1} was obtained for 60 wt% of I-carrageenan and 40 wt% of sodium iodide at room temperature. The temperature dependent conductivity plot of the polymer electrolyte seems to obey Arrhenius relation. Low activation energy of 0.021 eV was observed for the maximum ionic conductivity samples. From AC impedance data, dielectric parameter was obtained. The magnitude of dielectric constant was found to increase with the increase of temperature. Low relaxation time was observed from loss tangent analysis for the sample which possess maximum ionic conductivity.

Key words: I-Carrageenan, Sodium iodide, Solution casting technique, AC impedance, Arrhenius relation.

Hard water Tolerance of Mixed Surfactant Systems in Hard Water by the Polysorbate-80 –Sodium Dodecyl Sulphate Surfactants

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The objective of this research is to evaluate the new types of surfactant based on renewable materials for estimation of water hardness. By applying green chemistry approaches we aim to minimize the adverse environmental effect, hardwater intolerance created by the existing surfactants. The tensiometer have been used to determine the surface active properties like critical micelle concentration, free energy of micellization, surface excess concentration and surface area demand per molecule. The effect of incorporation of polysorbate-80 on the water hardness tolerance of anionic surfactant sodium dodecyl sulphate and the sodium salt of linear alkyl benzene sulphonate has been investigated with the help of a digital Nephelometer. No turbidity was observed upto 250 ppm hardness of water beyond 10% level of incorporation of Polysorbate 80.

A Note on A Sum equal to the Product

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In this presentation, we discuss the integral solutions of the Diophantine equation $DE: \left(\alpha_1^j + \alpha_2^j + \cdots + \alpha_n^j\right) = (\alpha_1 \alpha_2 \cdots \alpha_n)^j$, where $\alpha_i \geq 0$ $(i = 1,2, \cdots, n)$ are integers and $j \in \boldsymbol{N}$.

Influence of Cesium Chloride (CsCl) Dopant on Gamma Ray Irradiated Potassium Hydrogen Phthalate (Khp) Crystals and its Characterization

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Potassium hydrogen phthalate (KHP) crystals doped with 1M% to 4M% Cesium Chloride (CsCl) were grown by slow evaporation solution growth technique have been examined. The Characterization of Gamma-ray beam using Cobalt-60 irradiated KHP and doped crystals were made by Powder X-ray diffraction, Fourier Transform Infrared spectroscopy, UV-visible spectroscopy, Photoluminescence analysis and Laser Raman spectroscopy analysis. The structural difference between pure KHP and Cesium Chloride doped KHP crystals has been studied using Powder XRD analysis. Functional groups and modes of vibrations were identified by FTIR analysis. The UV-visible absorption spectra have been recorded to find the variation in the cut-off wavelength.

Vibrational spectral analysis and different stretching modes are discussed using the Laser Raman spectrum using 514.5 nm emission of Argon-ion source for the pure and doped KHP crystals. Photoluminescence analysis showed broad peaks from green to violet emissions 544.08nm, 600.60nm, 601.47nm, 603.31nm, and 604 nm respectively for Pure Potassium hydrogen phthalate and 1M% to 4M% CsCl doped KHP crystals. It was found that Cesium Chloride doped Potassium hydrogen phthalate semi-organic crystals to be very high energy scintillating material; due to its wide application effect of Gamma-ray using cobalt-60 different concentrations of Cesium chloride doped KHP Crystals.

Detection of the turn-on with high brightness for metal sensors; Rhodamine derivative with ferrocene conjugate

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Design and access of fluorescent chemosensors for heavy and transition metal cations is an area of passionate research movement in the environmental and bio-clinical arena.i The rhodamine based circuitries is an ideal candidate for construct OFF-ON fluorescent chemosensors and molecular logic could result in smaller and more efficient devices and soft materials.ii Rhodamine derivatives are non-fluorescent, whereas ring-opening of the corresponding spiro-lactam gives rise to strong fluorescence emission with a pink colored product. Inspired by this strategy, spiro-lactam of the ring-opening amide process was utilized for the detection of metal ions.iii The addition of metal cation leads to a spiro-cycle opening via coordination or irreversible chemical reaction, resulting in an appearance of pink color and orange fluorescence adduct. Currently, considerable attention has been focused on fluorescent chemosensors for the selective and rapid determination of the toxic heavy metal ions. So far, a vast number of molecular systems have been devoted to the development of metal ion selective chemosensors.iv Turn-on type metal sensors have photoexcited by UV light response to the targeted HTM cation. Rhodamine is a molecule used extensively as a fluorescent labeling reagent and a dye laser source because of its excellent photophysical properties, such as extended absorption and emission wavelengths elongated to the visible region, high fluorescence quantum yield, and significant absorption coefficient.v Therefore, we investigated the dense functionality of rhodamine derivative with ferrocene adduct the use of effective new functionalization of ferrocene. The investigation of these rhodamine derivatives as new metal ion sensors are currently in progress. The details on the synthesis of ris-rhodamine derivative with ferrocene conjugate and its metal sensing property will be presented in the poster. The ppb level fluorescent detection limit for metal ion suggests the possibility of practical applications in toxicology and environment sciences. Sensor ferrocene which contains two rhodamine carboxhydrazone arms exhibited the best selectivity chromogenically and fluorogenically, demonstrating that the robust chelating mode of ferrocene was helpful in creating a high selectivity toward heavy metal ions. Our future research efforts will concentrate on the development of new testing methods to improve the recognition ability of ferrocene and its derivatives toward different ions in the practical environment and media.

Integral Solutions of Exponential Diophantine Equation

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Many researchers have been devoted to finding the solutions $(x,,)$ in the set of non-negative integers, of Diophantine equations of the type $p^x + q^y = z^2$, where the values p and q are fixed. In this presentation, we show that the exponential Diophantine equation $4^x + 18^y = 22^z$, where $x, y, z \in \mathbf{N} \cup \{\mathbf{0}\}$ has exactly one positive integer solution $(1,1,1)$.

Treatment of 2,4,6-Trichlorophenol Wastewater using Agricultural Waste Products as an Adsorbent

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The present work discusses the adsorptive removal of 2,4,6-trichlorophenol (2,4,6-TCP) from aqueous solution by using low cost carbonized agricultural waste coir pith. The important adsorption factors like agitation time, adsorbent dosage, initial adsorbate concentration, and the initial pH were examined by batch mode studies. The adsorption kinetic process was fast, reaching equilibrium in 50 min for 10 and 20 mg/L and 100 min for 30 and 40 mg/L 2,4,6-TCP concentrations. Lagergren first-order, second-order, Bangham's and intra particle diffusion model were used to fit the experimental data. The experimental kinetic data revealed an excellent agreement with the second order kinetic model. The adsorption data obeyed Freundlich isotherm. Acidic pH was favorable for the adsorption of 2,4,6-TCP. Desorption studies showed that chemisorption plays a major role in the adsorption process. The change in entropy (ΔS^0) and heat of adsorption (ΔH^0)of coir pith carbon was estimated as 57.06 J/mol/K and 18.69 kJ/mol, respectively.

On Certain Inequalities for the sum of some integer (ζ) power of all divisors of Positive integer (n)

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Let ζ be a real number and $n \geq 1$ a positive integer. Let $d_1, d_2, \cdots d_k$ be all distinct divisors of n. Put $\sigma_\zeta(n) = \sum_{i=1}^{k} d_i^\zeta$ for the sum of ζ^{th} power of all divisors of n. In this presentation, we obtain certain inequalities for σ_ζ.

Synthesis, Characterization And Electrical Studies Of Solid Polymer Electrolyte Based On Poly Vinyl Alcohol/Gum Arabic/Ammonium Bromide

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In this study, we report on poly (vinyl alcohol) (PVA)/gum arabic (GA)/ NH_4Br membranes as solid polymer electrolytes (SPEs) for possible application in electrochemical devices. The samples were prepared with 10 to 50% of NH_4Br as a source of ions and subjected to electrochemical, structural, morphological characterizations. The best results were obtained for PVA/GA with 20 % of NH_4Br. This sample exhibited the highest ionic conductivity of 4.75381×10^{-7} Scm^{-1}.The PVA/ GA electrolytes were predominantly amorphous according to X-ray diffraction (XRD) data.

Keywords: Solid polymer electrolyte, Gum arabic. Poly (vinyl alcohol), Ammonium bromide, Ionic conductivity

Synthesis and Characterization of Spinel Co_3O_4 Loaded KCC-1 for Organic Transformations

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KCC-1 belongs to a new family of nanosilica known as dendritic fibrous nanosilica (DFNS). In this work, KCC-1 was synthesized in micro-emulsion medium generated by CTAB in *p*-xylene and water interphase. TEOS was used as silica source. The synthesis of KCC-1 was carried out at 120 °C by refluxing a mixture of CTAB, urea and TEOS in p-xylene/water mixture for 12 hours. The product obtained was filtered and calcined at 550 °C in the presence of air for 6 hours. The same reaction was carried out in the presence of Co_3O_4 to get the Co_3O_4 Loaded KCC-1. Thus synthesized materials are characterized by various analytical techniques like XRD, SEM and FT-IR. The catalytic activity was evaluated by performing aldol type condensation reaction with variety of aldehydes.

Positive Integral Solutions of Quadratic Diophantine Equation

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The integer 1233 has the astounding property $1233 = 12^2 + 33^2$. In this presentation, we find the four-digit numbers $\overline{\zeta\eta\tau\theta}$ which satisfy the property $\overline{\zeta\eta\tau\theta} = (\overline{\zeta\eta})^2 + (\overline{\tau\theta})^2$ using the theory of numbers and Diophantine analysis.

Synthesis of $AgFeO_2$/GO Composite for Photocatalytic Degradation of Environmentally Hazardous Pollutant

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The study demonstrates the facile synthesis of silver ferrite ($AgFeO_2$), graphene oxide (GO) and the representative composites to mineralize organic dye pollutant. The materials were synthesized by means of soft-chemical routes like solvothermal and hydrothermal techniques to obtain a unique morphology of the composites. The GO and $AgFeO_2$ composite enhanced electron movement, improved visible-light absorption, and delayed recombination of charges. It was observed that the composite was promising in photocatalytic degradation of MB dye (around 90%) under light-emitting diode (LED) irradiation (9W, 220V). The decomposition data was analyzed for reaction kinetics. In addition, the composite possessed fair reusability for repeated cycles. Hence, the as-synthesized composite applied for photocatalysis bring up a reliable system for the decontamination.

Keywords
Nanocomposite; photodegradation; LED irradiation; reusability; dye degradation.

Knoevenagel Condensation of Aldehydes and Malononitrile

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Conventional Knoevenagel condensation reaction involves the usage of non-recoverable or reusable bases like sodium ethoxide. In this work, we report a heterogeneous catalyst, Co_3O_4 Loaded KCC-1 for performing Knoevenagel condensation in ecofriendly solvent medium at ambient temperature conditions. The effect of various substituents present in the aromatic ring of aldehydes was also studied. It was found that the usage of the above mentioned catalyst improved the reaction rate and as well as the catalyst can be used for the particular reaction for 20 cycles without loss of activity. Based on the product selectivity a plausible mechanism also proposed.

A note on $\tau^* i$ – open sets in topological spaces

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In this paper, we define a new class of open sets called $\tau^* i$ - open sets in topological spaces. Also, we study some of the basic properties and the relations between some other classes of open sets and $\tau^* i$ - open sets is investigated. Furthermore, we define $\tau^* i$ - continuous mapping and prove some characterization of $\tau^* i$ - continuous mapping.

Application of tin-oxide nanostructures for LED assisted photo-mineralization of organic pollutant in water

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The present work illustrated the photocatalytic degradation of an organic dye by using SnO_2 catalyst under LED irradiation. The work systematically evaluated the as-synthesized material for its morphology, the electronic band level, elemental composition, and the zeta potential. Further, the demonstration of photodegradation of a model pollutant, methylene blue was carried out to determine the efficiency of SnO_2. The maximum degradation obtained was ~83% corresponding to 30mg of catalyst within 90 minutes. Also, the kinetics and possible mechanism involved in the photocatalysis is illustrated. The present work emphasize on the ease of catalyst synthesis, the energy efficient photon source, and overall performance of SnO_2 to achieve maximum degradation of the dye. Finally, the catalyst has its importance in practical applications like water and wastewater treatment wherein, dyes could be eliminated with ease.

Keywords
Tin-oxide; photocatalysis; LED assisted; characterization; dye removal.

Synthesis and characterization of alumina surface modified with graphitic carbon nitride

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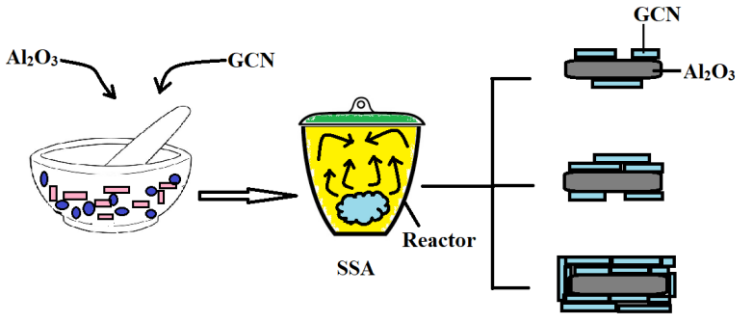
The present study is focused on the surface modification of inorganic aluminium oxide with organic graphitic carbon nitride material. A thermal spreading technique was applied to study the possibility of loading carbon nitride over alumina surface. The results reveal that, alumina surface can be successfully modified with carbon nitride and the thickness of carbon nitride material could be systematically varied. The changes in the surface morphology of resulting materials, interaction between the two phases and their structural changes have been studied. The layer thickness could be progressively increased by altering the loading of carbon nitride. The catalytic applicability of alumina supported carbon nitride in the photocatalytic decomposition of methylene blue dye is under progress.



