



Phones : 040-32519687
040-31001618
Direct : 040-31001617
Mobile : 98663 08257
Fax : +91-40-24220320
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Geethanjali College of Engineering and Technology

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Sy.No. 33 & 34, Cheeryal (V), Keesara (M), Medchal District. - 501 301.

Prof. (Dr) S. UDAYA KUMAR

B.E., M.E., M.Tech (Hons.) (New Zealand), Ph.D

PRINCIPAL

To

3rd March, 2022

Smt. Sangeeta Talwar, Sr. Accounts Officer - II,
Govt. of India, Ministry of Defence, Defence R&D Organization (DRDO)
Directorate of Extramural Research and Intellectual Property Rights,
5th Floor, Old LASTEC Building, Metcalfe House, Delhi - 110054.
Phone: 011-23818131

Dear Madam,

Subject: Response to your email on "Observation under Equipment Head" dated 24.02.2022 with reference to the submission of documents for 3rd year Release of GIA out of DRDO Project Funds (ERIP/ER/1504754/M/01/1719) - regarding.

With reference to your feedback on the above subject for the project titled "Development of Novel Carbon Nanotube/polymer Nanocomposite Materials for EMI Applications", the following actions were taken by us.

S.N.	Feedback from DRDO	Follow-up action taken by Geethanjali College of Engineering and Technology
1	The carry-forward balance shown under Equipment Head is incorrect. It should be carried forward as per bal. available as on 31.3.21 i.e. Rs. 12659.	It was corrected in the updated Provisional Statement of Expenditure Accounts (attached)
2	In case of Exp. As per Stat. of Accts. is correct i.e. Rs. 2,39,341/-, then submit the Revised ink-signed Equipment List.	The actual cost of equipment incurred is Rs. 21,55,841/- as mentioned in the already submitted ink-signed Equipment List earlier. So, there is no need of sending a modified equipment list.
3	In case Exp. As per Equipment List is correct, i.e. 21,55,841/-, then refund the differential amount of excess expenditure shown i.e. 83,500/- in favour of CDA (R&D), New Delhi through EMRO instead of DD.	Yes, Expenditure as per Equipment List is correct, i.e. Rs.21,55,841/-; Rs. . 83,500/- was refunded in favour of CDA (R&D), New Delhi through EMRO on 02/03/2022 with SBI Collect Ref. No. DUI6346470. Updated Utilization Certificate and Provisional Exp. Statements are enclosed for the F.Y. 2021-22.

All the above documents are enclosed in triplicate. I request you to kindly release funds for Financial Year 2020-21.

Prof. Dr. S. Udaya Kumar
Principal Investigator

Sponsored by TEJA EDUCATIONAL SOCIETY, HYDERABAD
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Phones : 9533791618, 7306295152

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UTILIZATION CERTIFICATE

FOR THE FINANCIAL YEAR 2021-2022 (From 1-4-2021 to 31-10-2021)

1.	Title of the Project / Scheme	Development of Novel carbon nanotube/polymer nanocomposite materials for EMI applications
2.	Name of the Institution	Geethanjali College of Engineering and Technology
3.	Principal Investigator	Prof. S.Udaya Kumar
4.	DRDO Letter No. and date of sanctioning the project	ERIP/ER/1504754/M/01/1719 Date 2-4-2018
	Date of Start of the Project	20-7-2018
5.	Head of account as given in the original sanction letter	Major Head – 2080 Minor Head – 004
6.	Amount brought forward from the previous financial year quoting DRDO letter No. & date in which the authority to carry forward the said amount was given.	Rs. 84,460/-
7.	Amount received during the financial year (Please give no. and date of DRDO sanction letter for the amount)	NIL
8.	Amount of interest accrued, if any, from the grants	Rs. 2,804/-
9.	Total amount that was available for expenditure (excluding commitments) during the financial year (SL. No 6 +7+8)	Rs.87,264/-
10.	Actual expenditure (excluding commitments) incurred during the financial year (upto)	Rs.2,51,014/-
11.	Balance amount available at the end of the financial year.	Rs. – 1,63,750/-
12.	Unspent balance refunded, if any (Please give details of Cheque No. etc.)	NIL
13.	Amount allowed to be carried forward to the next financial year	NIL




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(contd...)

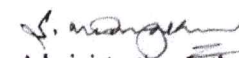
UTILIZATION CERTIFICATE

FY 2021-2022 (From 1-4-2021 to 31-10-2021)

Certified that sum of Rs.7.98 lakh was sanctioned as grants-in-aid during the Year 2019-2020 in favour of Geethanjali College of Engineering and Technology. Instt) vide DRDO letter No. ERIP/ER/1504754/M/01/1719 dated 2-4-2018. A sum of Rs. 7.98 lakh released vide Letter No. ERIP/ER/1504754/M/01/1719 dated 24-11-2020, an amount of Rs. 2,804 /- accrued as interest (if any) during the year and Rs. 84,460/- on account of unspent balance of the previous year, and fund available for the current financial year is Rs.87,264/- and a sum of Rs. 2,51,014 /- has been utilized for the purpose for which it was sanctioned and that the balance of Rs. -1,63,750/- at the end of the year shall be adjusted toward the grants-in-aid payable (as sanctioned.) during the year i.e. 2020-21.


Prof. Dr. S. UDAYAKUMAR
Principal Investigator
4/3/2022


Accounts/Finance Officer
B. Malleshwari


Administrative Authority
(with official seal)
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Geethanjali College of Engg. and Tech.
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2. Certified that I have satisfied myself that the conditions on which the grants- in-aid was sanctioned have been fulfilled/are being fulfilled and that I have exercised the following checks to see that the money was actually utilized for the purpose for which it was sanctioned.


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AUDITED/PROVISIONAL STATEMENT OF EXPENDITURE ACCOUNTS

FOR THE FINANCIAL YEAR 2021-2022 (1-4-2021 to 31-10-2021)

- (a) Title of the Project: Development of Novel carbon nanotube/polymer nanocomposite materials for EMI applications
- (b) Sanctioned letter no. & date: ERIP/ER/1504754/M/01/1719, Date: 2-4-2018
- (c) Principal Investigator: Prof. S. Udaya Kumar
- (d) Date of Start of the Project: 20-7-2018
- (e) Total Sanctioned cost of the Project: in Rs.45.81 lakh
- (f) Grant received (Rs.) in I yr. Rs.30.39 lakh II yr 7.98 lakh III yr --
- (g) Total Grants received so far: Rs. 38.37 lakh

S No.	Sanctioned Heads	Funds Sanctioned for the year (third year) in Rs Lakhs	Funds released (3rd year) Rs lakh	Carried forward from Previous year Rs.	Funds available (iv+v) Rs	Expenditure incurred during the FY Rs.	Balance (vi-vii) Rs	Commitments Rs	Total expenditure (vii+ix) Rs
i	ii	iii	iv	v	vi	vii	viii	ix	x
(a)	Staff	3.90	-	-226435	-226435	124000	-350435	39565	163565
(b)	Equipment	--	--	12659	12659		12659	12659	12659
(c)	Operation & Maint	--	--	-	0		0	0	0
(d)	Expendables	2.50	-	147168	147168	36240	110928	360928	397168
(e)	Travel	0.50	-	62146	62146		62146	112146	112146
(f)	Contingencies	0.25	-	23984	23984		23984	48984	48984
(g)	Research Consultant	0.29	-	58000	58000		58000	87000	87000
(h)	Procured Service	--	--	-	0		0	0	0
	Institutional over head	0	-	39000	39000	0	39000	39000	39000
	Interest (earned from 01/4/2021 to 31/07/2021)		2804	4470	7274		7274	7274	7274
	18/9/2020: returned excess JRF HRA @6% to DRDO (R&D)			-36532	-36532		-36532	-36532	-36532
	Interest returned Rs. 7274 (from 31/4/2020 to 31/7/2021) to DRDO					7274	-7274	-7274	0
	Refund of Equipment Budget Dt.02/3/2022 SBI Collect Ref No DU16346470					83,500	-83500	-83500	83,500
	TOTAL	7.44	2,804	84460	87264	251014	-163750	580250	831264

Name and Signature of Principal Investigator: *S. Udaya Kumar*
 Date: 4/3/2022

Name and Signature of Accounts Officer: *B. Malleshwar*
 Date: 03/03/2022

Signature of Administrative Authority: *S. Udaya Kumar*
 Date: 4/3/2022
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रक्षा लेखा प्रबन्धक
Controller General of Defence Accounts
रक्षा मंत्रालय, भारत सरकार
Ministry of Defence, Govt of India

e-Military Receivable Order (e-MRO)

SBI CMPOC, Survey no 26 , Gachibowli , Hyderabad-500019

Date: 02-Mar-2022

e-Receipt for State Bank Collect Payment

SBCollect Reference Number	DUI6346470
Bank Reference Number	CHI8221630
Category	PCDA R AND D NEW DELHI - UNITS
Name of Office/Sub off to which eMRO relates	DCDA R and D Delhi
Name of the Organisation	DRDO
Name of the Unit	Dte of ER AND IPR
Postal Address	5th Floor Old LASTEC Building Metcalfe Road Delhi
Nature of Payment	MISCELLANEOUS
Reference No.	1719
AMOUNT IN RS. (ROUNDED)	83500
Transaction charge	0.00
Total Amount (In Figures)	83,500.00
Total Amount (In Words)	Rupees Eighty Three Thousand Five Hundred Only
Remarks	Towards refund of Equipment budget for the project titled Development of Novel Carbon Nanotube/polymer Nanocomposite Materials for EMI Applications
Notification 1	
Notification 2	


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Phone: Off: +91-40-23158665
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Web : www.jntuh.ac.in
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JAWAHARLAL NEHRU TECHNOLOGICAL UNIVERSITY HYDERABAD
(Established by Govt. Act No.30 of 2008)
Kukatpally, Hyderabad – 500 085, Telangana (India)

PROJECT COMPLETION CERTIFICATE

SUB: - Project completion certificate – refund of unspent balance upon submission of Utilization Certificate.

Sir/Madam,

It is acknowledged that the project sanctioned to

1. **D. Mohan**, Sreenidhi Institute of Science & Technology
2. **Dr. K. Anitha Sheela**, JNTUH College of Engineering Hyderabad
3. **Mr. P. Sudhakar**, Geethanjali College of Engineering and Technology

With Procs No.JNTUH/TEQIP-III/CRS/2019/ECE/07 dated on 22-07-2019 under collaborative Research scheme; TEQIP-III JNTUH is completed. Out of the sanctioned amount of Rs 2,99,000/-, utilized amount (including Interest) is Rs 3,01,061/- and unspent amount for Rs NIL is refunded. In this connection Utilization certificate is submitted by Investigators in compliance to the above.