Coprime Irregular Graphs: Pentagonal Snakes

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A *k-edge-weighting* of a graph $G=(V,E)$ is a mapping $\Phi: E(G) \rightarrow 1,2,3,\dots,k$, where k is a positive integer. For a vertex $v \in V(G)$, the sum of edge-weights appearing on the edges incident at v under the edge-weighting Φ and is denoted by S_Φ. An k-edge-weighting of a graph G is a *coprime irregular edge-weighting* if $\gcd(S_\Phi(v), S_\Phi(u)) = 1$ for every pair of adjacent vertices u and v in G. A graph G is said to be *coprime irregular* if G admits a coprime irregular edge-weighting. In this paper, we prove that the Pentagonal Snakes, Double Pentagonal Snakes and corona of these graphs are coprime irregular.

Medicinal Plant Using Ground State Stabilization of Natural Antioxidant Curcumin by Keto-Enol Tautomerisation

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Curcumin is a medicinal agent that exhibits anti-cancer properties and bioactive pigment in Turmeric has a huge therapeutic value. It has a keto-enol moiety that gives rise to many of its chemical properties. A recent study has shown that keto-enol tautomerisation at this moiety is implicated the effect of curcumin. The tautomerisation of curcumin in methanol, acetone and acetonitrile are used in nuclear magnetic resonance (1 H, 13C) spectroscopy. It was characterized using UV, IR and Raman spectral values. The molecular electrostatic potential surface of the Curcumin has been visualized in electropositive potential in the region of the CH3? group and most electronegative potential in the two-oxygen atom has very strong binding group. In the following, the modality of structural and thermo dynamical parameters, electrophilicity (x), chemical potential (l), chemical hardness (g) and electronic charge transfer confirms the local reactivity. The rate constant of tautomerisation of curcumin shows strong temperature dependence. Molecular electrostatic potential and Temperature dependence of various thermodynamic properties like C0 p;m; S0 m; and H0 m is increase with increase in temperature for monomer and dimer of various electrical fields.

Keywords: Curcumin NMR UV HOMO-LUMO MEP

Cobalt Oxide Catalyzed CO-PROX Catalysis

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It has been demonstrated in the recent literature that, supported transition metal catalysts can exhibit superior CO-PROX performance than that of noble metal-based catalysts. In the preferential oxidation of CO in presence of excess hydrogen, the full conversion of CO must happen with the catalyst from the beginning to certain period of time. In the beginning of the reaction, the catalytically active species must exhibit good stability, otherwise, the CO conversion drops below 100%. The changes in the metal oxidation states may affect the catalyst performance after certain period of time. Other challenges include, the co-presence of water and CO_2 and coke formation. The supported Co_3O_4-based catalysts demonstrated the capacity of attaining 100% CO conversion in the temperature range, that is far below to that of complete reduction of Co_3O_4 into Co^0. Furthermore, the problems related to the carbonate-driven deactivation and inhibiting effects of water were also comparatively less for supported Co_3O_4-based catalysts, particularly with Co-Mn combinations which have attracted much attention. This paper highlights recent developments of cobalt catalysts for the CO-PROX reaction.

Locating Edge domination in H-graphs

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Let G = (V,E) be a graph. For $e_1 \in E(G)$, N (e_1) denote the neighborhoods of e_1 in G. A set D of E(G) is a locating edge dominating set if every two distinct edges e_1, $e_2 \in E(G) - D$ satisfy that $; \emptyset \neq N(e_1) \cap D \neq N(e_2) \cap D \neq \emptyset$ .The locating edge domination number $\gamma_L'(G)$ is the minimum cardinality of locating edge dominating set. The H- Graph of path P_n is the graph obtained from two copies of path P_n with the vertices $x_1, x_2, \ldots..,x_n$ and $y_1, y_2, \ldots..y_n$,by joining the vertices $x_{(n+1)/2}$ and $y_{(n+1)/2}$ if n is odd and $x_{(n/2)+1}$and $y_{n/2}$ if n is even. we will analyze the locating edge dominating number of H – graph.

Cis-Bromidobis(1,2-diaminoethane-j2N,N00) (ethylamine kN)cobalt(III) dibromide

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In the title complex, [CoBr(C2H7N)(C2H8N2)2]Br2, the CoIII centre has adistorted octahedral coordination environment, and is surrounded by four Natoms in the equatorial plane, with an additional N atom and the Br atomoccupying theaxial positions. The complex is isostructural with the Clcompound for which the X-ray structure has also been reported [Anbalagan,Mahalakshmi & Ganeshraja (2011). J. Mol. Struct. 1005, 45–52]. In the crystal,the complex cation and the two counter-anions are linked via N—H Brhydrogen bonds, forming a three-dimensional network.

Adsorption Studies For The Removal Of Ni(II) Ions Using Commercial Iron Oxide (CIO)

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The adsorbent Commercial Iron Oxide (CIO) was purchased commercially and purified by acid treatment to improve adsorption capacities. Adsorption experiments were carried out by using Batch method to compare the sorption behavior of CIO towards the Ni(II) ions. The study was conducted on the basis of parameters such as a function of initial concentration of the adsorbate, adsorbent dosage, contact time and pH. Freundlich and Langmuir isotherm models have been tested. The applicability of various first order kinetic equations like Natarajan-Khalaf, Lagergren, Elovich and Power functions equations were tested. The optimum conditions of the various factors for the

maximum removal of the Ni(II) ions al ions by using CNO was found 77.1% at the optimum concentration of 50ppm, optimum dose rate 3.57g/L, optimum contact ime 10min, optimum ph 6.6 Optimum stirring speed 135rpm.

Designing of Single Sampling Plan under New Weibull-Pareto Distribution

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Sampling plans are used in manufacturing industries to make a decision on the disposition of the lots based on quality characteristic. Acceptance sampling plan is a technique used to accept or to reject the lot on the basis of information obtained from the sampling inspection. Acceptance sampling plans involve minimum time and cost when compared to 100% inspection. In general, sampling plans based on time truncated life test are used to examine the lifetime of the products with less cost of inspection. This paper proposes the designing of single sampling plan for assuring mean lifetime of the products by assuming that the lifetime of the product follows New Weibull-Pareto distribution. The optimal plan parameters are determined by considering two specified points on the operating characteristic curve. An illustrative example is given in order to describe the sampling procedure of the proposed plan.

Investigation on spectral and optical properties of L-Alanine doped Glycine Phosphite (GPI) ferroelectric single crystal

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The pure and L-Alanine doped glycine phosphite (GPI) compound was synthesized in deionized water at lower temperature. The solubility was examined for the both glycine phosphite compound in water. pH of the solution was optimized to grow the single crystals. Single crystals of the GPI and LAGPI were grown in 15 days by slow evaporation. Infrared spectral study was taken and analyzed for the grown crystals. Optical transparency was evaluated to the GPI and LAGPI crystal by UV-Vis spectroscopy. The Optical bandgap was evaluated for the pure and doped GPI crystals. It was analyzed with the other dopants of the glycine. The L-alanine dopant effect was evaluated and presented.

Keywords:

Ferroelectric crystal, Single Crystals, Solution growth method, FTIR spectroscopy, Doped Single Crystals

NMR Spectral and Crystal Structure Studies of a Ketonic Mannich Base

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The conformational aspects of a ketonic Mannich base, 1,3,5-trimethyl-2,6-diphenylpiperidin-4-one (TMP) in the solution state has been ascertained by ^{1}H and ^{13}C NMR spectroscopy. The influence of substituents on chemical shifts in ^{1}H and ^{13}C NMR spectral pattern of the molecular system has also been discussed. The solid-state characterization by means of single crystal X-ray diffraction gives insights into the molecular packing through stabilizing interactions present in the molecular crystal besides the preferred conformation of the six-membered aza heterocycle in the solid-state.

Designing of single acceptance sampling plan based on time truncated life test under new Weibull-Pareto distribution

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In this study, we design the single acceptance sampling plan for assuring percentile life time of the products under new Weibull-Pareto distribution based on time truncated life test. The new Weibull-Pareto distributed percentile life time of the item is considered as its quality characteristic where the shape parameter is assumed to be known. For various percentile ratios, the optimal plan parameters of the single acceptance sampling plan such as sample size and acceptance number are determined by utilizing the methodology of two points on the operating characteristic curve. Tables are constructed for various values of shape parameter of new Weibull-Pareto distribution with the intention of choosing the optimal parameters.

Novel synthesis and characterization of copper molybdate nano particles as a super capacitive Materials

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Copper molybdate nanoparticles have been synthesized by microwave assisted combustion method in an aqueous medium. Structural features of the prepared NPs samples were investigated by using Powder X-ray diffraction. The surface morphology has been examined by Scanning Electron Microscopy and the chemical compositional stoichiometry was confirmed by Energy dispersive X-ray analysis technique. It is found that the crystal is of orthorhombic structure. Fourier transform infrared spectra have been used to identify the structural coordination and functional groups vibrations of the prepared NPs. The electrochemical properties of the resultant copper molybdate have been investigated and can be used for super capacitive material.

Keywords: Copper molybdate, XRD, Combustion method, Supercapacitor.

Fluorescence and Filter Characterizations of L-Alanine Potassium Nitrate (Lapn) – A Comparative Analysis in Macro and Nano Scaled Crystals

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LAPN crystals are having massive opto-electronic relevance, stage matching, frequency harmonizing and power communication and in supplementary utilities. Macro crystals have smallest amount applications by measurement determine up to nano form of LAPN. Macro crystals are position in ordered by slow evaporation solution growth method and nano crystal by milling method. LAPN are prepared by 5h of stirring for 25 days and crystals specialty is SHG. The nano outline of LAPN crystals are of 216 nm and 25 nm correspondingly. The band gap is 3.08 eV which is emission of 403 nm as emission FL value for macro scaling and 379 nm for nano scaling with band gap of 3.2717 eV. As the size of the sample from macro to nano of 21nm, the FL value varies by 24 nm in decremented value and energy value varied by 0.1917 eV as incremental one. Influx value of 1.9799 microns of LAPN represents that the macro influx and 2.0975 microns in nano scale represents that it is good and better prospects in filter utility and in beam displacement of waves compared to the macro scaling which is the matching part of nano scaling. So, the LAPN macro and nano crystals are used in filter applications also as the data are represented.

Design of a cumulative results plan for new Weibull-Pareto distributed percentile life assurance

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The purpose of using acceptance sampling is to dispose the lot of submitted products based on sample information only instead of inspecting each and every product. When quality characteristic considered for inspection is destructive nature or inspection is expensive, conventional sampling plans will not be appropriate since they need large sample size. Hence, the conditional sampling plans which achieve sample size reduction by utilizing cumulative results obtained from preceding/successive lots are used in this situation. So, this article proposes the designing of chain sampling plan, one of the conditional sampling plans, to provide percentile life assurance of the product where the lifetime follows new Weibull-Pareto distribution. In order to accomplish both producer and consumer expectations simultaneously, two points which consist of producer and consumer quality levels along with their risks on the operating characteristic are considered in this design. Tables provide the optimal plan parameters for different percentile ratio values. A real time example is given so that one can easily understand the sampling procedure of the proposed plan. Finally, it is shown that how the proposed plan outperforms the existing sampling plan by a comparative study.

Structural, intramolecular interaction and molecular orbital investigations on NLO active picrate salts of 4-Dimethylaminopyridine by computational methods

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Quantum chemical computations of 4-Dimethylaminopyridinium picrate have been performed at HF and DFT/B3LYP with 6-311++G(d,p) levels to reach the optimized geometry, Frontier molecular orbitals, Mulliken charge distributions and the NLO properties. The FMO analysis clearly illustrates the intermolecular N-H ⋯ O affects the charge transfer in the event of hydrogen bonding. Molecular electrostatic potential analysis reveals the potential sites for hydrogen bonding interactions. Population analysis clearly shows the existence of the accretion of positive and negative charge on atoms and their bonding interactions. Hirshfeld surface analysis has been investigated and the intermolecular interactions through 2D fingerprints were

discussed. Nonlinear optical efficiency is 12 times higher than that of standard urea.

Keywords: DFT; HOMO-LUMO; Mulliken charge; Hirshfeld surface; Nonlinear Optics

Effect of Ascorbic Acid in the Phytofabrication of Silver Nanoparticles using Fresh Cloves Aqueous Extract of Syzigium Aromaticum

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In recent years there is a tremendous growth in the interdisciplinary world of nanotechnology across the globe and emergence of its potential applications remains as a big revolution to the industry. Fusion of green nanotechnology and medicine represents one of the major breakthroughs of modern science with the aim of developing nanomaterials for diagnosis, treatment, prevention of various diseases and overall improving health for the beneficial of mankind. In the present study phytofabrication of silver nanoparticles (AgNPs) was carried out by using fresh cloves aqueous extract of syzygium aromaticum in the presence of ascorbic acid as a reducing, stabilizing and capping agents. Here, we have reported biofabrication of AgNPs from cloves aqueous extract having spherical shape with face centered cubic structure showing an average particle size of 70-90 nm. There is a tremendous increase in surface energy during the formation AgNPs which makes the extract of cloves biocompatible to the receptor site. Phytofabricated AgNPs were characterized by UV-spectroscopy, FTIR, XRD, SEM, AFM and TGA studies.