REGISTRAR



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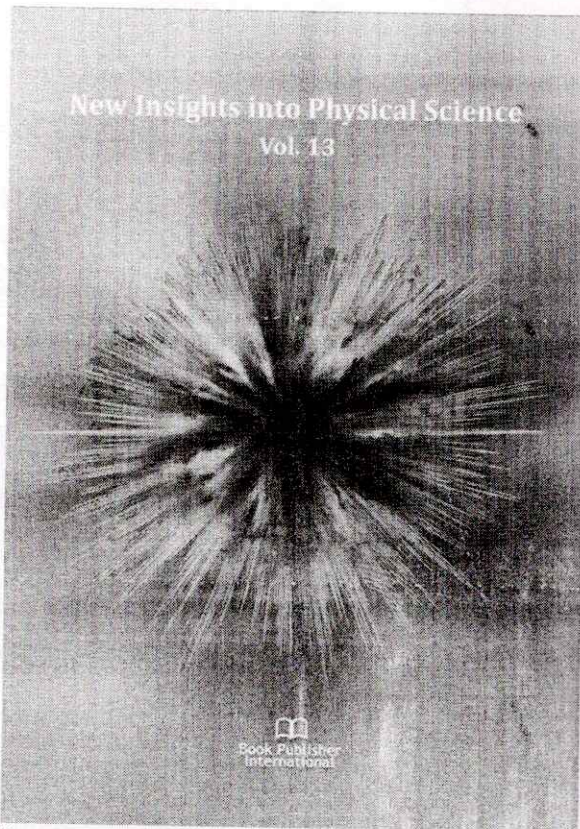
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A Frame Work for Decimal Floating Point Multiplier Using Vinculum Multipliers

G. Sreelakshmi ; Kaleem Fatima ; B. K. Madhavi

New Insights into Physical Science Vol. 13, 27 February 2021, Page 152-162

<https://doi.org/10.9734/bpi/nips/v13/6866D> (<https://doi.org/10.9734/bpi/nips/v13/6866D>)

Published: 2021-02-27

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A Novel MAC Protocol with Fusion Center and Adaptive Full-Duplex Communication for Cognitive Radio Networks

Appala Raju Uppala^{1,2}, C. Venkata Narasimhulu³ and K. Satya Prasad^{4*}

¹Department of ECE, Jawaharlal Nehru Technological University, Kakinada, India; ²Geethanjali College of Engineering and Technology, Hyderabad, India; ³LORDS Institute of Engineering and Technology, Hyderabad, India; ⁴Vignan's Foundation for Science, Technology & Research, Guntur, India

ABSTRACT

Cognitive radio network is an intelligent and adaptive communication technology used to effectively utilize the radio spectrum to provide better communication. It enables the secondary (unlicensed) users to communicate over vacant channels without disrupting the communication of the primary (licensed) users. This paper proposes a novel contention-free MAC protocol for full-duplex and half-duplex cognitive radio networks. A novel concept of a fusion center-based channel allocation scheme is proposed to provide better channel allocation and reduced energy consumption. The proposed technique is compared with the existing techniques in terms of the average number of channels being sensed by each user, average wait time, collisions, throughput, and average energy consumption. The number of collisions increases as the maximum allotted time of communication increases in existing approaches. The experiment is performed with 20, 40, 60, and 80 s. The existing approaches show for 20 s, the number of collisions is 65, 61, 68, and 62; for 40 s, the number of collisions is 93, 96, 95, and 92; for 60 s, the number of collisions is 122, 126, 133, and 130; for 80 s, the number of collisions is 176, 170, 173, and 175. The proposed method approaches the number of collisions will become zero as the maximum allotted time of communication increases. The experimental results show that the proposed approach performs better than existing approaches. Moreover, it can be observed that the average waiting time of secondary users when a collision occurs is reduced with the application of a fusion center-based channel allocation scheme.

KEYWORDS

Cognitive radio network; Dual-threshold; Full-duplex; Fusion center; Half-duplex; MAC protocol; Spectrum sensing

1. INTRODUCTION

The traffic encountered by the current day cellular network is huge due to the sharp increase in the use of mobile devices. This phenomenon raised attention towards determining appropriate outcomes for better usage of the spectrum. The cognitive radio network (CRN) and full-duplex (FD) mode of communication can provide an effective solution to the growing traffic and achieve maximum spectrum utilization [1]. These technologies majorly concentrate on increasing the utilization of the spectrum and efficiency of the network. Research has to be carried out on adaptive broadcasting techniques at the physical and MAC layers in both traditional networks and cognitive radios.

Generally, the CRN is non-time slotted. Hence, the transmission over the channels need not be continuous. The users can become active at any point of time after being inactive. Classical spectrum sensing strategies like listen before talk (LBT) is example of non-time slotted

networks. Such techniques generally fail to transmit the data without collisions in turn reducing the integrity of the model. This leads to collisions on a large scale when the primary users take over the channel or become active. Some of the studies in [2–5] projected the FD spectrum sensing for resolving this issue. In such approaches, the broadcasting secondary user maintains the sensing of the licensed users steadily all along the broadcasting slot, and after identifying the signal of the licensed user, the transmission gets paused to avoid collision [2]. Such techniques increase the security risks and thus the throughput of the system reduces as the collision causes the data corruption and the sender has to resend the data.

The dynamic utilization of the spectrum provided by the CRN has proved to be useful in allotting the spectrum effectively to the secondary users' (SUs) when the channels are idle [6, 7]. False detection of the channels will lead to the collision on the return of the primary users' (PUs) [8]. To improve the performance of the CRN sys-

*Present address: Department of ECE, Jawaharlal Nehru Technological University, Kakinada, India

Brain Tumor Segmentation, Detection and Grading in MRI Images

Kethu Sneha Latha¹ Yepuganti Karuna² Saladi Saritha³

^{1,2}School of Electronics and Communication Engineering, Vellore Institute of Technology, Vellore,
³Geethanjali College of Engineering and technology, Hyderabad, Telangana.

E-mail: kethusnehalatha@gmail.com¹, karun@vit.ac.in², saritha.saladi3188@gmail.com³

Abstract:

The most common malignant brain tumours are gliomas, and they come in a variety of grades, each of which has a significant impact on the patient's chance of survival. Magnetic resonance imaging (MRI) tumour grading and segmentation are normal and crucial for treatment preparation and diagnosis. A deep learning approach was developed to meet this clinical need, that associates tumour segmentation using U-net which is a convolutional neural network (CNN) and tumour grading using transfer learning using a Vgg19 and a completely associated classifier. T1-postcontrast, FLAIR and T1-precontrast MRI images of 110 patients with LGG were used to train and evaluate. DSC for segmentation model's and tumour detection accuracy are 0.875 and 0.937, correspondingly. At the MRI image level, the grading model classifies LGG with specificity, accuracy, sensitivity, and of 0.922, 0.907, and 0.893, correspondingly. In MRI images this study shows conventional tool for automated and simultaneous LGG tumour segmentation, detection, and grading in clinical settings.

Keywords: Glioma, Segmentation, Magnetic resonance imaging, Classification, Grading, Brain tumor.

I. INTRODUCTION

The most common malignant brain tumours are gliomas [1], through various grades based on tumour malignancy and growth rate [2]. Gliomas are categorised by the World Health Organization (WHO) into four grades [2,3]. Astrocytoma, oligoastrocytoma, and oligodendroglioma are some of the histological types of LGG. Grades of gliomas, as well as tumour location, shape, and size, are crucial in determining existence and treatment options [4]. As a result, designing conventional techniques to automate tumour segmentation and grading to improve patient results would be advantageous.

MRI is a non-invasive brain imaging technique that can deliver accurate images of the brain. As a result, it's widely used for tumour characterization and diagnosis. Brain tumour segmentation

[1841]



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RESEARCH ARTICLE

Carrier transport mechanism in bottom gate thin-film transistor with SnO as active layer for CMOS displays

Vallisree Sivathanu, Trupti Ranjan Lenka ✉, Vishal Goyal, Hieu Pham Trung Nguyen

First published: 11 November 2021

<https://doi.org/10.1002/jnm.2975>

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Abstract

In this work, we report on four tin monoxide (SnO) thin-film transistor (TFT) grain boundary (GB) models of carrier transport considering the native defects in the thin film, interface traps, and GB deep/tail states. The changes in the activation energy and the GB barrier potential on the application of gate electric field are thoroughly investigated. The shift in Fermi level and the charge carrier transport mechanisms are examined for the two-channel model by the application of external potential. Four models are developed to study the impact of phase transformation of SnO material on the TFT characteristics. Among the four developed models which are considered as four different cases, Case (iv) shows excellent performance and the simulation results revealed that the location of Fermi level closer to the mid gap are suggested to favor the ambipolar behavior. Also, the influence of SnO material thickness and the effect of different dielectrics on the ambipolar device characteristics are examined aiming at optimized performance of the device. The developed optimized model will help the process engineers in tuning the SnO material parameters for achieving better performance in both p-type and n-type TFTs when employed in CMOS based displays.

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DATA AVAILABILITY STATEMENT

Data sharing not applicable to this article as no datasets were generated or analysed during the current study.

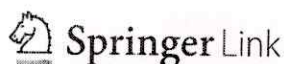
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Original Contribution | [Published: 08 October 2021](#)

Implementation of an Adaptive Neural Network-Based Controller for Improving the Conversion Efficiency of Solar Photovoltaic Module

[Kakarla Deepti](#) , [P. Srihari](#) & [K. Manjunath Achari](#)

Journal of The Institution of Engineers (India): Series B
103, 477–489 (2022)

37 Accesses | [Metrics](#)

Abstract

This research article proposes an intelligent artificial neural network-based fuzzy logic controller developed for tracking the exact maximum power point (MPP) under varying conditions of temperature and irradiance. The hybrid soft computing method combines learning abilities of an adaptive artificial neural network (ANN) and incremental conductance algorithm (INC)-based fuzzy logic controller (FLC) to handle uncertain data. The adaptive neural fuzzy inference system (ANFIS) is trained with the dataset generated for output voltage, current and all possible varying conditions to estimate the duty cycle of converter as maximum power point capturing device. ANFIS is developed in Takagi–

ARCHIVES

Implementation of MAC Protocol for Analysis of Traffic in Smart Cities

👤 Appala Raju, Uppala, C. Venkata Narasimhulu and K. Satya Prasad

Abstract

Human beings made Smart Transportation system as an essential need in their daily activity in the present era. For avoiding the road accidents in the present busy lives, it is necessary to create an application which is capable of transferring the emergency information between the vehicle and roadside units. This paper explains such network. The betterment of safety and no safety message delivery will be done by the MAC protocol. Threats occurring with 802.11p MAC protocol will be observed here. Hybrid MAC is capable of accessing two channels simultaneously, so that it can provide better performance during increased traffic load. MAC layer protocol is a challenging architecture for the vehicular network system. It is because of frequent changes in the topology of the vehicular network, huge quality of service requirements, infrastructure inadequacy, and automobile nodes during high speed. If the position of the vehicle is nearer to the network then the operation of the algorithm begins. New vehicles generate the request for sending the message. If there is any availability of the channel, then the channel is allocated and initiates the communication. If it is an old vehicle then it directly goes to the communication monitoring. The vehicle will be in a queue position if there is no availability of channels. When the channel becomes free then it gives first priority to the vehicles which are in the queue. The main aim of the Hybrid MAC protocol is to ensure that all vehicles get a proper channel accessing for conveying their message. Hybrid MAC is capable of reducing the loss of packet, delay in overall function, and collision reduction.