Selection of Sksp-2 Sampling Plan for Resubmitted Lots

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Skip lot sampling plan is one of the cost-saving plans in terms of time and effort. Skip lot sampling plans are widely used when the quality of the submitted product is extremely good. In this paper, we construct a table and provide a procedure to select the parameters of skip lot sampling plan of type SkSP-2 for resubmitted lots for given acceptable and limiting quality levels. Advantages of the proposed sampling plan are discussed.

Crystal structure, hydrogen bonding interaction and physical properties of p-toluenesulfonate salt of β-alaninine for optoelectronic device application

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A novel single crystal of β-alaninium p-toluenesulfonate has been grown by solvent slow evaporation method. Single crystal XRD analysis of the single crystal confirms the molecular structure and unit cell dimensions. In structural analysis, chain and ring motifs lead to the hydrophilic layers at z = 0, 1/2 and 1 which is sandwiched between the hydrophobic layers at x = 1/4 and ¾. FTIR and FT-Raman spectra have been recorded to confirm the vibrational modes of the crystal. Optical behavior has been studied by UV-Vis-NIR analysis. Thermal properties of BAPT crystal has been investigated by TG-DTA measurements. Mechanical nature of material was studied through Vicker's micro hardness studies. From dielectric measurements, relative dielectric permittivity values and theoretical values of polarizability values were determined. The third order NLO responses BAPT was analyzed by the Z-scan technique.

Keywords:
Single crystal XRD; Hydrogen bonding; Hardness; Dielectric constant; TGA/DTA; Z-Scan method.

Nickel oxide as a catalyst for electro-oxidation of urea

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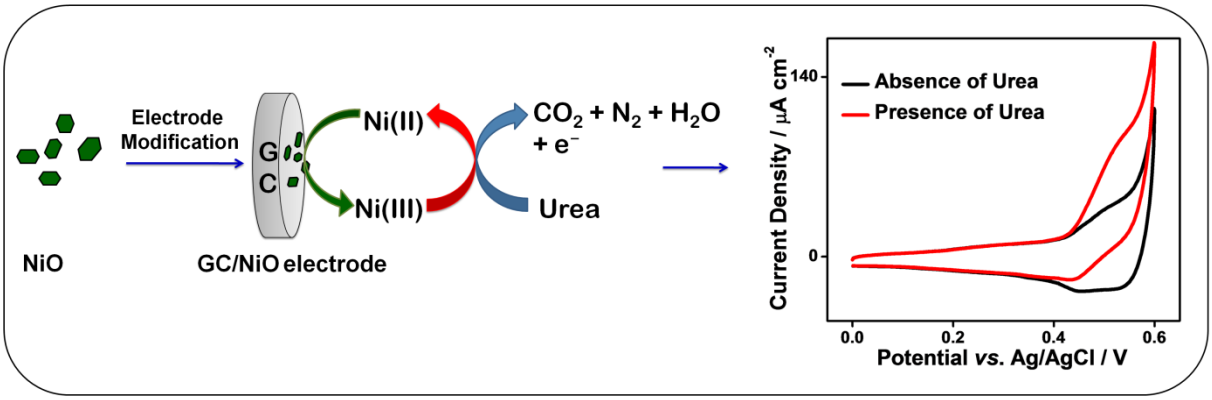
Nickel oxide nanosheets are synthesized through one-pot hydrothermal method. The NiO nanosheets are characterized by using X-ray diffraction (XRD), diffuse reflectance spectroscopy (DRS), Fourier transform infra-red spectroscopy (FT-IR), ramman spectroscopy, high resolution transmission electron microscopy (HRTEM), selected area electron diffraction (SAED) analyses and electrochemical analysis. Electrocatalytic activity of NiO nanosheets modified glassy carbon (GC) electrode is examined towards electro-oxidation of urea in 0.1 M NaOH solution using cyclic voltammetry and amperometry techniques. GC/NiO nanocomposite modified electrode disclosed higher current density for electro-oxidation of urea over bare electrodes used in this work. NiO nanosheets modified electrode was successfully used to design an electrochemical sensor for urea sensing and the detection limit was calculated to be 1 µM using amperometry i-t curve technique. In addition to good electroanalytical

performance, the present sensor displayed good stability and acceptable anti-interference ability in the presence of many-fold higher concentration of relevant interferents. The NiO nanocomposite modified electrode can be successfully used for the determination of urea in wastewater samples.



Schematic representation of electrocatalytic oxidation of glucose urea at GC/NiO modified electrode.

The Global Convexity Graph of Bistar

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Let G=(V,E) be a graph. A function g: V → [0, 1] is called a global dominating function (GDF) of G, if for every $v \in V$, $g(N[v])= \sum_{u\in N[v]} g(u) \geq 1$ and $g(\overline{N(v)})=\sum_{u\notin N(v)} g(u) \geq 1$. A GDF g of a graph G is called minimal (MGDF) if for all functions f: V → [0, 1] such that $f \leq g$ and $f(v) \neq g(v)$ for at least one $v \in V$, f is not a GDF. In this paper we determine the global convexity graph of Bistar.

Preparation of transition metal ion's doped CdS Quantum dots for selective optical metal ions sensing application

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Transition metal ions have cruel effects on the human health and environment even at low concentration level. However these ions play an important role in biology as nutritional microelements as well as associated with various kind proteins and enzymes. Hence the detection of these ions is important task in recent days. Semiconductor quantum dots (QD) have received much attention and widely used in quantitative detection of metal in ultra trace level. We have developed a simple methodology for the synthesis of transition

metal ion (Cu^{2+}, Mn^{2+}) doped CdS QD with visible emission region. The doped QDs were characterized by various instrumental methods such as UV-Vis, PL, HRTEM, XRD, FT-IR techniques to study the morphology, optical, structural properties, etc. The QDs exhibit cubic zinc blend structure with a size of ~5 nm. Enhancement of fluorescence intensity was observed for CdS quantum dots after doping with metal ions. Such a fluorescence property can be utilized for quantitative and selective sensing of particular metal ions in presence of other interfering ions. The proposed method is easy and simple method for the selective detection of metal ion from water sources.

Keywords: Metal ions sensor, Quantum dots, Optical sensing, Transition metal.

Electron deficient receptor for selective colorimetric recognition of cyanide and fluoride ion

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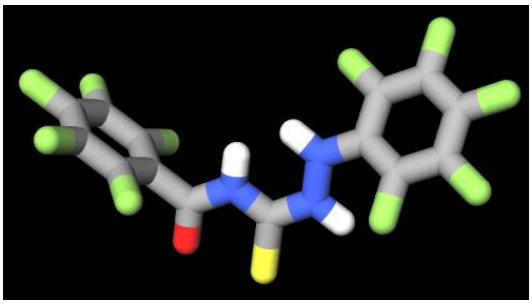
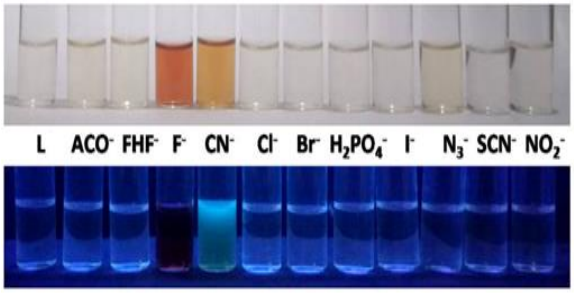
We have designed and synthesized a sensor **L**, as an strong selective colorimetric chemo-sensor for cyanide and fluoride ion. The acetonitrile solution contains **L** with tetrabutylammonium salts of cyanide, and fluoride results sudden color change from faint yellow to red. The chemosensor **L** produced an enhancement of absorbance intensity while addition of cyanide and fluoride ion. The recognition ability of the receptor **L** towards variety of anions is studied by naked-eye colorimetric experiments, UV–Vis spectrometry, Emission Spectrometry and IR Spectrometry.





A Study of couple stress fluid flow in an inclined channel in Non Oscillatory Flow with Hall Current

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This paper is devoted to the study of MHD couple stress fluid in an inclined channel in Non oscillatory flow with Hall current. The analytical solution has been carried out by using the long-wave approximation and low Reynolds number. Closed form expressions for velocity, temperature and concentration are developed. The solutions are obtained by solving analytically and the results are presented graphically for different values of parameters entering into the problem.

Solvent effects of Tridax Procumbene, Agalypa Indica and Turmeric for Dye-sensitized solar cell using green route synthesis

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The dye-sensitized solar cell (DSSC) provides a technically and economically credible concept in P-N Junction photovoltaic devices. In contrast to the conventional system, where the semiconductor assumes both the task of light absorption and charge carrier transport the two functions are repeated here. Light is absorbed by a sensitizer which is recharged to the surface of wide band of the solid. Carriers are transported in the conduction band of the semiconductor to the charge collector. The uses of sensitizer have a broad absorption band in conjunction with oxide films of nanocrystalline morphology permits to convert a large fraction of sunlight. Nearly quantitative conversions of incident photon into electric current are achieved over a large spectral range extending from the UV to the near IR region. Overall solar cells to current conversion efficiencies (IPCE) over 10% have been reached. There are good percept's to produce these cells at lower cost than conventional devices. Here we report DSSC were fabricated using natural dyes extracted from Tridex Procumbene Agalypa Indica and Turmeric, using ethanol as extraction solvents. The extraction absorbed on TiO_2 shows synergistic light absorption and photosensitization compared with mixed extracts. Among these Tridax procombenes extract alone shows the best sensitization performance related to interaction between the dye and TiO_2 surface is discussed. In the efficiency conversion the Tridax procombenes extract sensitization DSSC was improved up to 1.234%. By changing the p^H the stability was also improved.

Key words: P-N Junction photovoltaic devices, nanocrystalline, Tridex Procumbene, Agalypa Indica, Turmeric, DSSC.

A Mathematical Model for Rotating Disc Electrodes

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Rotating disc electrodes are used to analyze electrochemical reactions in electrochemical cells and various rotating types of machinery. This model contains a system of fully coupled and highly non-linear equations. This manuscript outlines the steady-state solution of rotating disc flow coupled through the fluid viscosity, to the mass-concentration field of chemical species and heat transfer of power-law fluid over a rotating disk. In addition, a simple analytical expression (Padé approximation) of velocity component/ self-similar velocity profiles is derived from the short and long-distance expression. Our analytical results are compared with simulation results, and satisfactory agreement is noted.

Structural, optical and magnetic properties of Gd doped CdTe quantum dots for spintronics applications

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Mercapto succinic acid capped pure and gadolinium (Gd) doped cadmium telluride (CdTe) QDs were synthesized in the aqueous phase and their structural, optical and magnetic behavior were studied. XRD result reveals the cubic zinc belende crystalline structure for the pure and Gd:CdTe QDs and the variations in the particle size and lattice parameter with the doping concentrations of Gd^{3+} ions. UV-vis absorption spectra shows that the changing in the energy band gap (E_g) of the QDs by varying the dopant concentration. The enhanced fluorescence behavior of Gd:CdTe QDs was analyzed by fluorescence spectroscopy. Quantum yield calculation showed that the Gd:CdTe QDs possess a maximum yield of 67% for the 10% Gd doping. XPS analysis confirms the formation of thiol capped Gd:CdTe QDs. Room temperature ferromagnetic behavior (RT-MF) of Gd:CdTe QDs was revealed by VSM measurement. Hence, the prepared Gd:CdTe QDs were proposed to be a potential DMS material for room temperature spintronics applications.

Enhancing the performance Direct Absorption Solar Collectors by the use of nanoparticles

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Renewable energy is the best alternative to fossil fuels having minimum environmental impact. One of the methods of generating renewable energy is through solar energy. An average solar cell can convert 13 to 15% of the energy falling on them to usable energy. Direct Absorption Solar Collectors (DASCs) can achieve a maximum efficiency of 90% if tested with silver nanofluids. Nanoparticles of some materials will have a larger impact in increasing the efficiency of DASCs. These solar collectors have advantages of minimum radiation loss, conduction and convection losses. Depending on shape, volume fraction and size of nanoparticles the efficiency of DASCs can be tuned to achieve better results.

On βω-Closed Sets in Topological Spaces

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The objective of this paper is to instigate a new sort of closed sets namely βω-closed set in topological spaces. This new class of closed set placed between β-closed sets and ω-closed sets. Several characterizations and some of their properties are obtained. A new type of space namely $T_{\beta\omega}$ –space is also introduced. The connection between this type of space and other existing spaces are also investigated.

Facile synthesis of ZnO/NiO:rGO nanocomposite *via* hydrothermal method for high-performance supercapacitor applications

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In this work, ZnO/NiO:rGO nanocomposite (ZNR) have been successfully synthesized through the one pot hydrothermal method. The synthesized powder samples have characterized by XRD analysis to confirm the formation of ZnO and NiO crystalline phases. The FT-IR studies confirm the functionalization of the prepared of rGO nanosheets and its presence in the ZNR sample. The Raman spectrum of the prepared GO and rGO elucidates the reduction GO with lower structural defects. The SEM micrographs of the prepared rGO sheets and ZNR sample confirms the ultrathin rGO nanosheets have dispersed in ZnO/NiO particles. The high purity of the ZNR was confirmed by EDS analysis. The electrochemical performances of the modified working electrode were studied by three electrode system under 1 M KOH electrolyte solution. The working electrode exhibited maximum of 622.3 Fg^{-1} of specific capacitance at the current density of 1 Ag^{-1}. Also, it delivers maximum of 4500 W kg^{-1} power density and 77.8 W h kg^{-1} energy density. The retention of 78.8% capacity after 5000 GCD cycles was one of the key advantages for long term applications.

Molecular Docking Study of Substituted N-Methyl Piperidone with TNF-A Protein

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Tumor necrosis factor- alpha (TNF-α, cachexin, or cachectin) is a cell signaling protein (adipokine) involved in systemic inflammation. TNF-α is a bioactive cytokine an important component of the inflammatory and pain pathways. Inhibition of TNF can decrease the inflammatory response, and this approach has been used in therapy of auto-immune conditions. The molecular docking study using MAESTRO v 9.3.5, implemented in the Schrödinger software, was carried out to investigate the binding mode of interactions between the synthesized compound and the protein theoretically. The synthesized compound (3-isopropyl-1-methyl-2,6-diphenylpiperidin-4-one) was docked against Tumor necrosis factor-alpha (TNF-α) protein to find the plausible interactions in the active site of the protein. Molecular docking results with van der Waals and Coulomb interaction energies of the docked compound are discussed. The synthesized substituted piperidone compound shows the docking score – 6.52 kcal/mol. The carbonyl group present in the Piperidone ring has hydrogen bond interaction with amino acid CYS 532. Also compound has very good hydrophobic interaction with all amino acid present in the active site. The glide energy of the docked compound is -28.425 kcal/mol. The molecular docking study revealed that the synthesized compound fit well into the active site of the Tumor necrosis factor (TNF-α) protein.

Equitable Irregular Edge-Weighting of Corona graphs

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A *k-edge-weighting* of a graph $G=(V,E)$ is a mapping $\Phi: E(G) \rightarrow 1,2,3,\dots,k$, where k is a positive integer. For a vertex $v \in V(G)$, the sum of edge-weights appearing on the edges incident at v under the edge-weighting Φ and is denoted by S_Φ. A k-edge-weighting of a graph G is a *equitable irregular edge-weighting* if $|S_\Phi(v) - S_\Phi(u)| \leq 1$ for every pair of adjacent vertices u and v in G. A graph G is *equitable irregular* if G admits a equitable irregular edge-weighting. In this paper, the admissible of equitable irregular edge-weighting of the graphs $K_r o K_s$, $P_r o K_s$, $K_r o P_s$, $and\ P_r o P_s$ are discussed.

Investigation of structural and intrinsic green emission of ZnO synthesized by low temperature sintering method

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Zinc oxide was prepared by sintering of zinc acetate at different temperatures in reducing atmosphere and enhancing defect related green emission. Photoluminescence of ZnO showed deep level green emission around 500 nm was associated with oxygen vacancies which were created while sintering in reducing atmosphere. The prepared ZnO characterized

by X-ray diffraction and Rietveld refinement analysis to study their structural information which confirms the wurtzite hexagonal phase. The shape and surface morphology are examined using Scanning Electron Microscopy (SEM) which indicates partially hexagonal structure with average particle size is about 1μm. The distribution of electrons in the unit cell and bonding behavior is determined by Maximum Entropy Method reveals that the mixed ionic and covalent character of ZnO which are supports the PL investigation.

Keywords: ZnO, X-ray diffraction, Rietveld Refinement, SEM, MEM, photoluminescence

L-Tryptophan single crystals: An approach of Physio-chemical and Quantum chemical investigation

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In this work, optically transparent better quality single crystals of L-Tryptophan (LTP) were grown by slow evaporation solution growth technique using methanol as a solvent. The crystalline nature and functional groups of LTP have been identified through powder X-ray diffraction and Fourier transform infrared (FTIR) studies, respectively. The optical transmittance window and the lower cut-off wavelength of the LTP single crystal have been explored by UV–Vis–NIR studies. Dielectric and photoconductivity performances have been probed for the grown crystal. In order to analyze the mechanical strength of single crystal sample, Vickers hardness measurement and void percentage analysis were performed. Second order nonlinear optical (NLO) characteristic was examined using Nd:YAG laser study. In addition to that, quantum chemical calculations on LTP have been performed by density functional theory (DFT) calculations employingB3LYP method with 6–311++G(d,p) basis set. The computed value of first order hyperpolarizability was determined to be two times greater than that of urea. These experimental and computational investigations obviously proposed that LTP could be an attractive material for nonlinear optical applications.

Regular Generalized Regular ρ – Closed Sets in Topological Spaces

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In this paper, we define and study new class of closed sets called regular generalized regular ρ-closed sets (briefly rgrρ-closed sets) and regular generalized regular ρ-open sets (briefly rgrρ-open sets) in topological spaces and investigated some of their fundamental

properties. In addition, we presented the perception of continuity using regular generalized regular ρ-closed sets and regular generalized regular ρ-open sets in topological spaces.

Structural and electronic properties of lead-free $Na_{0.5}K_{0.5}NbO_3$ ceramic solid solution

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Lead-free $Na_{0.5}K_{0.5}NbO_3$ ceramic was synthesized by solid state reaction method. The synthesized sample was characterized by X-ray diffraction. The results of X-ray diffraction analysis show that the prepared ceramic displays typical perovskite based structure with tetragonal crystal structure and space group *P*4*mm*. The crystal structure of $Na_{0.5}K_{0.5}NbO_3$ powder was determined by Rietveld refinement analysis. The spatial arrangements of the electron distribution and bonding nature of the sample have been analyzed through maximum entropy method. Charge density analysis reveals the ionic in nature between Na and O atoms and the covalent in nature between Nb and O atoms. Based on the previous reports, the lead-free $Na_{0.5}K_{0.5}NbO_3$ ceramic considered as promising candidates for ferroelectric and dielectric components.

Keywords: Ceramics, X-ray diffraction, Maximum entropy method, electronic structure.

Ni(II) Schiff base complex: Synthesis, spectral investigation and catalytic oxidation of alcohols

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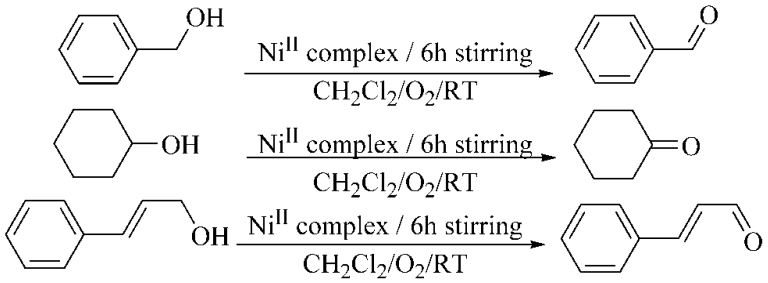
Air stable Ni(II) Schiff base complex viz. [Ni(L)(PPh_3)] [where L is dianions of Schiff base ligand respectively] have been synthesized and characterized by analytical and spectral (electronic, FT–IR, ^1H, ^{13}C and ^{31}P NMR) methods. The assignment of all the aromatic carbon-hydrogen resonances is made on the basis of ^1H–^{13}C HSQC spectrum of the complexes. The Schiff base ligand behave as a bibasic tridentate ligand and get bonded through ONO mode. A square planar structure has been proposed on the basis of spectral data. Thermal and air stability of the complexes offer the advantage of oxidation of alcohols



Catalytic oxidation of alcohols

The Fractional Path Cover of a Graph

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Let G=(V,E) be a graph. A *path cover* or *path partition* of a graph G is a collection P of paths (not necessarily open) in G such that every edge of G is in exactly one path in P. The *path partition number* π of G is the minimum cardinality of a path partition of G. The path partition number π of G is also call the *path covering number* of G. In this paper we introduce the concept of fractional path cover.

Preparation and characterization of CuO nanostructures on copper substrate for using anodization

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Nanostructured copper oxide (CuO) thin films were prepared on copper substrate through an anodization deposition technique using sodium hydroxide (NaOH) as oxidizing agent at various current densities. The resultant CuO thin films were characterized by X-ray diffraction (XRD), scanning electron microscopy (SEM), energy dispersive X-ray spectroscopy (EDX) and UV-Visible-Near-Infrared (UV-Vis-NIR) spectrophotometer. The XRD patterns of CuO thin films confirmed the presence of diffraction peaks correspond to CuO. Only peaks of Cu and O observed in EDX spectrum of CuO thin film sample disclose its pristine nature. The SEM image revealed the presence of CuO nanorods with 80-100 nm width having net-like morphology.

Keywords: CuO nanorods, CuO thin films; oxidizing agent; Energy conversion

Synthesis and Characterizations of Silver Nanoparticles-Reduced Graphene Oxide Hybrid Using Lemon Extract as a Reducing Agent

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Here, we report the synthesis of silver nanoparticle-reduced graphene oxide (AgNPs-rGO) hybrid for facile and eco-friendly method. Silver nanoparticles (AgNPs) were successfully deposited on reduced graphene oxide (rGO) sheets to form (AgNPs-rGO) hybrid using lemon extract as a reducing and stabilizing agent. The products form a stable aqueous solution without any surfactant stabilizers and this makes it possible to produce (AgNPs-rGO) hybridon a large scale using low-cost solution processing technique. The synthesis of nanohybrid was monitored at different ratio of reducing agent (1:1, 1:2, 1:4) and characterized using UV-Visible (UV-Vis) absorption spectrum, X-ray diffraction (XRD) and Raman spectroscopy analyses. From UV-Vis absorption spectrum, the (AgNPs-rGO) (1:1) hybrid result shows the sharp peak at 433 nm indicating the accomplishment formation of AgNP on the surface of rGO sheets. Completely spherical Ag nanoparticles (NPs) were found at (AgNPs-rGO) (1:1) hybrid with an average particle size of 21 nm. Furthermore, (AgNPs-rGO) (1:1) hybrid exhibit fast electron-transfer kinetics for electrochemical reaction of Fe $(CN)_6^{3-/4-}$ redox couple, suggesting the potential applications for electrocatalysis and electrochemical sensor.

Neighbourhood Connected Strong Domination In Graphs

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Let $G = (V, E)$ be a simple, connected, undirected graph. A set$S \subseteq V$ is said to be a neighbourhood connected strong dominating setof G if S is a strong dominating set of G and $< N(S) >$ is connected.This paper initiates a study on neighbourhood connected strong domination number and also we determine such number for some standard graphs. Further we obtain some bounds on this parameter.

Review of filler added polymer electrolytes for the application of energy storage devices

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This review paper describes the advantages and characteristics of filler added polymer electrolytes in solid-state batteries. The applications of fillers in polymer electrolyte and the differences between polymer electrolytes (with filler and without filler) are discussed. The review focuses on filler added systems which have received particular attention from electrolytes which are free from fillers [1]. The effects of fillers in polymer electrolytes are reflected in the performance of devices. We discuss the features and performance of different type of fillers added polymer hosts based on some important and recently published literature [2]. Recent progress of some approaches used in improving the performance of the polymer electrolytes is highlighted. This review includes the technological applications of some electrical energy storing/converting devices like batteries, electrochemical capacitors, fuel cells and solar cells [3].

Keywords: Polymer electrolyte; Filler; Batteries and Fuel cell.

Synthesis and characterization of Jatropha Curcas latex coated magnetite nanoparticles for antimicrobial activity

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Jatropha Curcas (JC) latex coated magnetite nanoparticles (MNPs) were synthesized using the crude latex of Jatropha curcas in a cheaper and greener way in an open-air environment. DLS, UV-visible spectroscopy, FTIR spectroscopy, powdered XRD, and FE-SEM were used for the characterization of the MNPs. From the images of FE-SEM,the size ranges of the synthesized JC-Fe_3O_4 NPs was found to be between 20-42 nm . The effect of synthesized magnetic nanoparticles in wastewater treatment (bacterial portion) had been studied, as well as antibacterial (against both gram-negative and gram-positive bacteria), antioxidant, and cytotoxic activity were also performed . This study will lead to a development of nanoparticles for the efficient antimicrobial activity in future.

Some Special Classes of Equitable irregular graphs

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A *k*–edge-weighting of a graph G = (V,E) is a map $\boldsymbol{\varphi}$: $\boldsymbol{E(G)} \rightarrow \{\mathbf{1},\mathbf{2},\mathbf{3},\ldots\boldsymbol{k}\}$, where $\boldsymbol{k} \geq \mathbf{1}$ is an integer. The sum of edge-weights appearing on the edges incident at the vertex *v* under is denoted by $\boldsymbol{S_{\varphi}(v)}$. A k-edge - weighting of G is equitable irregular if $|\boldsymbol{S_{\varphi}}(u) - \boldsymbol{S_{\varphi}(v)}| \leq \mathbf{1}$, for every pair of adjacent vertices u and v in G. The equitable irregular strength $\boldsymbol{S_e}(G)$ of an equitable irregular graph G is the smallest positive integer k such that there is a k-edge weighting of G. In this paper, we discuss the equitable irregular edge-weighting for Jahangir graphs, Double fan graphs, Closed sun flower graphs and Antiweb-gear graphs.