📖 Volume 11 | 06-Special Issue

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International Journal of Energy Research / Volume 45, Issue 7 / p. 10527-10537

RESEARCH ARTICLE

Modeling and performance optimization of two-terminal Cu₂ZnSnS₄-silicon tandem solar cells

Vallisree Sivathanu, Thangavel R, Trupti Ranjan Lenka ✉

First published: 14 February 2021

<https://doi.org/10.1002/er.6540>

Citations: 1

Summary

A dual-junction Cu₂ZnSnS₄-Silicon (CZTS-Si)-based tandem configuration is modeled and analyzed for its viability as a solar cell. The top and bottom modules in the tandem structure are validated by comparison with experiment. Initially, the designed tandem structure yields very low efficiency of 3.18%, and the various loss mechanisms are identified and investigated. The current mismatch between top and bottom cells and parasitic absorption (photon losses) are suggested to be the major causes limiting the short circuit current and hence the efficiency of the device. We optimize the material parameters within experimentally achievable limits in order to obtain current matching, and the optimized thicknesses of copper zinc tin sulfide (CZTS) and silicon (Si) absorbers are found to be 150 nm and 250 μm, respectively. The simulation results revealed that the photon losses are reduced, and overall absorption in the longer wavelength region has enhanced with the replacement of cadmium sulfide (CdS) by zinc sulfide (ZnS) buffer and careful optimization of the front layers of the device. The maximum predicted efficiency of tandem structure is >20% by minimizing the recombination centers within the experimentally obtainable ranges and improving the carrier separation process.


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DATA AVAILABILITY STATEMENT

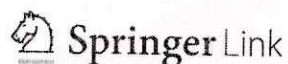
The data that support the findings of this study are available from the corresponding author upon reasonable request.

Citing Literature

<https://onlinelibrary.wiley.com/doi/10.1002/er.6540>


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Original Research Article | Published: 21 February 2022

Modeling and Simulation of CZTS Thin-Film Solar Cell for Efficiency Enhancement

Rabin Paul, S. Vallisree, T. R. Lenka & F. A. Talukdar

Journal of Electronic Materials **51**, 2228–2235 (2022)

160 Accesses | [Metrics](#)

Abstract

CZTS solar cells have been utilized as a replacement for CIGS and CdTe solar cells in thin-film technology. With the better absorption coefficient of this material, it has achieved efficiency higher than 13%. In this work, the performance of a CZTS thin-film solar cell (TFSC) is analyzed by replacing intrinsic ZnO (i-ZnO) with Mg-doped ZnO as window layer material. i-ZnO has good optical and electrical characteristics, but the optical, electrical,

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Improved Convolutional Neural Network Based Cooperative Spectrum Sensing For Cognitive Radio

Appala Raju Uppala^{1*}, Venkata Narasimhulu C², and Satya Prasad K³

¹ Research Scholar, Department of ECE, Jawaharlal Nehru Technological University
Kakinada Andhra Pradesh, India

Associate Professor, Geethanjali College of Engineering and Technology,
Hyderabad, Telangana, India

[e-mail: rekharajuppala2009@gmail.com]

² LORDS Institute of Engineering and Technology, Hyderabad,
Telangana, India

[e-mail: narasimhulucv@gmail.com]

³ Vignan's Foundation for Science, Technology & Research
Guntur, India

[e-mail: prasad_kodati@yahoo.co.in]

*Corresponding author: Appala Raju Uppala

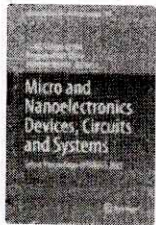
Received October 24, 2020; revised January 29, 2021; accepted May 16, 2021;
published June 30, 2021

Abstract

Cognitive radio systems are being implemented recently to tackle spectrum underutilization problems and aid efficient data traffic. Spectrum sensing is the crucial step in cognitive applications in which cognitive user detects the presence of primary user (PU) in a particular channel thereby switching to another channel for continuous transmission. In cognitive radio systems, the capacity to precisely identify the primary user's signal is essential to secondary user so as to use idle licensed spectrum. Based on the inherent capability, a new spectrum sensing technique is proposed in this paper to identify all types of primary user signals in a cognitive radio condition. Hence, a spectrum sensing algorithm using improved convolutional neural network and long short-term memory (CNN-LSTM) is presented. The principle used in our approach is simulated annealing that discovers reasonable number of neurons for each layer of a completely associated deep neural network to tackle the streamlining issue. The probability of detection is considered as the determining parameter to find the efficiency of the proposed algorithm. Experiments are carried under different signal to noise ratio to indicate better performance of the proposed algorithm. The PU signal will have an associated modulation format and hence identifying the presence of a modulation format itself establishes the presence of PU signal.

Keywords: Cognitive radio, Cooperative spectrum sensing, Primary user, Simulated annealing, Neural network.

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Micro and Nanoelectronics Devices, Circuits and Systems pp 227–236

Performance Analysis of HIT-CZTS Tandem Solar Cell Towards Minimizing Current Losses

Sivathanu Vallisree & Trupti Ranjan Lenka

Chapter | First Online: 10 September 2021


497 Accesses

Part of the Lecture Notes in Electrical Engineering book series (LNEE, volume 781)

Abstract

In this work, we report on Heterojunction with intrinsic thin layer-Cu₂ZnSnS₄ (HIT-CZTS) tandem solar cell modelled using Silvaco TCAD simulator. Initially the HIT and the CZTS solar cells are modelled and validated. Then the tandem structure is designed using HIT as bottom module and CZTS as top module and various loss mechanisms are investigated. From the simulation study, it is revealed that current mismatch among the top and bottom modules has contributed to low short-circuit current density and hence the efficiency of

https://link.springer.com/chapter/10.1007/978-981-16-3767-4_21


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Test pattern generation using thermometer code counter in TPC technique for BIST implementation

K. Jamal ^a, K. Manjunatha Chari ^a, P. Srihari ^b

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Abstract

This paper introduces a newly pattern generation with Test-Per-Clock technique for Built-In-Self-Test implementation. This proposed test vector generation generates Multiple Single Input Change vectors. Each pattern enforced in SIC vector as scan chain. To generate minimal transition sequence of test patterns, a scalable SIC counter and Thermometer Code Counter implemented. The proposed Multiple SIC vector generator is adaptable to both Test-Per-Scan, Test-Per-Clock techniques. This method developed a theory to evaluate MSIC scheme. Survey outcome demonstrates that, applying Multiple SIC test patterns on ISCAS C432 benchmark reduces the power consumption due to uniform distribution and lesser transition generated test patterns.

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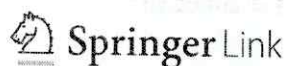
Keywords

Test-Per-Scan (TPS); Design under test (DUT); Multiple SIC (MSIC); Thermometer Code Counter (TCC); Test-Per-Clock (TPC)

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The stability, structural, electronic, and optical properties of hydrogenated silicene under hydrostatic pressures: a first-principle study

V. Kumar & R. Santosh

Journal of Molecular Modeling **27**, Article number: 278 (2021)

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Abstract

The structural, electronic, and optical properties of hydrogenated silicene have been studied under different hydrostatic pressures using first-principle calculations. The binding energy and band structure have been calculated for chair (C-) and boat (B-) structures, which are having good stability at 0 GPa, 3 GPa, 6 GPa, 9 GPa, 12 GPa, 15 GPa, and

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1/16

Insulation integrity of grading high insulating spacer with functionally graded material in a Gas Insulated Busduct

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 Published Online: 12 October 2020

A. Rukmananda, G. V. Nagesh Kumar, M. Aruna Bharathi, and Sravana Kumar Bali



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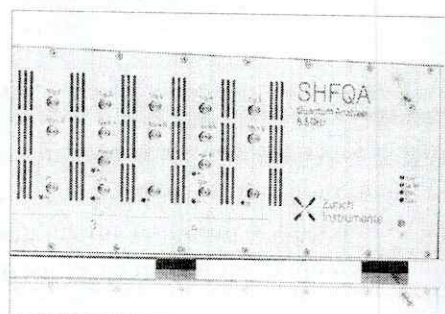
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Design and analysis of grading high plate type spacer in a single phase gas insulated busduct for reduction of electric field stress

AIP Conference Proceedings 2269, 030046 (2020); <https://doi.org/10.1063/5.0019502>

Synthesis and characterization of $\text{LiMn}_{1.5}\text{Ni}_{0.5}\text{O}_4$ by sol-gel method for cathode material & its application in Li-ion battery

AIP Conference Proceedings 2269, 030048 (2020); <https://doi.org/10.1063/5.0019660>

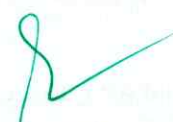


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Insulation Integrity of Grading High Insulating Spacer with Functionally Graded Material in a Gas Insulated Busduct

A. Rukmananda¹, G.V. Nagesh Kumar^{2,a}, M. Aruna Bharathi³, Sravana Kumar Bali^{4,b}

^{1,2}Department of EEE, JNTUA College of Engineering Pulivendula, India.

³Department of EEE, Geethanjali College of Engineering and Technology, Cheeryal, Keesara, Hyderabad, Telangana, India.

⁴Department of EEE, GITAM Deemed to be University, Visakhapatnam, India.

a) Corresponding author: drgvnk14@gmail.com

b) sravanbali@gmail.com

Abstract. High voltage power equipment is becoming more compact and under high stress, resulting in loss of insulation. The construction of insulators plays a vital role in enhancing the system's reliability. For GIS, the solid supporting structures called spacers are vulnerable to increased stress and are concerned about their functionality. The point of contact of the conductor, gas and spacer called the triple point junction in the air-insulated bus duct is a highly stressed area and is responsible for significant insulation failures. GIS switchgear design requires comprehensive field distribution in the supporting structures called spacers, which is critical for the system's healthy operation. In this paper, high grade material is used for post form spacers with specific permittivity for controlling field stress distribution on the spacer surface. Electric field calculations for different grades are calculated and compared and the stress reduction is carried out with the insertion of metal inserts.