One Step Deposition of Monodispersed Silica Nanospheres Using Stöber Method and their Size Predication through Adaptive Neuro- Fuzzy Inference System

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Highly monodisperse nanostructures is becoming the centre of focus in the field of material science towards the application of sensors, photocatalysis, gas sensing, antibacterial activity, drug delivery and energy applications. In the present work, demonstration of synthesis of monodisperse silica nanospheres were achieved using stober method and deposition of as prepared monosphere on thin film was done using vertical deposition. Different parameters were optimized during synthesis process such as ethanol, water, ammonia and tetraethyl orthosilicate (TEOS). Prepared substrates were characterized using SEM & XRD. SEM characterization clearly show the presence of monolayer of nanosphere with a size ranging from 100 – 200 nm mostly due to aggregation of the sample and XRD analysis shows amourphous nature of SiO_2 film. Adaptive Neuro- Fuzzy Inference System (ANFIS) method was used in the present work as a simulation tool in order to optimize the experimental parameters. Results of ANFIS clearly show that our experimental condition well matches with the theoretical results indicating a good and successful attempt.

Synthesis and characterization of Cinnamomum tamala leaf extractcoated magnetite nanoparticles for wastewater treatment

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Removal of organic pollutants (through adsorption), toxic metal ions, and harmful bacteria can give us clean and purified drinking water from wastewater resources. In this regard, *Cinnamomum tamala* leaf extract coated CT-Fe_3O_4 nanoparticles were synthesized, using a cheaper and greener way in an open-air environment with the use of

aquas leaf extract of *Cinnamomum tamala* (CT). Characterization of CT-Fe_3O_4 had been performed by DLS, UV-visible spectroscopy, FTIR spectroscopy, powdered XRD, and FE-SEM. The size ranges of the CT-Fe_3O_4 was found to be within the range 26-35 nm by FE-SEM analysis. The effect of synthesized magnetic nanoparticle in wastewater treatment (bacterial portion), dye adsorption (MB), toxic metals (Cu^{2+}, Co^{2+}) removal as well as antibacterial, antioxidant, and cytotoxic activity had been studied. This report lead to an enhance the resources of clean and pure drinking water in the future.

Economic Scheming of SkSP-3 involving destructive and Non-destructive testing of cross member automobile spare parts

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This paper demonstrates the development of an economic designing and evaluating procedure for the Skip-lot sampling plan-3 under the conditions of Poisson distribution. The designing of feasible cost model under certain conditions imposed in essential construction of single sampling plan to study the economic designing of special purpose plan such as SkSP-3 at various stages of inspection of lots at the production unit is emphasized. The cost behaviour of spare parts with respect to plan parameters through the sensitivity analysis and furthermore, cost curves deals with determining the optimal plan parameters are presented in the tailor made tables for the Industrialist. Efficiency gain is exclusively given for the stochastic representation of the cost function in destructive and non-destructive testing.

Detail investigation of Ce doping on Zn/CdO thin films for opto-electronic applications by nebulizer spray pyrolysis

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Cerium doped with transparent conducting oxide zinc doped cadmium oxide thin films were coated in highly cleaned glass substrate by a nebulizer spray pyrolysis technique. The effect of Cerium percentage films were characterized as electrical studies by XRD, AFM, UV-Vis spectroscopy. XRD results show that all deposited CdO films are polycrystalline and well-crystallized along (111) plane with simple cubic structure using conventional Debye Scherer's formula. The structural study revealed that the surface roughness of the film decrease as the doping concentration increase. Energy dispersive x-

ray EDX, atomic force microscope AFM and elemental mapping analysis confirm the presence of Cd, Zn and Ce elements and the films were near stoichiometric. Raman spectra of CdO film showed the presence of Raman peaks was located at 300 cm^{-1}, 590 cm^{-1}, and 1100 cm^{-1}, which belonged to TO and LO modes of vibration of Cd-O bond . The optical energy gap of the film increased from 2.53 to 2.73eV after doping with cerium from 0 wt% to 5 wt % respectively. Ce doping of 5wt% showed improved property of the film with low resistivity 3.98×10^{-4} Ω cm.

Keywords: Nebulized Spray Pyrolysis, Zn doped CdO (ZCO) thin film, Ce doping, structural, optical properties.

Study on Interaction Capabilities of Ternary Liquid Mixtures by Thermodynamic Parameters at 308.15K

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Experimental densities, viscosities and ultrasonic velocities were measured for ternary liquid mixtures of diethylmalonate+ 1, 4-dioxane with nitrobenzene at 308.15K and atmospheric pressure over the entire range of mole fractions. The calculated thermodynamic properties and some excess parameters such as V^E, ΔK_s, $\Delta\eta$, ΔV_F, ΔL_F, $\Delta\beta_T$, were calculated from measures values and applied to Redlich – Kister polynomial equation to determine the appropriate coefficients. The deviations of the ternary mixtures from its ideal behaviour were determined and the interaction ability of the liquids in the ternary liquid mixtures was studied.

NOTIONS VIA R $^{\#}$- OPEN SETS IN TOPOLOGICAL SPACES

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In this paper we have introduced a new class of sets called $\rho^{\#}$- open sets and $\rho^{\#}$- interior in topological spaces. Further the notions of $\rho^{\#}$- kernel, $\rho^{\#}$- derived, $\rho^{\#}$- border, $\rho^{\#}$- frontier and $\rho^{\#}$- exterior of the set using $\rho^{\#}$- open set is investigated. Some fascinating results that demonstrates the connection between $\rho^{\#}$- frontier and $\rho^{\#}$- open sets are obtained.

FTIR, FT-Raman spectra, DFT calculations, NLO and electronic properties of 5-bromo-6-chlorotoluene

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The vibrational spectra of 5-bromo-6-chlorotoluene (BCT) have been recorded using the FTIR (4000-400 cm^{-1}) and FT-Raman (3500-50 cm^{-1}) spectroscopies. The complete assignments of normal modes of BCT were carried out from the experimental data and confirmed by the total energy distribution (TED). The density functional theory (DFT) with 6-311++G(d,p) basis set have been used for calculating the optimized parameters, vibrational frequencies and intensities. The dissimilarity between the experimental and computed frequencies of normal modes is found to be very small. The nonlinear optical property of the investigated molecule has been studied by computing the first hyperpolarizability and dipole moment values. The frontier molecular orbital analysis which is the key factor for biological activity has been discussed. In addition, the Mulliken's charge and molecular electrostatic potential (MEP) analyses of molecule have been examined.

Tripodal molecular pocket for anions: Selective colorimetric detection of azide through Metal-π···hole interactions

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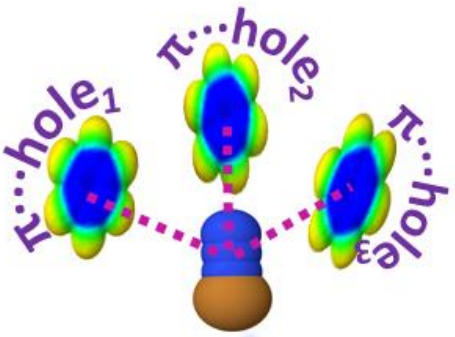
Tris amine based C_3v symmetric tripodal molecular pocket has been prepared and metal complex of **L** having M^{n+}- π··· hole as recognizing elements, becoming a potential and selective colorimetric chemo sensor for perfect linear recognition of N_3^-, generate a Metal−NNN- π··· hole unit inside the tripodal cavity. Systematic UV-Vis spectrometry and IR spectrometry Systematic spectrometric and naked-eye colorimetric studies reveals that, this chemo sensor is also colorimetrically recognizing the cyanide ion by cavity via Cu-N_4-π···hole.



Functions In Bipolar Valued Multi Fuzzy Subhemirings Of A Hemiring

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In this paper, bipolar valued multi fuzzy subhemiring of a hemiring is introduced and their properties are discussed, particularly homomorphism and anti-homomorphism functions are used in the theorems. The theorems are very useful to further theory development. In 1965, fuzzy set was introduced by Zadeh after that the fuzzy set was extended into varies types of fuzzy sets, bipolar valued multi fuzzy set is one of this.

Structural and Electron Density Distribution Analysis of Strontium Tungstate

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Scheelite type $SrWO_4$ material was prepared via simple co-precipitation technique. The crystalline purity of prepared $SrWO_4$ was investigated by powder X-ray diffraction characterization. In-depth structural details of tetragonal structured $SrWO_4$ were carried out by the Rietveld refinement method. The nature of the chemical bond between atoms and distributions of electrons in the single unit cell were examined through high-resolution maximum entropy method (MEM). The MEM results provide the 3-dimensional unit cell, 2-dimensional miller maps and 1-dimensional electron density profiles of $SrWO_4$ material.

Keywords: $SrWO_4$; Rietveld Refinement; MEM; Electron density distribution

Synthesis, Characterization, Biological Evaluation and Computational Prediction of Novel Aminophenol Derived Schiff Base Metal Complexes

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This research work deals with a series of novel Schiff base ligand andmetal complexes derived from2,2'-Dichlorobenzil, 2-amino-phenol, and metal chlorides were reported. The synthesized metal complexes were characterized by multispectral techniques such as UV-Visible, FT-IR, NMR, ESI-mass analysis. Moreover, metal complexes strive for their biological future. Biological studies such as antimicrobial, cytotoxic studies and free radical scavenging studies were performed. The antimicrobial evaluation indicated that the compounds were the best antimicrobial agents against selected microorganisms due to complexation. The in vitro anticancer activities of metal complexes in MCF-7, HepG2, and HBL-100 cell lines were investigated using MTT assay and confirmed that the combined complexes have a higher potency than the ligand. The antioxidant studies have revealed that metal complexes have the desirable ability to eliminate the hydroxyl radical rather than the free ligand.Molecular docking investigations have also been performed to demonstrate the binding affinity of compounds with biological entities such as protein and DNA. The prediction of in-silico ADMET properties found that compounds based on Lipinski's rules obtain significant drug-like properties.

Entire Labeling of Plane Graphs

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For a plane graph $G = (V, E, F)$ we define a labeling $\varphi: V \cup E \cup F \rightarrow \{1,2, \ldots ,k\}$ to be an entire k-labeling. The weight of a face f under an entire k-labeling φ, $W_{\varphi}(f)$, is the sum of labels carried by that face and all the edges and vertices surrounding it. An entire k-labeling $\varphi$is defined to be a face irregular entire k-labeling of the plane graph G if for every two different faces f and g of G there is $W_{\varphi}(f) \neq W_{\varphi}(g)$. The entire face irregularity strength, denoted *efs* (G), of a plane graph G is the smallest integer k such that G has a face irregular entire k-labeling. We discuss about some estimation of entire face irregularity strength and determine the precise values for graphs from families of plane graphs.

Experimental and Finite Element Analysis of Energy Storage from Diesel Engine Exhaust using Alumina Packed Pebble bed Heat Exchanger

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Alumina is widely used material in the family of engineering ceramics. The materials from which this high performance of technical grade. Aluminum oxide commonly referred to alumina, possesses strong bonding characteristics of material. Aluminum oxide is in the form of pebbles packed bed is a promising concept for fusion blanket. The main objective of this study is to measure the thermal energy storage Al_2O_3 as function of average bed temperature. The Al_2O_3 pebbles are 4 mm to 10 mm and are randomly dumped and packed in a 450 mm long hollow tube of 45 mm inner diameter. The tube was fully covered the asbestos ropes to reduce the heat loss. Hot air from a source was allowed to flow into the packed bed at various inlet conditions of velocity varying from 1 m/s and 2 m/s. The spheres were heated from inlet temperature of 28^{o}C.The experimental work was done in the heat exchanger is given to air in the multistage compressor and diesel engine exhaust. Waste heat energy was stored in the heat exchanger. The experimental results showed that the increased the porous media temperature, increased the outer surface temperature, increased the heat transfer rate with increase of the average bed temperature of 301 K to 371 K.

Keywords: Alumina (Al_2O_3) pebbles, Sensible heat storage, Pebble Bed Heat Exchanger, Porous media, Finite Element Analysis.

A Novel Sheet-Like $CoMn_2O_4$ Nanoparticle: An Affordable Visibly Active Driven for the Degradation of Organic Pollutants

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In this work, the novel sheet-like $CoMn_2O_4$ nanoparticles were prepared by a simple hydrothermal method. The crystal structure and microstructure of as-prepared samples were confirmed by the XRD, SEM, EDAX, TEM, DRS, PL spectroscopy technique and photochemical analysis. The $CoMn_2O_4$ nanoparticles shows superior photocatalytic activity in the visible region towards the degradation of Ciprofloxacin(CIP) based on the enrich recombination of electron-holes pairs. The photodegradation rate of as

prepared samples for CIP belongs to first-order kinetics. The $CoMn_2O_4$ nanoparticles showed excellent photocatalytic activity even after 6 consecutive cycles and plausible mechanism of the CIP degradation reaction was proposed by trapping experiment. The above set of results strongly evidenced that the $CoMn_2O_4$ might be a good photocatalytic material for the environmental application.