INTRODUCTION

Gas Insulated Busduct (GIB) is becoming the most popular technology in India due to its compactness, ideal use in restricted areas. The high demand for electrical power and energy efficiency in urban areas made it necessary for power consumers to boost the voltage network. Gas Insulated Busducts provides an excellent alternative to the above-mentioned issue and have been operating around the globe for over 30 years. The most challenges faced by the GIB is failure of Insulating spacers as they are the weakest insulating link (weak link) and they can lose their strength due to corona effect or metallic particles. The rapid rise in the power density of electrical equipment and electronic equipment highlights the need for thermally conductive but electrically insulating products. The surges or any event of flashovers will damage of spacer and hence a spacer material has to be chosen to get rid of these situations in regular testing in plant or onsite. It is enormously essential as SF₆ systems should be viewed as self-restoration. Cycloaliphatic resins consist of greater track resistance when compared with biphenyl resins with reduced mechanical strength. Aluminum-based fillers along with epoxy resins are used to create general strength even though they have a demerit of greater allowability and greater thermal expansion coefficient. Due to the defects like protrusions, voids, depressions, cracks, delaminations and poor adherence to electrodes the life of the spacer can be decreased as the conductor is positioned in the middle of the spacer. From the survey of GIB used in the context of India it was observed that the maximum rate of its failures is because of material failures, improper selection of materials. Few other reasons like corrosion, loose particles effect the overall failures in the GIB.

This work focuses on design of Optimal Spacer in GIB using various insulating materials and analysis will be carried by determining electric breakdown strength, thermal conductivity, temperature resistance, corona resistance, and specific energy storage in dielectrics. Later, design of disc type and cone type FGM (Functionally Graded

Synthesis and charecterization of $\text{LiMn}_{1.5}\text{Ni}_{0.5}\text{O}_4$ by sol-gel method for cathode material & it's application in Li-ion battery

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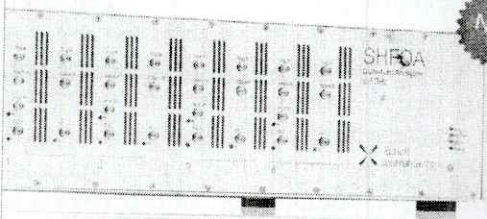
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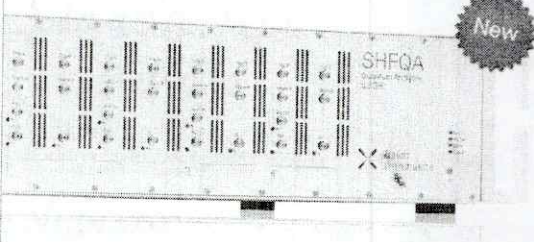
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Analyzing and Predicting Cyber Security Violations using Machine Learning Techniques

¹Veeramakali T

Associate Professor, CSE Dept., Vel Tech Rangarajan Dr Sagunthala R & D Institute of Science and Technology, Tamilnadu.
drveeramakalit@veltech.edu.in

²G. Swapna

Asst.Professor, CSE Dept., Geethanjali College of Engineering and Technology, Hyderabad.
g56swapna@gmail.com

³P Ila Chandana Kumari

Assoc. Professor, CSE Dept., Hyderabad Institute of Technology and Management, Hyderabad.
ilachandana@gmail.com

⁴V N L N Murthy

Assistant Professor, CSE Dept., Vardhaman College of Engineering, Hyderabad.
vlnlmurthy@gmail.com

Abstract — To deepen our insight into the evolution of a threat situation, study of cyber incident data sources is an essential process. This is a relatively recent subject for science and many experiments still have to be conducted. Throughout this article, we present statistical analysis of the 12-year cyber hacking operation (2005-2017) violation incident data set which includes attacks by malware. We prove that, in comparison to the literary results, breach sizes and inter-arrival times for hacking breaches can be modeled instead of distributions, since they have an auto-correlation. In order to adapt the time of the intercom and the scale of the violation, we suggest complex stochastic process models. We also prove that the inter arrival periods and the violation scale can be estimated from these models. We perform quantitative and qualitative pattern research on the data set to achieve a better understanding of the growth of hacking infringement incidents. We derive a variety of observations into cyber security, including the challenge of cyber hacking in its scale, but not in its severity.

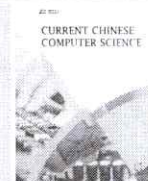
Keywords: Cyber risk analysis, Hacking breach, breach prediction, data breach cyber threats, trend analysis, cyber security data analytics and time series.

Introduction

An information breakdown is the protection for the transfer, transmission, stolen or as any use of important, safe or confidential information by an unapproved person. The breakdown of data is the purposeful or unintended intrusion into a non-trustworthy realm of safe or private/classified data. This

RESEARCH ARTICLE

Leaf Image Classification with the Aid of Transfer Learning: A Deep Learning Approach



Srinivasa Rao Dammavalam^{1,*}, Ramesh Babu Challagundla², Vangipuram Sravan Kiran¹, Rajasekhar Nuvvusetty³, Lalith Bharadwaj Baru¹, Rohit Boddeda⁴ and Sai Vardhan Kanumolu¹

¹Department of Information Technology, VNR Vignana Jyothi Institute of Engineering and Technology, Hyderabad, India; ²Department of CSE, Geethanjali College of Engineering and Technology, Hyderabad, India; ³Department of Information Technology, Gokaraju Rangaraju Institute of Engineering and Technology, Hyderabad, India; ⁴Department of CSE, VNR Vignana Jyothi Institute of Engineering and Technology, Hyderabad, India

Abstract: Background: Crop diseases are a primary hazard to nutrient safety, which proves to be a serious problem in many places in the world due to the unavailability of essential aid. Typically agriculturalists or specialists perceive the plants with a naked eye for detection and identification of an illness. Machine vision models, in specific Convolutional Neural Networks (CNNs) have directed an impact in feature extraction to a greater extent. Since 2015, numerous solicitations for the automatic classification and recognition of crop illnesses have been established.

Methods: In this paper, we proposed, analyzed, and assessed various state-of-the-art models proposed over a decade. These models are pre-trained with the finest parameters where we modeled a design-oriented method with numerous leaf-images and classified them into infection and healthy class for each type of leaf independently.

Results: Through our examination, we concluded that VGG models stand-alone with many cited prototypes and give on par results. As declared, these VGG models (VGG16 and VGG19) are utilized for feature extraction, and further, we augmented a set of dense layers and train them consequently for classification. The performances of various machine vision prototypes were pictorially perceived and their sophisticated architecture is not only capable of extracting detailed features but also repressed many loop-holes. The performance is assessed and computed for several types of leaf images and the accuracy scores attained were more than 97.5% for VGG16 and 96.72% for VGG19.

Conclusion: AUC-ROC curves were portrayed to illustrate its inspiration in defining an accurate classification where VGG16 and VGG19 have at least 96.6% and 95% area under the curve (AUC) which resembles their robustness.

Keywords: Leaf classification, deep learning, transfer learning, automated plant diagnosis, CNNs.

1. INTRODUCTION

The trick of competent plant disease fortification is carefully connected to the difficulties of supportable cultivation and weather variation. Investigation outcomes designate that weather variation can change phases and amounts of pathogen improvement; it can also change host confrontation, which leads to physiological variations of host-pathogen connections. The condition is more difficult by the fact that today; diseases are increasing globally. New diseases can transpire in places where they were formerly unknown, where there is no native ability to find proper medication.

Cultivation has a huge impact on the production of food, especially with the increasing population. The plant diseases are intimidating the yield of the crop. Plant diseases can have a major impact on decreasing crop production in farming and forestry. Initial discovery and identification of plant diseases oblige to take suitable actions.

There are numerous methods to identify plant pathologies. Some diseases do not have any noticeable indications related, or appear only when it is too late to act. In these circumstances, it is essential to accomplish refined examination, typically by resources of influential microscopes. In some circumstances, the marks can only be perceived in portions of the electromagnetic band that are not obvious to the naked eye.

*Address correspondence to this author at the Department of Information Technology, VNR Vignana Jyothi Institute of Engineering and Technology, Hyderabad, India; Tel: 0423042761; E-mail: dammavalam2@gmail.com

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Multi-Otsu's image segmentation for Mammograms using Artificial Bee Colony (ABC) Algorithm

Mamindla Ajay Kumar¹, Dr. Y Ramadevi²

¹Research Scholar, OU., Department of CSE, GCET.

Ajaymamindla.cse@gcet.edu.in

²Department of CSE, CBIT, Hyderabad
yrd@cbit.ac.in

Abstract:

Clear-cut image segmentation of mammogram images is indispensable in malignant tumor detection. This paper is attempted to propose a nature-inspired optimized method for mammogram image segmentation by adopting Otsu's multi-level thresholding algorithm as a fitness function into the ABC algorithm. Moreover, in image segmentation, Multi-level thresholding algorithms come across with insufficient exploration and low exploitation on search space. Hence, to solve this problem a Metaheuristic optimized algorithm is leveraged. This is achieved by using the ABC algorithm to explore the population space and exploit the specified population space to select the finest threshold values. Thereafter, the output of ABC is used to segment the mammogram image using the multi thresholding method. In this work, the proposed method is exercised with a total of nine images from the MINI MIAS database. Besides, to assess the performance of the proposed method different threshold levels are used to segment mentioned images. It was witnessed that the performance of the wished-for method is effective and efficient to segment the mammogram images in terms of measures like PSNR, SSI, and computational time.

Keywords: Artificial bee colony, Otsu, Multi-level Thresholding, Mammogram, Breast cancer

1. Introduction

1.1 Medical Image Segmentation

Mammogram images are currently most widely adopted technique in clinical practice to detect the breast cancer as it is easily accessible and cost-effective. For early detection of malignant tumors in mammogram images, many methods have been proposed [12]. Breast cancer mainly affects middle-aged women for different reasons. Over the past twenty years, several methods are demonstrated to segment the medical images like X-ray, CT (computed tomography)-scan, Magnetic Resonance Imaging (MRI) Mammogram, etc. [1]. Homogeneous gray level values of pictorial muscle in preprocessed mammogram images exhibits effective intensity. Cancer detection false positive rate depends on the accuracy of image segmentation [16]. Image segmentation increases the visibility of microcalcification in processed mammogram images. In computer vision algorithms image segmentation plays a significant role [6]. There are six types of image segmentation methods, threshold-based, Artificial Neural Network (ANN) based, edge-based, clustering-based, watershed-based, region-based, and PDE-based methods[8]. Thresholding is the most popular segmentation method in medical image processing. In the bi thresholding method, the grayscale image is divided into two intensities i.e forefront and background. But, multi thresholding divides the images into many homogeneous regions [13].

1.2 Otsu's Multi Thresholding

In automatic global threshold case studies, gray level images can be effectively segmented into bimodal (foreground or background) or multi classes using a non-parametric and unsupervised Otsu's thresholding algorithm. It is centered on a very simple idea: exhaustively search for the threshold that reduces the weighted within class variance defined as α_w^2 [22]. The class variances are given by (1) and (2) respectively

$$\alpha_0^2 = \sum_{i=0}^n (i - \mu_0)^2 \Pr(i/C_0) = \sum_{i=0}^n (i - \mu_0)^2 p_i / w_0$$

Three Point Boundary Value Problems Associated with First Order Fuzzy Difference Systems-Existence and Uniqueness via the Best Least Square Solution

N.Swapna¹, S. Udaya Kumar²

¹Department of Electronics and Computer Engineering, SreeNidhi Institute of Science and Technology Yamnampet(V), Ghatkesar, Telangana, INDIA

²Geetanjali college of Engineering and Technology, Cheeryala(V), Keesara(M), Medchal Dist. Telangana, INDIA.