Rho Weakly Generalized Closed Sets in Topological Spaces

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The aim of this paper is to introduce a new class of sets called rho weakly generalized closed sets (briefly ρwg-closed sets) and a new class of functions called rho weakly generalized continuous functions (briefly ρwg-continuous) in topological spaces. Some of their properties and characterizations are deliberated.

Structural and Functional Characterization with Electrical conducting Properties of solid polymer electrolytes

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In recent years, there has been a growing demand for high-energy density rechargeable lithium batteries for portable electronic products because of their advantages including safety, high-energy density, high single cell voltage, geometry and no memory effect. However, the ionic conductivity of polymer electrolytes is generally low, often too low for practical application. To improve the basic requirements of the polymer electrolyte, various processes have been used such as electrochemical stability towards lithium battery electrodes, compatibility with the electrode, materials, reasonable ionic conductivity, sufficient thermal stability and good mechanical stability Proton conducting Ammonium nitrate mixed PVDF-PVP solid polymer electrolytes are prepared by simple solution casting techniques. The prepared polymer electrolytes are characterized by XRD, FTIR and AC impedance Analysis. The structural identification of the solid polymer electrolytes are done by XRD analysis. The functional groups present in the polymer matrix are confirmed through FTIR analysis. Ac impedance analysis is used to find the ionic conductivity of solid polymer electrolytes. The maximum ionic conductivity is obtained for 8wt% of NaNO3 added PVDF-PVP solid polymer electrolytes. Activation energy is the main role to the transmit of ions to improve the electrical conductivity of the sample.

A study of the corrosion inhibition of aluminium in alkaline medium

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Materials are precious resources of a country. Our material resources of iron, aluminum, copper, chromium, manganese, titanium, etc. are dwindling fast. Someday there will be an acute shortage of these materials. So we should preserve these valuable resources. In the field of corrosion inhibition, the scientists are seeking better and more efficient ways of combating the corrosion of metals. Inhibitors are used to protect materials from corrosive environment or deterioration of metals from corrosion process. In this work inhibition of aluminium metal corrosion by CMCis a result of adsorption of ions at the metal surface forming a protective layer.This layer prevents corrosion of the aluminium metal.

To study the effect ofCarboxymethyl cellulose (CMC) as corrosion inhibitor foraluminium in alkaline media. The corrosion inhibition of CMC on aluminium in 1.0 N NaOH has been evaluated by potentiodynamic polarization, linear polarization, electrochemical impedance spectroscopy and weight loss measurements. Results obtained show that Carboxymethyl cellulose is ananodic inhibitor and it inhibits aluminium from corrosion through adsorption mechanism. It shows 80% inhibition efficiency at 250 ppm of CMC and 25 ppm of Zn^{2+}. It infers a synergistic effect exist between CMC-Zn^{2+}. FTIR spectra reveal that the protective film consists of CMC-Al^{3+} complex and $Zn(OH)_2$. AFM clearly reveals that surface roughness of inhibited aluminium sample is less than uninhibited aluminium.

Synthesis and Electrical Properties of solid polymer electrolyte based on Ammonium nitrate doped PVDF-PVP polymers

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Solid-state batteries support greater energy density, which gives larger capacities, and utilize solid electrolytes, which are demonstrably safer. Proton conducting solid polymer electrolytes are mostly used in Proton Exchange membrane Fuel cells and Proton batteries. Ammonium nitrate mixed Polyvinylidene fluoride (PVDF)- polyvinyl pyrrolidone (PVP) [PVDF-PVP] solid polymer electrolytes are prepared simple solution casting techniques. Electrical properties of polymers are analysed using measured ac impedance data. DC conductivity and ac conductivity with hopping frequencies are

identified to solid polymers which are follows the Johnsher's power law. Using Johnsher's power law, dc conductivity of solid polymer electrolyte is calculated and Higher conductivity is obtained 8wt% of $NaNO_3$ added PVDF-PVP for 6.26×10^{-7} S/cm. Maximum dielectric constant is obtained for higher conducting samples. From the Tangent analysis, the relaxation humps are shifted to higher frequency to confirm the conductivity increases upto 8wt% of $NaNO_3$ added system.

Biodegradable packaging material using food waste – An alternative to existing non-biodegradable polymer packaging materials

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It is essential to work on in finding an alternative packaging material to replace the existing synthetic packaging material which is non-biodegradable and hazardous to the environment. The new material must be biodegradable as well as economic so that it will be affordable to all. In this concern we developed a polymer biocomposite with food waste as filler material. The developed polymer biocomposite with food waste as filler possess appreciable tensile strength and thermal stability. The matrix material was Polylactic acid (PLA), a thermoplastic which is completely biodegradable, as matrix and pomegranate peel powder (PPP), a food waste obtained after consuming, as reinforcement and thus made PLA/PPP green composites. The main aim of this project work is to add value to the waste PPP by using it as reinforcement in polymer composites. In PLA/PPPcomposites, PPP was loaded in 5 wt. %, 10 wt. %, 15 wt. %, 20 wt. %, and 25 wt. % of PLA. The PPP was found to be distributed uniformly in PLA. Thus, the obtained composite films were characterized by XRD, FTIR and TGA.

Structural, vibrational and electronic properties of 3-methoxy-2,4,5-trifluorobenzoic acid using DFT calculations

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The vibrations of 3-methoxy-2,4,5-trifluorobenzoic acid (MFBA) molecule have been examined by recording Fourier transform infrared (FTIR) and FT-Raman spectroscopy. Experimental data and quantum chemical studies from DFT calculations employing B3LYP method with 6-311++G(d,p) basis set were used for studying the complete

vibrational assignment and analysis of the fundamental modes of the molecule. In addition, the molecular electrostatic potential and Mulliken charges have also been calculated. The results of lower the value of HOMO-LUMO energy gap and NBO analyses suggests the possibility of intramolecular charge transfer in the molecule. Furthermore, NLO properties of the molecule have been identified by calculating the first hyperpolarizability and total dipole moment.

A Green Pathway for the Synthesis of Amidoalkyl-2-naphthols Derivatives Using Commercial Clay as Solid Acid Catalyst

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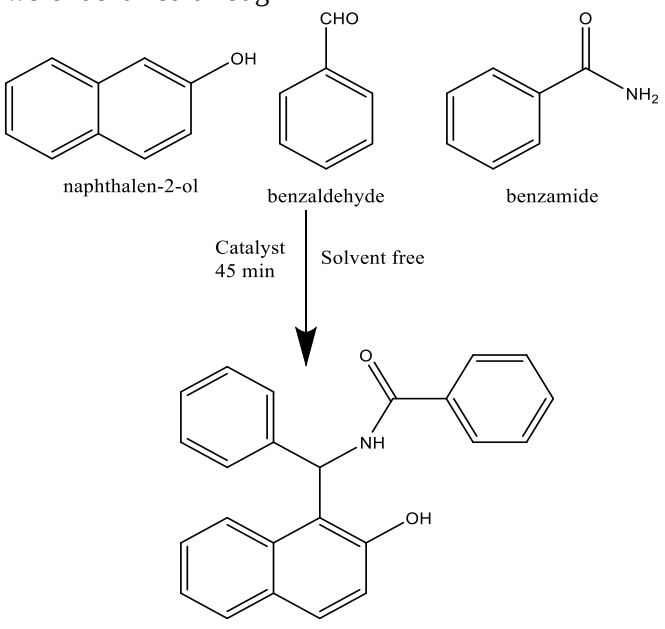
An efficient and green protocol for the one-pot three component synthesis of amidoalkyl-2-naphthols derivativesusing Commercial Clay as Solid acid Catalysthas been developed. The synthesized amidoalkyl-2-naphtholsderivatives were identified through physical and spectroscopic methods. Solvent free reaction conditions, good yield of products, easy isolation of products and recovery and sustainable usage of catalyst are the salient features of this method.



N-((2-hydroxynaphthalen-1-yl)(phenyl)methyl)benzamide

Synthesis of Perovskite-Type Lanthanum Nickel Ferrite Nanoparticles by Auto-Combustion Method

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Lanthanum Nickel Ferrite ($LaFe_{1-x}Ni_xO_3$) (x=0.1, 0.3) nanoparticles were synthesized by auto-combustion method in order to analyze the structure and magnetic properties. The crystalline nature and the functional group analysis are confirmed using X-ray Diffraction (XRD), Fourier Transform Infrared Spectroscopy (FT-IR). The morphology and composition observations are ascertained from Scanning Electron Microscopy (SEM) and Energy Dispersive analysis by X-ray (EDAX). Magnetic properties are analysis from Vibrating Sample Magnetometer (VSM). XRD studies reveal that the prepared samples have perovskite phase orthorhombic structure. FT-IR spectra confirm the presence of metal oxygen bonds of O-Fe-O and Fe-O in the FeO_6 octahedra. A very sensitive, inexpensive and simple method was used for the first time to attribute auto-combustion method parameters for the formation of nickel doped lanthanum ferrite.

Thermal behavior of Sevelamer Carbonate and non-isothermal decarboxylation kinetics using TGA to obtain activation energy as a parameter for sameness.

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Sevelamer carbonate is an orally administered ion exchange resin contains polymeric amine that binds phosphate and it is used to treat chronic kidney disease patients to remove excess phosphate. It is marketed as "Renvela" in the tablet form. Because it is insoluble in aqueous media and thus cannot be absorbed into the systemic circulation, studies of *in vivo* bioequivalences cannot be performed for generic formulations of *Renvela*. In order to prove the equivalence, the FDA suggested in vitro studies and sameness studies. The sameness mentions a variety of physicochemical characteristics including carbonate content. Alongside the carbonate content, the comparison of decarboxylation characteristics can offer additional assurance on the sameness. In this work, we have determined the 'activation energy (*Ea*), of decarboxylation of sevelamer using a Thermogravimetric analyzer (TGA), which can be used as a novel characteristic under sameness. Differential scanning calorimeter (DSC) was used to determine overall thermal behavior. Non-isothermal kinetics of decarboxylation in combination with a well-accepted Coats-Redfern model-fitting method was used to determine the activation energy (E_a) and the pre-exponential factor (A) of the decarboxylation. A total of 13 different models were tested of solid-state reaction in which the second-order model suits better with an excellent correlation of 0.9926. The resultant values of the Arrhenius parameters; E_a and A are 25 kcal/mol and 1.23007 x 10^{12} Sec^{-1}, respectively.

E-Nose : A Smart Gas Sensing System

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In markets, variety of sensors is available for different purpose of human needs. Sensors make dramatic change in the all the fields. Sensors are separated in different categories such as liquid sensors, gas sensors etc. Chemicals are the substance which is in solid, liquid and gaseous form. It is used to sense the liquid, solid and gaseous substances. There are lot of technology to make a sensor. In ancient days, sensor's size was large and also expensive one. Nowadays, Manufacturers and researchers use nanotechnology for making compact and intelligent sensors. In this article, we discuss about the structure of sensor arrays, impacts, advantages and disadvantages and future focus of sensors.

Graphitic-Carbon Nitride Nanosheets Modified TiO_2 Nanotubes with Enhanced Photoelectric Conversion Efficiency in Dye-sensitized Solar Cells

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Dye-sensitized solar cells (DSSCs) were fabricated by using g-C_3N_4 modified TiO_2 nanotubes (TiO_2 NTs/g-C_3N_4) as photoanode materials. TiO_2 NTs/g-C_3N_4 nanocomposites with different weight percentage (1, 2, 3, 4 and 5 wt%) of g-C_3N_4 loaded on TiO_2 NTs were synthesized by hydrothermal method. The characterization of the as-prepared nanomaterial was done with SEM, XRD and DRS. The photovoltaic performance of the different wt% of TiO_2/g-C_3N_4 photoanodes based DSSCs employing imidazole based liquid electrolyte were investigated. N719 dye was used as sensitizer and platinum coated FTO was used as counter electrode. The experimental results showed that the photoelectric conversion efficiency of DSSCs was obviously improved after modified by g-C_3N_4 nanosheets. The results demonstrate that the (3 wt%) TiO_2 NTs/g-C_3N_4 photoanode DSSCs exhibited high efficiency (η) of 1.60% with short circuit photocurrent density (I_{sc}) of 5.00 mA cm^{-2}, open circuit voltage (V_{oc}) of 0.64 V and fill factor (*FF*) of 0.50, which is higher than that of pure TiO_2 NTs. The better photovoltaic performance exhibited by the optimum level of 3wt% of TiO_2 NTs/g-C_3N_4 photoanode DSSCs is due to the thin layer of g-C_3N_4 which can act as the blocking layer for electron backward recombination with electrolyte, which can be used as the functional material to increase the DSSC performance.

Flora-extract mediated CdO NPs via coprecipitation route

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Green protocol of synthesizing nanoparticles has emerged as an optional way to overcome the limitation of the conventional methods. Chemical-reducing and capping reagents are widely used in synthesizing metal oxide nanoparticles which limit the biomedical applications. The synthesis of metal oxide nanoparticle is in vogue due to their miraculous application in diverse fields. Among the all metal oxide nanoparticles, cadmium oxide nanoparticles (CdONPs) have attracted a great deal of attention due to its superior biological, chemical, and physical properties. In this study, we report the facile green synthesis of cadmium oxide nanoparticles (CdONPs) for the first time by an completely environmentally benign process using Rosa Damascus plant extract. The synthesized nanoparticles were characterized using techniques such as scanning electron microscope (SEM), Fourier transform infrared spectroscopy (FTIR), and X-ray diffraction technique (XRD). Using the plant extract, the XRD reveals that the small size of the nanoparticles is due to the broadening of the peaks. For the SEM image it can be observed that the nanoparticles were cluster in formation and fibrous in nature. The presence of characteristic Cd-O stretching modes in FTIR supports the phase purity of the Monteponite CdO nature of the nanoparticles. The prepared CdO sample will be further used for photocatalytic and antibacterial applications.