Abstract:

This paper presents a criteria for the existence and uniqueness of solutions to first order fuzzy difference system using QR-algorithm. Modified QR-algorithm is presented for fuzzy linear systems using singular value decomposition.

Keywords: Fuzzy Difference Systems, Modified QR-algorithm, Fundamental matrix, Decode algorithm.

AMS(MOS) classifications 34B15,93B05,93B15

1. Introduction:

Existence and uniqueness of solutions to initial value problems have a long mathematical history going back to Picards. The mere fact that f is continuous on R ensures existence of at least one solution to the initial value problem

$$y' = f(t, y), \quad y(t_0) = y_0 \quad (1.1)$$

on R . The situation is different for boundary value problems. Length of interval estimates are necessary to prove existence and uniqueness of (1.1). If f satisfies a lipschitz condition in the second variable, then (1.1) has a unique solution. The situation is different for first – order difference system..

$$y_{n+1} = A(n)y_n + f_n, \quad y(n_0) = y_0, \quad (1.2)$$

where A is an $p \times p$ continuous matrix, whose elements $a_{ij}(n)$ are all real or complex valued functions defined on $N_{n_0}^+$ and $y_n \in R^p(C^p)$ with components $y_1(n), y_2(n), \dots, y_p(n)$, defined on $N_{n_0}^+$. The corresponding homogeneous equation corresponding to (1.2) is

$$y_{n+1} = A(n)y_n, \quad y(n_0) = y_0 \quad (1.3)$$

(1.3) possess a unique solution on $N_{n_0}^+$ as can easily be seen by induction.



UnderTracker: Generating Robust Binaries Using Execution Flow Traces

Rajesh Kumar Shrivastava¹ · Chittaranjan Hota²

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Abstract

Programs are developed in a manner so that they execute and fulfill their intended purpose. In doing so, programmers trust the language to help them achieve their goals. Binary hardening is one such concept that prevents program behavior deviation and conveys the programmer's intention. Therefore, to maintain the integrity of the program, measures need to be taken to avoid code-tampering. The proposed approach enforces code verification from instruction-to-instruction by using the programmer's intended control flow. *UnderTracker* implements execution flow at the instruction cache by utilizing the read-only data-cache available in the program. The key idea is to place a control transfer code in data-cache and call it from instruction cache via labels. *UnderTracker* injects labels into the binary without affecting the semantics of the program. After the code execution starts, it verifies every control point's legality before passing the control to the next instruction, by passively monitoring the execution flow. We proposed a cache-based monitoring method to verify code integrity. In this, we used side-channel information to monitor the program's execution state. This monitoring system uses a sliding window scheme to detect the violation of code integrity with high reliability. This paper proposes an efficient technique, called *UnderTracker* to strengthen the binary integrity of an I/O intensive running program, with the nominal overhead of only 5-6% on top of the normal execution.

Keywords Superblock · Execution flow verification · Systems security · Cache-based monitoring

1 Introduction

An adversary can tamper code via a malicious form of the binary (executable file) hosted by a third-party. An adversary can also install malicious binary by applying phishing attacks. There are some possible scenarios when code tampering exploits happen listed as follows:

1. An adversary can directly change the application binary through a phishing attack.
2. An adversary can exploit the resource within an application.

3. An adversary can exploit code to inject malicious payload.

The code tampering method leaves an impact on both ways, technical and business. The technological implications of code modification include password leaking, theft of identification, unauthorized modification of code. On the other hand, the firm is also gets affected by revenue loss and damage to reputation.

There are various application programs available over the internet, which contains a malicious payload. For example, games are the most popular in this category. If a user doesn't want to pay for the game, they use some short-tricks to achieve extra power or life. This bypass allows them to enjoy the game without pay. The adversary has also injected spyware to steal user's information in this type of game bypass technique. They can steal your important data like banking id and password.

One of the most lucrative attack vectors present in a binary is the code reuse attack, and therefore it becomes paramount to protect it. Existing protection methods such as stack canaries (Marco-Gisbert and Ripoll 2013), Data Execution Prevention (DEP) and Address Space

✉ Rajesh Kumar Shrivastava
rajesh5479@gmail.com

Chittaranjan Hota
hota@hyderabad.bits-pilani.ac.in

¹ Geetahnajali Collage of Engineering and Technology, Hyderabad, India

² Birla Institute of Technology and Science, Pilani, Hyderabad campus, India

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QMCP: QoS Aware Multi-Channel Path Discovery for End to End Data Transmission Over Cognitive Radio Ad Hoc Networks

Nagul Shribala^(1*), P. Srihari⁽²⁾, B. C. Jinaga⁽³⁾

- (1) ECE Department, Jawaharlal Nehru Technological University, India
- (2) ECE Department, Jawaharlal Nehru Technological University, India
- (3) ECE Department, Jawaharlal Nehru Technological University, India
- (*) *Corresponding author*

DOI: <https://doi.org/10.15866/irecos.v11i12.10978>

Abstract

ICT (Information and Communication Technology) trends are fast emerging and globally leading to the substantial demand of spectrum channels used for wireless networks. Cognitive Radio (CR) is an emerging technology solution that shall work on dynamic spectrum channel allocation. In cognitive radio ad hoc networks (CRAN), it is often difficult to establish the path among nodes with direct channel. Hence it is obvious to establish the path through the set of channels in sequence. The constraint is quality of service (QoS). Path establishment by the multiple channels in sequence needs a dynamic channel assignment for ensuring an optimum utilization of the available resources, whilst minimizing the interference in a network. In this paper, the emphasis is on Multichannel transmission Path with optimal QoS fitness for Cognitive Radio Networks. The proposed model is called QoS aware Multi-Channel Path (QMCP) discovery for end-to-end data transmission over CRAN. The QMCP performs the evolutions using adaptive genetic algorithm on the initial multichannel paths discovered in order to obtain the best fit path. The QoS metrics defined in our earlier contribution are used in fitness function. Results from the study reflect the robustness of the proposed model which could certainly

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Software Defined Radio with LFSR and Hard Decision based Viterbi Decoder

Alajangi Rama Krsihna, Balaji Narayanam , P. Srihari

Abstract:

This paper describes about Software Defined Radio (SDR) design for the prospect of testing the Bit-Error Rate (BER) and power analysis of digital communication schemes (ASK, FSK, BPSK) using Xilinx system generator. The design was implemented using Xilinx and MATLAB Simulink. This design describes the process of channelization as it exploits to low power and high efficiency applications in communication industry (such as wireless, satellite and cellular systems) and Digital Signal Processors. A SDR is defined as radio in which some or all of the physical layer functions are software defined. The SDR radio frequently has to load various signals depending on their requirements, which may use different source coding, modulation schemes, channel coding and demodulation schemes. The conventional hardware based radio devices have an extent on cross functionality and a slight flexibility in mounting multiple waveform with high hardware cost. This problem is solved by Software Defined Radio (SDR) architecture with Fibonacci Linear Feedback Shift Register and Viterbi Decoder.

Issue: 02-Special Issue

Year: 2018

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Original Paper | [Published: 06 September 2021](#)

The stability, structural, electronic, and optical properties of hydrogenated silicene under hydrostatic pressures: a first-principle study

[V. Kumar](#)  & [R. Santosh](#)

Journal of Molecular Modeling **27**, Article number: 278 (2021)

146 [Accesses](#) | [Metrics](#)

Abstract

The structural, electronic, and optical properties of hydrogenated silicene have been studied under different hydrostatic pressures using first-principle calculations. The binding energy and band structure have been calculated for chair (C-) and boat (B-) structures, which are having good stability at 0 GPa, 3 GPa, 6 GPa, 9 GPa, 12 GPa, 15 GPa, and

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Applied Materials Today

Volume 27, June 2022, 101435

Thermo-photodynamic perspective of the simultaneous S-Scheme ternary heterostructure through Ag₃VO₄ shuttle for the increased photo-redox ability

Aneek Kuila ^a, Santosh Routu ^b, Pichiah Saravanan ^a ✉, Chuanyi Wang ^c, Detlef Bahnemann ^{d, e}

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Highlights

- A hierarchical directional heterojunction among InVO₄-Ag₃VO₄-gC₃N₄ was synthesised.
- DFT calculation revealed the agnostic interaction where Ag₃VO₄ acted as a bonding bridge and charge-transfer mediator.
- Induced redox ability of the constituents increased the thermo-photocatalytic property.
- A simultaneous S-scheme charge transfer is observed during the exciton transfer.

Abstract

A binary heterostructure bearing Ag₃VO₄ and InVO₄ is deposited over a 2D gC₃N₄ nano-bed through a multistep hydrothermal technique. Though the synthesis is non-directional, the formation of the junction is governed through Ag₃VO₄ acting as a shuttle for charge transfer between InVO₄ and gC₃N₄. Vacant d-orbital in the Ag₃VO₄ accommodated the incoming □ electrons from gC₃N₄ forming a covalent bond through Agostic interactions and was as

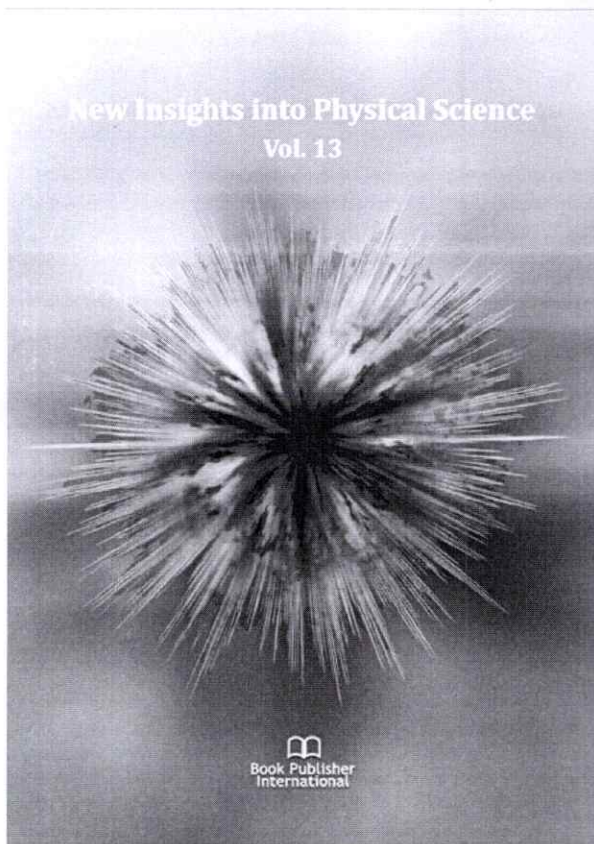
New Insights into Physical Science Vol. 13