Mechanical Properties of CFRP Composite Based on Two Thermoset Resins

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Carbon fiber reinforced plastic (CFRP) composites are used in the actual application areas, such as aerospace, automotive, and wind energy. In CFRP the reinforcement is carbon fiber, which provides the strength. The matrix is usually a polymer resin, such as epoxy and phenolic based to bind the reinforcements together. Because CFRP consists of two distinct elements, the material properties depend on these two elements. In this work, CFRP composite is prepared by two ways such as epoxy resin as well as phenolic resin based. Mechanical testing is used to realize the material properties before implementation of real time application. Hence tensile test, flexural test, impact test and compression test are performed. The result concluded that compressive and flexure strength of the epoxy resin based carbon fiber matrix is observed more when compared to the phenolic resin based carbon fiber matrix, this is due to the more adhesive properties of the epoxy resin than phenolic resin.

Textile effluent treatment using Graphene Oxide decorated Nickel Titanate (GO-$NiTiO_3$) nanofibers

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Graphene Oxide decorated Nickel Titanate (GO-$NiTiO_3$) nanofibers were fabricated by electrospinning technique. The effect of graphene oxide concentration on the properties of nickel titanate nanofibers were investigated by X-ray diffraction, Scanning Electron Microscopy and X-ray photon spectroscopy. The $NiTiO_3$ nanofibers decorated with 3 wt% of graphene oxide showed better photocatalytic activity through the degradation of Methylene Blue (MB) under visible light irradiation. This improved photocatalytic activity can be utilized for environmental remediation applications.

Keywords: Electrospinning, Nanofibers, Methylene Blue (MB), Photocatalytic activity.

Solid lubricant as environmental free cutting fluid in turning process

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Machining process involve high temperature due to plastic deformation which must be reduced to enhance cutting tool life as well as work piece surface damage. Generally, hydro carbon oil based cutting fluids are used but it creates environmental as well as operator health issue. Alternative cutting fluids are minimum quantity lubrication, vegetable oil as cutting fluid and cryogenic coolant. These methods have some limitations in terms of properties and supply. Solid lubricants powder are mixed with vegetable oil and applied to the machining zone become a good alternative cutting fluid. In this regard, a device is made and supply to the machining zone. Application of solid lubricant on textured tool leaving a continuous solid lubricating layer on the surface of the tool due to the thermal expansion by heat produced during machining. This thin layer led to reduced friction and temperature in the machining zone. Various solid lubricant powders such as Tungsten Disulfide (WS_2), graphite, boric acid, molybdenum disulfide, and calcium diflouride are commonly used in machining. In this work, Inconel 718 is machined using (WS_2) solid lubricant and analyzed that machinability intern of surface quality and temperature. The result revealed that WS_2 has texture II, hexagonal layered structure, high temperature resistance, oxidation resistance and good lubricity. The formed thin lubricated film due to plastic deformation in nature of thin, brittle nature and easily smeared and give low coefficient of friction. Solid lubrication leads to less environmental impact as well as eco-friendly in turning process.

Aqueous synthesis of CdTe Quantum Dots (QDs) decorated onto TiO_2 Nano rods

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In this paper, the well-aligned n-type TiO_2 Nano rods were synthesized directly on FTO Substrate by hydrothermal method and it was decorated with p-type CdTe Quantum Dots (QDs). The optical and structural properties of the prepared TiO_2 Nano rods were investigated respectively by means of UV-Visible and X-ray Diffraction Analysis. Results indicate that the CdTe QDs decorated TiO_2 Nano rods greatly enhance both the optical and structural properties. The absorption of UV and visible light occurs due to the p-n hetero-junction being constructed between p-type CdTe QDs and n-type TiO_2 Nano rods. From the XRD, we could observe that the prepared CdTe QDs decorated TiO_2 Nano rods are having the nano composite formation, retaining their individual structures. The other results will be discussed in detailed.

Keywords: CdTe QDs, TiO_2 Nano rods, CdTe QDs decorated TiO_2 Nano rods, Aqueous phase method

Facile One-Pot Green Synthesis of Mushroom Like Zinc Stannate Nanostructures

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An efficient microwave-assisted-one-pot synthesis was used to stimulate the growth of mushroom like nanofibrous zinctinoxide (NZTO) for photocatalytic application. The NZTO formation start at 2 min, and the complete transformation was observed after 5 min. Thus developed NZTO exhibited a uniform fibre interconnected to form a mushroom like architecture, which exhibits enhanced catalytic activity towards methylene blue degradation. The proposed method is facile, eco-friendly, fast and scalable synthesis of NZTO materials for environmental and energy applications.

Investigation of silver doped CdTe colloidal quantum dots as a light harvester in solar cell

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The pure CdTe QDs and Silver (Ag) (0.5 at. %, 3 at. %, and 5 at. %) doped CdTe QDs were synthesized through a colloidal process using 3-Mercaptoproponic acid (3-MPA) capping agent in an aqueous medium. The photophysical properties of highly luminescent Ag-doped CdTe and pure CdTe colloidal quantum dots are determined from UV-Visible spectra and Photoluminescence (PL) spectra which is red-shifted in higher wavelength based on different doping concentrations ($Cd_{1-x}Ag_xTe$ (X = 0, 0.005, 0.03, 0.05)). The structural, morphologies were studied by HRTEM and X-Ray diffractometer. The elemental compositions and the capping effect of the thiol group were studied by EDX and FTIR analysis respectively. The performance of solar cell device fabricated by sensitizing photoanode with Ag-doped CdTe QDs is found to get influenced by changes in these physical parameters. The efficiency of these devices is increased from 0.40%, 0.43%, 0.47%, and 0.51% with increasing dopant concentrations (0.5 at. %, to 5 at. %) with respect to pristine CdTe QDs. The incident-photon to current efficiency (IPCE) measurement of fabricated devices are tested and appraise of the short circuit current (J_{SC}) of the J-V measurement following the same movement while comparing with Integrated J_{SC} of IPCE.

Keyword: Colloidal, Quantum dots, CdTe, Doping, Solar cell

Facile Synthesis of Dy_2WO_6/ZnO@GO nanocomposite via Simple hydrothermal method: An efficient catalyst for the mitigation of carcinogenic organic dye

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In this scenario, a novel Dy_2WO_6/ZnO@GO (DWZG) nanocomposite material was made by the simple hydrothermal route was confirmed by various characterization techniques. The P-XRD was explained the crystalline nature of the as-prepared materials, the obtained diffraction peaks reveal good crystalline nature of as prepared Dy_2WO_6/ZnO@GO nanocomposite. The morphology of the DWZG materials has been fungi like irregular hexagonal Dy_2WO_6/ZnO incorporate on GO sheet. The presenting elements and the oxidation state of Dy, C, O and W and Zn were confirmed by X-

ray Photoelectron Spectroscopy analysis. Interestingly, Dy_2WO_6/ZnO@GO catalyst having an efficient activity in the degradation process than that undoped Dy_2WO_6, ZnO and GO materials and the degradation efficiency was above 97% corresponds to methylene blue (MB) degradation within 35 mins. In Reactive Oxidative Species study, hydroxyl and superoxide radical's quenchers are the main reactive species in the MB degradation process. On the other hand, the recycling test has confirmed the stability and reusability of the catalysts.

Synthesis of $Cd_xZn_{(1-x)}S$ Alloy Nanocatalyst for visible active photocatalyst: Metal Complexes as Single Source Precursor by Microwave irradiation Method

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In the present study, we report the synthesis of high quality $Cd_xZn_{(1-x)}$ S semiconductor nanocrystals alloy was obtained by microwave irradiation method from metal complexes [$Cd(DTC)_2$], $Zn(DTC)_2$] as single source precursors. The structural and optical properties of the prepared nanoparticles were characterized by X-ray diffraction (XRD). The XRD pattern reveals that crystal structure and lattice plane of the prepared $Cd_xZn_{(1-x)}S$ alloy nanoparticles. Scanning electron microscopy (SEM) images were demonstrates that the $Cd_xZn_{(1-x)}S$ alloy nanoparticles are spherical shaped morphology. The UV-Vis. spectra exhibited a blue-shift with respect to the bulk samples which is attributed to the quantum size effect. The prepared nanoparticles ware examined for photodegradation against commercial textile dyes in aqueous medium.

Key words: Metal complex, single source precursor, Microwave Irradiation, $Cd_xZn_{(1-x)}S$, Photodatradation.

Antibacterial Organic cotton using microcapsules of Eugenol

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Organic cotton, an eco-friendly textile was cultivated and processed using methods and materials that have a low impact on the environment. Cotton was more prone to microbial attack due to their hydrophilic nature. Microbial infestation on cotton textiles can be prevented by different functional finishing methods. In the present work microencapsulation of eugenol, the core material with gum acacia as wall material was carried out by co-acervation method and applied on fabric by pad dry cure method. The light microscopic analysis proved the formation of eugenol microcapsules and the Scanning Electron Microscopic Analysis confirmed the impregnated microcapsules on

the fabric. The antibacterial efficacy of the fabric against the gram negative bacteria (E-coli) was studied by agar diffusion method. The prominent zone of inhibition developed for gram negative bacteria proved the biocidal action of eugenol. The fabrication of antibacterial organic cotton using microcapsules of eugenol with biodegradable polymer gum acacia was non toxic and environmentally benign method.

Electrical Properties of Lithium Ion Conducting Poly Vinyl Alcohol / Poly (Vinyl Pyrrolidone) Polymer Electrolytes Doped with Zirconium Oxide

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Lithium ion conducting polymer blend electrolyte films based on poly(vinyl alcohol) (PVA) and poly(vinyl pyrrolidone) (PVP), 25Mwt% of lithium acetate dihydrate ($C_2H_7LiO_4$) salt and different wt% of Zirconium oxide have been prepared by using a solution cast technique. The polymer blend electrolyte has been characterized by XRD, FTIR, SEM and impedance analyses. The XRD study reveals the amorphous nature of the polymer electrolyte. The FTIR study confirms the complex formation between the polymer and salt. The ion conductivity of the prepared polymer electrolyte has been found by AC impedance spectroscopic analysis. The PVA/PVP blend system with a composition of 50wt% PVA: 50wt% PVP: 25wt% Lithium acetate exhibits the highest conductivity at room temperature. With the concentration, different wt% of Zirconium oxide is added and polymer electrolytes have been prepared to increase the conductivity. The conductivity is found to increase with increase in temperature. Conductivity studies show that addition of ZrO2 slightly enhances ionic conductivity at 303 K. The temperature dependent conductivity of the polymer electrolyte follows the Arrhenius relationship which shows hopping of ions in the polymer matrix.

Corrosion Studies of Ni-W-P Alloy by Electrodeposition Method

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Nickel tungsten alloys has a large pool of applications in industry field. Corrosion of those alloys pose an issue for long term uses. This work attempts to prepare a nickel tungsten phosphorous alloy with more corrosion resistant by electro deposition. Rather than adding additive or coating a inhibitor this method is more tranquil work just by changing the preparation parameters. Nickel tungsten phosphorous alloy was prepared by electro deposition bath, the bath was optimized by varying the temperature, current and pH for best results in corrosion protection. Characterization of so done variations were reported by XRD, SEM, Hull Cell experiments. The corrosion studies was done by potentio dynamic studies and nyquist plots. The variation done in bath, their characterization differences and their corrosion resistant qualities were tabled and showed in graph. The best corrosion resistant variant and its preparation parameters was reported.

Investigations on structural, spectroscopic, electro-optical properties of 4,7-dihydroxycoumarinby Density functional theory calculations

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Density functional theoretical computations of 4,7-dihydroxycoumarin have been studiedwith 6-31 G(d,p) levels to reach the optimized geometry, FT-IR-FT-Raman spectra, charge distributions and hyperpolarizability calculations. FMO analysis indicates the electron delocalization and also it small value of energy gap point out the bioactive of material. . The molecular orbital parameters of the title compound have been calculated by FMO analysis. Population analysis has been studied and discussed. Furthermore, time dependent-DFT analysis has been investigated to explain the electronic properties of the present molecule.Microscopic NLO parameters of the title compound have been calculated and it exhibits an excellent nonlinear optical efficiency. The chemical reactivity of the 4,7-dihydroxycoumarinhas been visual demonstrated by Molecular electrostatic potential surface analysis

Keywords: Computational calculations; MEP, Mulliken charge distributions; HOMO-LUMO; Electronic property, TD-DFT

Study on the Influence of Azeotropic Mixture Pre-Treatment on the Dyeing and other Physico-Chemical Properties of Pet-Cotton Blended Fabric

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Dyeing of polyester with dispersed dyes is a highly complex phenomenon. Pre-treatment of blended fabric with azeotropic mixture at room temperature. The effect of pre-treatment of fabric to induces the dyeing behavior.The effect of pre-treatment on the physico-chemical properties of the treated fabric material has been studied using SEM,FTIR,DSC,XRD.The results are presented and discussed.