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(<https://stm.bookpi.org/NIPS-V13/issue/view/51>) **A Frame Work for Decimal Floating Point Multiplier Using Vinculum Multipliers**

G. Sreelakshmi ; Kaleem Fatima ; B. K. Madhavi

New Insights into Physical Science Vol. 13, 27 February 2021, Page 152-162

<https://doi.org/10.9734/bpi/nips/v13/6866D> (<https://doi.org/10.9734/bpi/nips/v13/6866D>)

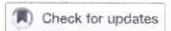
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A Novel MAC Protocol with Fusion Center and Adaptive Full-Duplex Communication for Cognitive Radio Networks

Appala Raju Uppala ^{1,2}, C. Venkata Narasimhulu ³ and K. Satya Prasad ^{4*}

¹Department of ECE, Jawaharlal Nehru Technological University, Kakinada, India; ²Geethanjali College of Engineering and Technology, Hyderabad, India; ³LORDS Institute of Engineering and Technology, Hyderabad, India; ⁴Vignan's Foundation for Science, Technology & Research, Guntur, India

ABSTRACT

Cognitive radio network is an intelligent and adaptive communication technology used to effectively utilize the radio spectrum to provide better communication. It enables the secondary (unlicensed) users to communicate over vacant channels without disrupting the communication of the primary (licensed) users. This paper proposes a novel contention-free MAC protocol for full-duplex and half-duplex cognitive radio networks. A novel concept of a fusion center-based channel allocation scheme is proposed to provide better channel allocation and reduced energy consumption. The proposed technique is compared with the existing techniques in terms of the average number of channels being sensed by each user, average wait time, collisions, throughput, and average energy consumption. The number of collisions increases as the maximum allotted time of communication increases in existing approaches. The experiment is performed with 20, 40, 60, and 80 s. The existing approaches show for 20 s, the number of collisions is 65, 61, 68, and 62; for 40 s, the number of collisions is 93, 96, 95, and 92; for 60 s, the number of collisions is 122, 126, 133, and 130; for 80 s, the number of collisions is 176, 170, 173, and 175. The proposed method approaches the number of collisions will become zero as the maximum allotted time of communication increases. The experimental results show that the proposed approach performs better than existing approaches. Moreover, it can be observed that the average waiting time of secondary users when a collision occurs is reduced with the application of a fusion center-based channel allocation scheme.

KEYWORDS

Cognitive radio network; Dual-threshold; Full-duplex; Fusion center; Half-duplex; MAC protocol; Spectrum sensing

1. INTRODUCTION

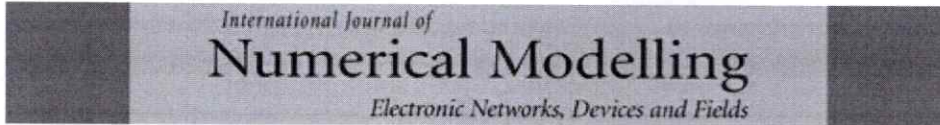
The traffic encountered by the current day cellular network is huge due to the sharp increase in the use of mobile devices. This phenomenon raised attention towards determining appropriate outcomes for better usage of the spectrum. The cognitive radio network (CRN) and full-duplex (FD) mode of communication can provide an effective solution to the growing traffic and achieve maximum spectrum utilization [1]. These technologies majorly concentrate on increasing the utilization of the spectrum and efficiency of the network. Research has to be carried out on adaptive broadcasting techniques at the physical and MAC layers in both traditional networks and cognitive radios.

Generally, the CRN is non-time slotted. Hence, the transmission over the channels need not be continuous. The users can become active at any point of time after being inactive. Classical spectrum sensing strategies like listen before talk (LBT) is example of non-time slotted

networks. Such techniques generally fail to transmit the data without collisions in turn reducing the integrity of the model. This leads to collisions on a large scale when the primary users take over the channel or become active. Some of the studies in [2–5] projected the FD spectrum sensing for resolving this issue. In such approaches, the broadcasting secondary user maintains the sensing of the licensed users steadily all along the broadcasting slot, and after identifying the signal of the licensed user, the transmission gets paused to avoid collision [2]. Such techniques increase the security risks and thus the throughput of the system reduces as the collision causes the data corruption and the sender has to resend the data.

The dynamic utilization of the spectrum provided by the CRN has proved to be useful in allotting the spectrum effectively to the secondary users' (SUs) when the channels are idle [6, 7]. False detection of the channels will lead to the collision on the return of the primary users' (PUs) [8]. To improve the performance of the CRN sys-

*Present address: Department of ECE, Jawaharlal Nehru Technological University, Kakinada, India



RESEARCH ARTICLE

Carrier transport mechanism in bottom gate thin-film transistor with SnO as active layer for CMOS displays

Vallisree Sivathanu, Trupti Ranjan Lenka ✉, Vishal Goyal, Hieu Pham Trung Nguyen

First published: 11 November 2021

<https://doi.org/10.1002/jnm.2975>

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Brain Tumor Segmentation, Detection and Grading in MRI Images

Kethu Sneha Latha¹Yepuganti Karuna²Saladi Saritha³

^{1,2}School of Electronics and Communication Engineering, Vellore Institute of Technology, Vellore,
³Geethanjali College of Engineering and technology, Hyderabad, Telangana.

E-mail: kethusnehalatha@gmail.com¹, karun@vit.ac.in², saritha.saladi3188@gmail.com³

Abstract:

The most common malignant brain tumours are gliomas, and they come in a variety of grades, each of which has a significant impact on the patient's chance of survival. Magnetic resonance imaging (MRI) tumour grading and segmentation are normal and crucial for treatment preparation and diagnosis. A deep learning approach was developed to meet this clinical need, that associates tumour segmentation using U-net which is a convolutional neural network (CNN) and tumour grading using transfer learning using a Vgg19 and a completely associated classifier. T1-postcontrast, FLAIR and T1-precontrast MRI images of 110 patients with LGG were used to train and evaluate. DSC for segmentation model's and tumour detection accuracy are 0.875 and 0.937, correspondingly. At the MRI image level, the grading model classifies LGG with specificity, accuracy, sensitivity, and of 0.922, 0.907, and 0.893, correspondingly. In MRI images this study shows conventional tool for automated and simultaneous LGG tumour segmentation, detection, and grading in clinical settings.

Keywords: Glioma, Segmentation, Magnetic resonance imaging, Classification, Grading, Brain tumor.

I. INTRODUCTION

The most common malignant brain tumours are gliomas [1], through various grades based on tumour malignancy and growth rate [2]. Gliomas are categorised by the World Health Organization (WHO) into four grades [2,3]. Astrocytoma, oligoastrocytoma, and oligodendroglioma are some of the histological types of LGG. Grades of gliomas, as well as tumour location, shape, and size, are crucial in determining existence and treatment options [4]. As a result, designing conventional techniques to automate tumour segmentation and grading to improve patient results would be advantageous.

MRI is a non-invasive brain imaging technique that can deliver accurate images of the brain. As a result, it's widely used for tumour characterization and diagnosis. Brain tumour segmentation

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Abstract

In this work, we report on four tin monoxide (SnO) thin-film transistor (TFT) grain boundary (GB) models of carrier transport considering the native defects in the thin film, interface traps, and GB deep/tail states. The changes in the activation energy and the GB barrier potential on the application of gate electric field are thoroughly investigated. The shift in Fermi level and the charge carrier transport mechanisms are examined for the two-channel model by the application of external potential. Four models are developed to study the impact of phase transformation of SnO material on the TFT characteristics. Among the four developed models which are considered as four different cases, Case (iv) shows excellent performance and the simulation results revealed that the location of Fermi level closer to the mid gap are suggested to favor the ambipolar behavior. Also, the influence of SnO material thickness and the effect of different dielectrics on the ambipolar device characteristics are examined aiming at optimized performance of the device. The developed optimized model will help the process engineers in tuning the SnO material parameters for achieving better performance in both p-type and n-type TFTs when employed in CMOS based displays.

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DATA AVAILABILITY STATEMENT

Data sharing not applicable to this article as no datasets were generated or analysed during the current study.

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Original Contribution | [Published: 08 October 2021](#)

Implementation of an Adaptive Neural Network-Based Controller for Improving the Conversion Efficiency of Solar Photovoltaic Module


Kakarla Deepti , [P. Srihari](#) & [K. Manjunath Achari](#)

Journal of The Institution of Engineers (India): Series B
103, 477–489 (2022)

37 Accesses | [Metrics](#)

Abstract

This research article proposes an intelligent artificial neural network-based fuzzy logic controller developed for tracking the exact maximum power point (MPP) under varying conditions of temperature and irradiance. The hybrid soft computing method combines learning abilities of an adaptive artificial neural network (ANN) and incremental conductance algorithm (INC)-based fuzzy logic controller (FLC) to handle uncertain data. The adaptive neural fuzzy inference system (ANFIS) is trained with the dataset generated for output voltage, current and all possible varying conditions to estimate the duty cycle of converter as maximum power point capturing device. ANFIS is developed in Takagi–


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International Journal of Energy Research / Volume 45, Issue 7 / p. 10527-10537

RESEARCH ARTICLE

Modeling and performance optimization of two-terminal Cu₂ZnSnS₄-silicon tandem solar cells

Vallisree Sivathanu, Thangavel R, Trupti Ranjan Lenka ✉

First published: 14 February 2021

<https://doi.org/10.1002/er.6540>

Citations: 1

Summary

A dual-junction Cu₂ZnSnS₄-Silicon (CZTS-Si)-based tandem configuration is modeled and analyzed for its viability as a solar cell. The top and bottom modules in the tandem structure are validated by comparison with experiment. Initially, the designed tandem structure yields very low efficiency of 3.18%, and the various loss mechanisms are identified and investigated. The current mismatch between top and bottom cells and parasitic absorption (photon losses) are suggested to be the major causes limiting the short circuit current and hence the efficiency of the device. We optimize the material parameters within experimentally achievable limits in order to obtain current matching, and the optimized thicknesses of copper zinc tin sulfide (CZTS) and silicon (Si) absorbers are found to be 150 nm and 250 μm, respectively. The simulation results revealed that the photon losses are reduced, and overall absorption in the longer wavelength region has enhanced with the replacement of cadmium sulfide (CdS) by zinc sulfide (ZnS) buffer and careful optimization of the front layers of the device. The maximum predicted efficiency of tandem structure is >20% by minimizing the recombination centers within the experimentally obtainable ranges and improving the carrier separation process.

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DATA AVAILABILITY STATEMENT

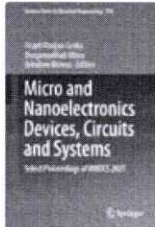
The data that support the findings of this study are available from the corresponding author upon reasonable request.

Citing Literature

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Micro and Nanoelectronics Devices, Circuits and Systems pp 227–236

Performance Analysis of HIT-CZTS Tandem Solar Cell Towards Minimizing Current Losses

Sivathanu Vallisree & Trupti Ranjan Lenka

Chapter | First Online: 10 September 2021

497 Accesses

Part of the Lecture Notes in Electrical Engineering book series (LNEE, volume 781)

Abstract

In this work, we report on Heterojunction with intrinsic thin layer-Cu₂ZnSnS₄ (HIT-CZTS) tandem solar cell modelled using Silvaco TCAD simulator. Initially the HIT and the CZTS solar cells are modelled and validated. Then the tandem structure is designed using HIT as bottom module and CZTS as top module and various loss mechanisms are investigated. From the simulation study, it is revealed that current mismatch among the top and bottom modules has contributed to low short-circuit current density and hence the efficiency of


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Improved Convolutional Neural Network Based Cooperative Spectrum Sensing For Cognitive Radio

Appala Raju Uppala^{1*}, Venkata Narasimhulu C², and Satya Prasad K³

¹ Research Scholar, Department of ECE, Jawaharlal Nehru Technological University
Kakinada Andhra Pradesh, India

Associate Professor, Geethanjali College of Engineering and Technology,
Hyderabad, Telangana, India

[e-mail: rekharajuppala2009@gmail.com]

² LORDS Institute of Engineering and Technology, Hyderabad,
Telangana, India

[e-mail: narasimhulucv@gmail.com]

³ Vignan's Foundation for Science, Technology & Research
Guntur, India

[e-mail: prasad_kodati@yahoo.co.in]

*Corresponding author: Appala Raju Uppala

*Received October 24, 2020; revised January 29, 2021; accepted May 16, 2021;
published June 30, 2021*

Abstract

Cognitive radio systems are being implemented recently to tackle spectrum underutilization problems and aid efficient data traffic. Spectrum sensing is the crucial step in cognitive applications in which cognitive user detects the presence of primary user (PU) in a particular channel thereby switching to another channel for continuous transmission. In cognitive radio systems, the capacity to precisely identify the primary user's signal is essential to secondary user so as to use idle licensed spectrum. Based on the inherent capability, a new spectrum sensing technique is proposed in this paper to identify all types of primary user signals in a cognitive radio condition. Hence, a spectrum sensing algorithm using improved convolutional neural network and long short-term memory (CNN-LSTM) is presented. The principle used in our approach is simulated annealing that discovers reasonable number of neurons for each layer of a completely associated deep neural network to tackle the streamlining issue. The probability of detection is considered as the determining parameter to find the efficiency of the proposed algorithm. Experiments are carried under different signal to noise ratio to indicate better performance of the proposed algorithm. The PU signal will have an associated modulation format and hence identifying the presence of a modulation format itself establishes the presence of PU signal.

Keywords: Cognitive radio, Cooperative spectrum sensing, Primary user, Simulated annealing, Neural network.

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Original Research Article | Published: 21 February 2022

Modeling and Simulation of CZTS Thin-Film Solar Cell for Efficiency Enhancement

Rabin Paul, S. Vallisree, T. R. Lenka  & F. A. Talukdar

Journal of Electronic Materials **51**, 2228–2235 (2022)

160 Accesses | [Metrics](#)

Abstract

CZTS solar cells have been utilized as a replacement for CIGS and CdTe solar cells in thin-film technology. With the better absorption coefficient of this material, it has achieved efficiency higher than 13%. In this work, the performance of a CZTS thin-film solar cell (TFSC) is analyzed by replacing intrinsic ZnO (i-ZnO) with Mg-doped ZnO as window layer material. i-ZnO has good optical and electrical characteristics, but the optical, electrical,

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PREDICTION OF BIOACTIVITY OF PHYTOCHEMICALS IN *Anethum graveolens* – AN *in silico* APPROACH

J. V. MADHURI*, K. SATISH AND LNS PRAKASH GOTETI

Geethanjali College of Engineering and Technology, Cheeryal, Hyderabad, India [JVM, KS]

Tech Mahindra Limited, Hyderabad, India [JVM, KS, LPG]

[* For Correspondence: E-mail: jvmadhuri.fe@gcet.edu.in]

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Original Research Article

ABSTRACT

Anethum graveolens is a popular herb widely used as flavouring agent and it yields essential oil. It is rich in polyphenols which exhibit antioxidant and carminative properties. In this work, phytochemical screening is performed to establish the presence of terpenoids, flavonoids and tannins etc. In food products, lipid peroxidation is common and to prevent it synthetic antioxidants like butylated hydroxyanisole (BHA), butylated hydroxytoluene (BHT) are used and they are carcinogenic in nature. So, there is an increasing demand for plant derived antioxidants. *Anethum graveolens* is a plant rich in antioxidants and the present study predicts the antioxidant and bioactivity of Limonene, Carvone, α -Phellandrene, Dillapiol, Geraniol and p-Cymene. *In silico* studies were carried out using PASS prediction tool and the bioactive compounds were predicted with $Pa > 0.7$. For these compounds, the bioactivity score is calculated and their potential medicinal value is discussed using Lipinski's rule of 5 analysis. From the study, it is observed that all the compounds have bioactivity and are potential antioxidants that may be used in health care, cosmetic and food and beverage industry.

Keywords: *Anethum graveolens*; bioactivity spectrum; phytochemical screening; bioactivity score; Lipinski rule of 5.

INTRODUCTION

Anethum graveolens (Dill) is an herb that belongs to the family of apiaceae. The genus name *Anethum* is originated from the Greek word aneeson or anecton, i.e strong smelling. It originates from the Mediterranean and West Asia [1]. *A. graveolens* is popularly known as Dill or

shapt. It is cultivated across the world and is known for its flavouring and curative properties. The experimental studies demonstrated the antimicrobial, stomachic, antioxidant, and carminative properties of Dill [2-5]. Flowers and leaves have high content of polyphenols when compared to fruits and hence are used for extracting essential oil.

20-21-311

A Framework for Developing Intellectual Property Perspective among Computer Science Students

Dr. J V Madhuri

Associate Professor

Geetanjali College of Engineering and Technology,
Cheeryal, Hyderabad

LNS Prakash Goteti

Principal Consultant in AI and Analytics

Tech Mahindra Limited,
Bahadurpally, Hyderabad

Corresponding Author: **Dr J V Madhuri**

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Abstract

Intellectual property rights are being discussed and have become as policy issues in this era of knowledge. Every organization, industry in every sector is striving hard to protect, create, and convert their intangible assets to tangible ones through intellectual property rights. In this scenario, young students comprising majority work force of information technology field are to be sensitized about intellectual property rights at the beginning of their career. With this background, as a facilitator of this course a frame work was developed to impart intellectual property rights education to computer science students. This paper discusses how students are introduced to concepts in a unit wise manner and as the course makes progress, how challenges are dealt pedagogically to reach the outcomes of the course.

Key words: Intellectual property rights, pedagogy, information technology, learning goals, critical thinking.

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Hard core proof of the polyvinyl alcohol as a reducer for the formation of gold nanoparticles

Anurag Gautam^{a,c,*}, Pragya Komal^{b,*}, Ram Sevak Singh^c, Prabhat Gautam^d, S.K.V. Manjari^b, R.S. Ningthoujam^{e,*}^a Department of Chemistry, Geethanjali College of Engineering and Technology, Cheeryal, Hyderabad, Telangana 501301, India^b Department of Biology, Birla Institute of Technology and Science, Pilani-Hyderabad Campus, Jawaharnagar, Shamirpet Mandal, Hyderabad, Telangana 500078, India^c School of Science, O. P. Jindal University, Raigarh 496001, Chhattisgarh, India^d Department of Chemistry, CMR Institute of Technology, Bengaluru, Karnataka 560037, India^e Chemistry Division, Bhabha Atomic Research Centre, Mumbai 400085, India

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TGA

ABSTRACT

In this paper, we report the direct synthesis of water dispersed gold nanoparticles encapsulated in polyvinyl alcohol (PVA), which acting as reducer to gold ion to gold metal and capping agent. The syntheses of the gold nanoparticles were carried with the direct addition of the aqueous HAuCl₄ solution to aqueous PVA solution at 50 °C. Initially, the PVA solution was prepared by using 2 g of PVA per 100 ml of distilled water in a round bottom flask which was placed in oil bath placed over the magnetic stirrer. Subsequently, the aqueous solution HAuCl₄ was added drop-wise to the PVA solution. Afterward, the solution was made viscous by heating at same temperature and casted in form of nanocomposites films. Various compositions of HAuCl₄ (0.2 wt%, 0.5 wt%, 1.0 wt% and 1.5 wt%) with respect to PVA (films of Au-PVA nanocomposites) were prepared. Upon drying in ambient condition these films were analyzed with XRD, SEM, EDX, TGA, UV-Visible, and IR techniques. The XRD analysis reveals the fcc crystal structure with crystallite size nearly 22 nm. The crystallite size is in agreement with that obtained by SEM analysis which is in range of 25–30 nm and particles are nearly spherical in shape. Furthermore, the UV-visible analysis showed the surface plasmon resonance (SPR) band at ~ 550 nm which confirmed the formation of gold nanoparticles. It is further supported by the EDX analysis that showed the gold peaks in the spectrum.

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1. Introduction:

Noble metal nanoparticles had an increased attention over the last decade and still fascinating the researcher to greater extent due to their unique photochemical properties [1–7]. In particular the gold nanoparticles have been unique characteristics such as tunable localized surface plasmon resonance enable them wide variety of application such as Förster resonance energy (FRET) sensor, photo-thermal therapy (PTT), catalysis, electronics, and energy storage devices [5–9]. For instance, spherical gold nanoparticles have extensively used in the FRET process because of no dipole moment it can interact with the donor from all faces in the visible region [9]. On the other hand the gold nanorods had been used as the sensor over wide range from visible to near infrared region due

to their tunable wavelength spectrum. Moreover, the PTT application of gold nanoparticles is due to the exceptionally high absorption cross-section through surface plasmon resonance (SPR) compared to the bulk gold that result in increase the localized temperature which is essential principle of the cancer treatment process [10]. All these properties are dependent on the size and shape of the nanoparticles, therefore, to control the size and the shape of the gold nanoparticles many methods have been used [11]. For instance, the chemical reduction method in which the gold ions are reduces to gold atoms with the application of suitable reducing agent. Commonly, used reducing agents are NaBH₄, hydrazine, and gaseous hydrogen [11–15]. Moreover, green synthesis process has also been developed in which the nature of the reducing agent was mild and the sources of the reducing agents were green plants [16]. Additionally, in a polyol process the reduction of the metal ions to metal were achieved by using the different molecules containing the OH functional group such as ethylene

* Corresponding authors.