Crystal growth and characterization of piperazinium salicylate nonlinear optical single crystal

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The piperazinium salicylate (PISA) organic nonlinear optical single crystal was grown by slow evaporation solution growth method using ethanol as a solvent. The crystal precision was confirmed by X-ray diffraction analysis. The chemical configuration and functional groups of the PISA crystal were confirmed by FT-IR and Laser Raman Spectroscopy analysis. Optoelectronics application was identified by the UV-Vis studies. It is revealed that the grown crystal has lower bandgap at 305 nm and the good transmission in the entire visible range. The luminescence property was identified by photoluminescence (PL) studies. PL spectrum of PISA crystal recorded with an emission peak at 415 nm in the near to violet region with an excitation wavelength at 360 nm. The thermo gravimetric and differential thermal analyses were carried out to study the thermal behavior of the grown crystal. Nonlinear optical property was confirmed by the study of Second harmonic generation.

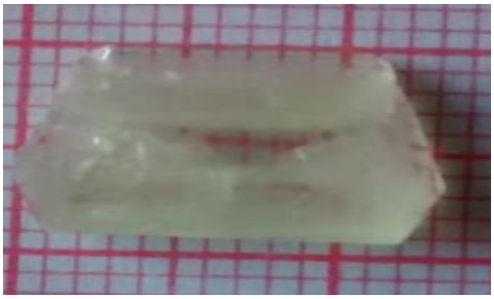

Fig.1 As-grown PISA crystal

Fabrication of Novel Zincs Selenide Nanostructures for Efficient Photocatalytic Degradation of Antibotic Drug

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Novel Zinc selenide nanoparticles (ZnSe NPs) through a simple hydrothermal technique. The crystalline structure, morphology and elemental compositions were investigated by X-ray diffraction (XRD), Scanning electron microscopy (SEM), and Energy Dispersive X-ray spectroscopy (EDX) analysis. The photocatalytic activity of ZnSe NPs was scrutinized for the degradation of Cefioxime (CF) under visible light irradiation. The obtained UV-vis spectroscopy results illustrate that ZnSe NPs could degrade above 98% CF aqueous solution within 70 min of visible light irradiation. Radical trapping experiments revealed that the hydroxyl radicals (•OH) plays predominant for the degradation system. This study showed that engineering the interfacial structures could provide a scientific basis for the design of efficient photocatalysts.

Enhancing the ionic conductivity of PEO/PVP based Na^+ ion conducting composite blend polymer electrolytes by Al_2O_3 nanofiller

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The conventional solution casting technique was used to yield polymer polymers PEO and poly PVP as polymer hosts, sodium nitrate ($NaNO_3$) as ion-conducting electrolytes with different wt.% of aluminium oxide (Al_2O_3) as nanofiller. Water has been used as a double distillation solvent. For these specific samples, AC impedance spectroscopy was performed between the frequency ranges of 42 Hz and 1 MHz. For poly (ethylene oxide) (PEO), poly (vinyl pyrrolidine) (PVP) polymer hosts, sodium nitrate ($NaNO_3$) film is formed at ~10^{-7} S cm^{-1} and enhanced to ~10^{-5} S cm^{-1} by addition of Al_2O_3 nanofiller at ambient temperature. Dielectric and Tan del parameters have been calculated from the AC impedance data. Increasing the nanofiller concentration was shown to increase the dielectric constant. It suggested plurality for relaxation. It was found that for different wt.% Al_2O_3, the maximum amount of tan del peaks went to the higher frequency side and therefore a lower relaxation time.

Keywords: Solution casting technique, Sodium ion conducing blend polymer, AC impedance spectroscopy, Ionic conductivity, Relaxation time.

Design of Dye sensitized Graphene Oxide Nanoparticles – An Excellent Photocatalysis for degradation of Organophosphate Pesticides

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The photo-degradation of organic pollutants using solar light is an attractive chemical process for water pollution control. In this study, we synthesized a novel highly efficient Dye sensitized Graphene oxide (Dye GO) photocatalyst for degradation of organophosphate pesticides Methyl parathion (MP). The phase structure, surface morphology and optical properties of the as-prepared Dye GO was characterized by X-ray diffraction (XRD), Scanning electron microscopy (SEM), Raman, Fourier Transform Infrared (FTIR) and Ultraviolet spectroscopy. The photocatalytic activity of the as-prepared Dye GO was assessed by degradation of MP under visible light irradiation. The results demonstrate that Dye GO displayed excellent photocatalytic performance for the degradation of MP. The effect of various factors such as catalyst concentration and initial substrate concentration as well as reaction kinetics were investigated. Furthermore, it could be easily recovered by simple filtration process after the photo degradation process. The work is expected to shed new light on the development of novel nanostructures for gathering visible light energy and on the improvement of new photocatalytic materials for the exclusion of environmental pollutants.

Preparation OF Vanadium Pentoxide (V_2O_5) thin film solar by Physical Vapour Deposition(PVD)

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V_2O_5 thin film was deposited by Physical vapour Deposition (**PVD**) method on glass substrate. The structural and optical and electrical properties were studied by means of X-ray diffraction (XRD), Fourier transforms infrared (FTIR) Spectroscopy, and UV-VIS Spectrophotometer. The morphology of the V_2O_5 has studied by scanning electron microscope. V_2O_5 η efficiency was studied by Solar Simulator.

Keywords: V_2O_5, Thin film Solar, Physical vapour Deposition (**PVD**) Technique

Conductivity and Dielectric studies of Biopolymer Electrolytes based on I-Carrageenan

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Solid Polymer electrolytes based on I-Carrageenan with sodium nitrate ($NaNO_3$) was prepared by using solution casting technique. The samples were subjected to AC impedance spectroscopy. AC impedance measurements were carried out in the frequency range of 42Hz to 1MHz. The same measurements was also carried out at different temperature for all the prepared samples. Maximum ionic conductivity 7.8369×10^{-5} Scm^{-1} was obtained for 20 wt% of sodium nitrate at room temperature. Arrhenius behaviour was observed from temperature dependent conductivity studies. Low activation energy of 0.0615 eV was observed for the maximum ionic conductivity samples. Dielectric parameter were obtained from AC impedance data. As the temperature increases, the magnitude of dielectric constant was found to increase.

Keywords: Solid polymer electrolyte, I-Carrageenan, Arrhenius Relation, AC Impedance technique, Activation energy.

DFT Study on Interaction Between Herb and Drug for Type 2 Diabetes

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The usage of herb induced drugs for the treatment of type 2 diabetes has become the present research in the medical field to reduce the side effects caused by the latter. Based on the above, we have studied theoretically the interaction of a commonly used drug (Metformin) with a herb (Ferulic Acid) applying density functional theory (DFT). The herb-drug was optimized at various positions and confirmed to be in their local minima through vibrational analysis at B3LYP/6-311++G** level. Study on the molecular geometry along with the interaction energy of the complexes confirmed the presence of interaction between the hydroxyl and amine group of the herb and drug respectively. The

calculation of Gibbs free energy and entropy exhibited the stability of the interacting structures along with the vibrational assignment which showed significant red and blue shifts in the complexes. Additionally, NBO analysis and molecular electrostatic potential (MEP) revealed the charge transfer between the complexes identifying an electrostatic interaction prevailing between the herb and drug. This study identifies the most convenient position for the herb-drug to interact which will aid the research community in understanding the nature of interaction prevailing in the complex at the atomic level.

Keywords: Metformin; Ferulic Acid; Herb; Drug; DFT; Type 2 Diabetes

Compatibility Studies of Polyblends Using Physical Methods-An Overview

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A Polymer blend is a mixture of at least two polymers that are blended together to create a new polymer material with different physical properties. Many researchers have analysed the miscibility nature of polyblends using physical techniques like measurement of relative viscosity, ultrasonic velocity, density and refractive index on different polymers in various solvents at different temperatures. These physical techniques are conducted on different compositions of polyblends and the miscibility natures of the blends are thus analyzed. If the variation of ultrasonic velocity with blend composition shows a linear relation, then the blend is assumed to be miscible; if it shows a S- type pattern variation then it is predicted as an immiscible blend and if tha variation is shown in between linear and non linear type, then the blend is assumed to be semi compatible. To confirm further various reconfirmation techniques are also available for this study. Based on vast interest in this area of research, an attempt has been made to provide an overview of various physical methods used to determine the compatibility nature of polymer blends along with various re-confirmation techniques like additive rule, optical studies, and glass transition temperature measurement using Differential scanning calorimetry.

Key words: Additive law, Adiabatic compressibility, Compatibility, Free volume, Internal pressure, Polyblends

Synthesis and Antibacterial Analysis of Nano Silver Coated Silk- A Green Approach

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Recent studies have proved that plant extracts act as a potential precursor for the eco-friendly synthesis of nanoparticles in non-hazardous ways because scientists are concerned about conventionally synthesizing nanoparticles by chemical method due to their toxicity and thus they prefer to develop environmental friendly process. Green synthesis of nanoparticles has emerged as a significant step in the field of nanotechnology. Green synthesis is considered as the best suited method because of wide variety of biomolecules present in them which not only act as reducing agent but also as stabilizing and capping agents. Plants are successfully used in the green synthesis of several

nanoparticles like gold, platinum, silver, zinc oxide, copper, palladium, etc.. Out of all metallic nanoparticles, silver NP grabs more attention because of its physical, chemical and biological properties. Furthermore silver nanoparticles are widely known for its antimicrobial properties against microbes such as bacteria, fungi and virus. Due to these proven properties, silver NPs are widely used in textile industry. This review explains a wider variety of plants that are used for rapid and single step protocol for synthesis of silver NPs coated silk and its antibacterial activity.

Keywords: Antibacterial activity, Green synthesis, Nanofluid, Silver NP

Theoretical investigation of intermolecular dihydrogen bonds in C_2H_2···HM and C_2H_4···HM (M=Li, Na and K) complexes - A DFT and ab-initio study

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Dihydrogen bonds (DHB) are difficult to appear owing to its weak interaction that arises due to charge separation between the molecules. This study aims to investigate the DHB formation in C_2H_2 and C_2H_4 with HM (M = Li, Na, and K) complexes using density functional theory (DFT) and ab-initio methods. It mainly focuses on the comparison of the performances of different functional of DFT and ab initio method on the intermolecular dihydrogen bonded complexes. The geometrical parameter and energy values agree with the formation of dihydrogen bonds in the complexes. Among the ethene and ethyne complexes, the smallest dihydrogen bond distance was formed by C_2H_2···HK and C_2H_4···HK respectively. C_2H_2 is found to form better DHB with alkali metal hydrides than C_2H_4. Among all the functionals, M06L was observed to predict shortest H···H bond distance, while M062X the longest. Natural bond orbital (NBO), quantum theory of atom in molecules (QTAIM) along with molecular electrostatic potential (MEP) analysis further confirms the dihydrogen bond formation.

Keywords: Dihydrogen bond; Density functional theory; Metal hydrides; Hybrid functionals.

Influence of Cesium Chloride (CsCl) Dopant on Gamma Ray Irradiated Potassium Hydrogen Phthalate (KHP) Crystals and its Characterization

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Potassium hydrogen phthalate (KHP) crystals doped with 1M% to 4M% Cesium Chloride (CsCl) were grown by slow evaporation solution growth technique have been examined. The Characterization of Gamma-ray beam using Cobalt-60 irradiated KHP and doped crystals were made by Powder X-ray diffraction, Fourier Transform Infrared spectroscopy, UV-visible spectroscopy, Photoluminescence analysis and Laser Raman spectroscopy analysis. The structural difference between pure KHP and Cesium Chloride doped KHP crystals has been studied using Powder XRD analysis. Functional groups and modes of vibrations were identified by FTIR analysis. The UV-visible absorption spectra have been recorded to find the variation in the cut-off wavelength. Vibrational spectral analysis and different stretching modes are discussed using the Laser Raman spectrum using 514.5 nm emission of Argon-ion source for the pure and doped KHP crystals. Photoluminescence analysis showed broad peaks from green to violet emissions 544.08nm, 600.60nm, 601.47nm, 603.31nm, and 604 nm respectively for Pure Potassium hydrogen phthalate and 1M% to 4M% CsCl doped KHP crystals. It was found that Cesium Chloride doped Potassium hydrogen phthalate semi-organic crystals to be very high energy scintillating material; due to its wide application effect of Gamma-ray using cobalt-60 different concentrations of Cesium chloride doped KHP Crystals.

Keywords: KHP, Gamma-ray irradiation, Powder X-ray diffraction, UV- visible analysis, photoluminescence analysis, Laser Raman spectroscopy analysis.

Electron deficient receptor for selective colorimetric recognition of cyanide and fluoride ion

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We have designed and synthesized a sensor L, as an strong selective colorimetric chemo-sensor for cyanide and fluoride ion. The acetonitrile solution contains L with tetrabutylammonium salts of cyanide, and fluoride results sudden color change from faint yellow to red. The chemosensor L produced an enhancement of absorbance intensity while addition of cyanide and fluoride ion. The recognition ability of the receptor L towards variety of anions is studied by naked-eye colorimetric experiments, UV–Vis spectrometry, Emission Spectrometry and IR Spectrometry.

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