E-mail addresses: ganurag13@gmail.com, anurag.fe@gcet.edu.in (A. Gautam), pragya@hyderabad.bits-pilani.ac.in (P. Komal), rsn@barc.gov.in (R.S. Ningthoujam).<https://doi.org/10.1016/j.molliq.2021.116112>

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Geethanjali College of Engineering and Technology
(Autonomous)
Cheeryal (V), Kosasa (M), Medchal Dist. (T.S.) - 501301

RESEARCH ARTICLE

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Synthesis, biological evaluation and docking studies of 1,2,4-oxadiazole linked 5-fluorouracil derivatives as anticancer agents

Ravi Kumar Bommerra¹, Shashikala Kethireddy², Rajeshwar Reddy Govindapur³ and Laxminarayana Eppakayala^{1*}

Abstract

Background: 1,2,4-oxadiazole derivatives exhibited significant anti-cancer activity when they were evaluated, against human cancer cell lines. They also showed anti-inflammatory, analgesic, diabetic, immunosuppressive, $\alpha_2\beta_2$ -receptor antagonist, antimicrobial, anti-helminthic, histamine-H3 and antiparasitic properties. A pyrimidine analog, 5-fluoro-uracil is a chemotherapeutic drug used for treating multiple solid malignant tumors. But its application is limited, as it has side effects like low bioavailability and high toxicity. Molecular docking is an exemplary tool, helps in identifying target and designing a drug containing high bio-availability and minimum toxicity.

Results: A set of 1,2,4-oxadiazole linked 5-fluorouracil derivatives (7a–j) were synthesized and their structures were confirmed by ¹HNMR, ¹³CNMR and Mass spectral analysis. Further, these compounds were investigated for their anti-cancer activity towards a panel of four human cancer cell lines such as (MCF-7, MDA MB-231), lung cancer (A549) and prostate cancer (DU-145) by using MTT method. Among them, compounds 7a, 7b, 7c, 7d and 7i demonstrated more promising anticancer activity than standard.

Conclusion: Synthesized derivatives (7a–j) of 1,2,4-oxadiazole linked 5-fluorouracil and investigated for their anticancer activity towards a panel of four human cancer cell lines.

Keywords: 5-Fluorouracil, Ataluren, Pyrimidine, Oxadiazole and anticancer activity

Background

Over the past few decades, heterocyclic rings containing nitrogen atoms have played a significant role in medicinal chemistry. They are considered as key templates for the development of new therapeutic agents [1]. Among all the nitrogenated compounds, pyrimidines are a more privileged class of six-membered heterocyclic organic units. They occupy a unique position in medicinal chemistry due to their wide range of biological applications [2–12]. Pyrimidines exist as an essential component in several

nucleic acids and therapeutic drugs, such as 5-Fluorouracil (1, 5-FU, Fig. 1) [13–16]. The USFDA-approved drug, 5-FU, is one of the most distinguishable chemotherapeutic drugs available. It was first synthesized by Heidelberger and co-workers [17]. It shows antitumor activity by inhibition of thymidylate synthetase enzyme leading to prevention of DNA synthesis [18], and has been used frequently for the treatment of various solid malignant tumors [19–21]. However, it has limited clinical applications because of several side effects, including poor tumor selectivity, toxicity, lower drug-resistance, gastrointestinal toxicity, and adverse effects on central nervous system [22, 23]. Previously, many researchers have developed several 5-FU contained compounds to overcome

*Correspondence: elxnkits@yahoo.co.in

¹ Sreenidhi Institute of Science and Technology (Autonomous), Yamnampet, Ghatkesar, Hyderabad, Telangana, India

Full list of author information is available at the end of the article



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20-21-35

The pK_a of Pentazole (HN_5)

Sanjeev Rachuru,^A Jagannadham Vandanapu,^{B,D} and Adam A. Skelton^C

^ADepartment of Chemistry, Geethanjali College of Engineering and Technology, Cheeryal-501301, Telangana, India.

^BDepartment of Chemistry, Osmania University, Hyderabad-500007, India.

^CDepartment of Pharmacy, School of Health Science, University of KwaZulu-Natal, Durban 4000, South Africa.

^DCorresponding author. Email: jagannadham1950@yahoo.com

Pentazole having the molecular formula HN_5 is an archetypical five-membered homocyclic inorganic aromatic molecule consisting of five nitrogen atoms. A hydrogen atom is bonded to one of the nitrogens. Even though the molecule does not contain a carbon it appears last in the series of the heterocyclic azole family; the family containing one to five nitrogen atoms. This series of heterocyclic azoles is pyrrole, imidazole, pyrazole, triazole, tetrazole, and the last one is the pentazole. Barring pentazole, the rest of the members of the azole family are heterocyclic organic molecules. The pK_a of $N(1)H$ -acidity values of all the azole members are known, except for that of pentazole. In the present work we endeavoured to determine the pK_a of pentazole by a graphical method and by performing theoretical DFT calculations.

Keywords: pentazole, pK_a , DFT.

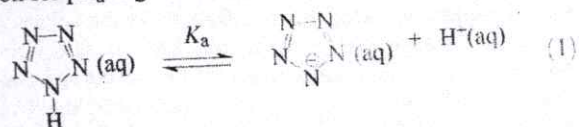
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Introduction

The chemistry of pentazole has a long debatable history.^[1-11] A century ago, the preparation of its silver salt AgN_5 was reported by Lipschitz^[1] and later it was refuted by Curtius et al.^[2] Though the X-ray crystal structure of a related compound, 4-dimethylaminophenylpentazole was reported,^[3] the synthesis of pentazole HN_5 was not.^[4] Subsequently, several papers appeared in the literature regarding pentazole and its substituted compounds reporting on their various aspects like their stability and its existence.^[5-11] The pK_a of pentazole has not been reported either by experiment, owing to its instability, or by theory in any of the earlier research articles. The only small report that appeared regarding the pK_a was by Katritzky et al.^[12] Owing to the difficulty in the synthesis of pentazole (if at all synthesised it is in a metastable state), the experimental pK_a has not been reported so far. This was the motivation to carry out theoretical studies. The theoretical study reported here sheds light on the fact that the pK_a determined by extrapolation method might not be correct. Further it is proposed that the pK_a values determined by SMD_{SSAS} (a solvation model based on a density-scaled solvent-accessible surface model) appear to be correct.

It is known that pK_a is the negative logarithm of K_a , the equilibrium constant of the acid dissociation reaction $HA \rightleftharpoons A^- + H^+$ in aqueous solution. In any graduate laboratory, experimental methods, like potentiometry, conductometry, and UV-visible spectroscopy, are available to determine the equilibrium constant K_a . The acid dissociation constant K_a is the quantitative measure of the strength of an acid in solution; yet the symbol pK_a , which is the negative logarithm of K_a , is more commonly used. At equilibrium, in the acid dissociation reaction

$HA \rightleftharpoons A^- + H^+$ the concentrations of HA , A^- , and H^+ will not change with the passage of time because the rates of the forward and backward reactions are equal.^[13] The acid dissociation reaction $HA \rightleftharpoons A^- + H^+$ for pentazole is shown in Eqn 1, the equation for K_a is given in Eqn 2, and the subsequent equation for pK_a is given in Eqn 3.



$$K_a = \frac{[A^-][H^+]}{[HA]} \quad (2)$$

$$pK_a = -\log_{10} K_a = \log_{10} \frac{[HA]}{[A^-][H^+]} \quad (3)$$

Methods

All the linear correlations were done using the *KaleidaGraph* software (Reading, PA, USA). The chemical structures were drawn using *Chemdraw*. *Gaussian 09* software was utilised for theoretical calculations.^[14] Density functional theory (DFT) was used to calculate the pK_a values. The reactant and the products were optimized and frequency calculations were performed using the *wB97XD*^[15] and *B3LYP* functional with 6-311+g(d,p) basis set. pK_a values were determined using the SMD continuum model. The pK_a values were determined by both default SMD (solvation model based on density) and SMD_{SSAS} (scaled solvent-accessible surface). Here the

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VARIOUS TECHNOLOGICAL PROCESSES

Enhanced Optical and Electrical Properties of Graphene Oxide-Silver Nanoparticles Nanocomposite Film by Thermal Annealing in the Air

Ram Sevak Singh^{a,b,*}, Aseem Rasheed^b, Anurag Gautam^c, Arun Kumar Singh^d, and Varun Raie

^a Department of Physics, O P Jindal University, Raigarh, Chhattisgarh, 496109 India

^b Department of Physics, National Institute of Technology Kurukshetra, Haryana, 136119 India

^c Department of Chemistry, Geethanjali College of Engineering and Technology, Cheeryal, Hyderabad, Telangana, 501301 India

^d Department of Pure & Applied Physics, Guru Ghasidas Vishwavidyalaya, Bilaspur, Chhattisgarh 495009 India

^e School of Materials Science and Engineering, Nanyang Technological University Block N4.1, Nanyang, 639798 Singapore

*e-mail: singh915@gmail.com

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Abstract—Here, we report the enhanced optical and electrical properties of graphene oxide-silver nanoparticles (GO-AgNPs) nanocomposite due to thermal annealing in air at different temperatures (150, 250, and 350°C). Our findings show that the optical properties of the GO-AgNPs film strongly depend on the annealing temperature. With an increase in annealing temperature, the optical absorption band and photoluminescence (PL) band are monotonically shifted towards a longer wavelength with a slight increase in absorbance. Interestingly, annealing of the nanocomposite film at 350°C in the air results in the nitrogen-doping from air into GO lattice. Unlike the PL bands in the near-ultraviolet (UV) range in cases of GO-AgNPs annealed at 150 and 250°C, this film exhibits pronounced multiple PL bands in the visible range, which are attributed to optical transitions associated with the localized nitrogen defects incorporated from air under thermal annealing and charge transfer between AgNPs and carbon. Mechanisms of the observed optical properties are also discussed. Furthermore, thermal annealing of the film also affects its electrical properties. The sheet resistance of the film reduces with the increase of annealing temperature and its lowest value ~ 21 Ω/□ with transmittance ~ 82% at 550 nm is achieved at 350°C.

Keywords: Thermal annealing in air, nitrogen-doped graphene oxide-silver nanoparticles, transparent conductive electrode, photoluminescence

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INTRODUCTION

Graphene has been recognized as a promising material that could be utilized in many areas that include electronics, optoelectronics, energy, and biochemistry [1–10]. However, experimentally synthesized pure graphene has some limitations such as lack of band gap in sp² hybridized structure, high sheet resistance [1], and less pronounced luminescence [11]. Modification of graphene structure is therefore needed to extend its effective utilization in various application sectors. Chemi-

cally synthesized graphene oxide (GO), in this scenario, has been an attractive and basic material. GO consists of sp² bonded carbon atoms with a large fraction of sp³ hybridized carbon atoms bound to oxygen-related functional groups. GO is an insulator and reduction of GO is demanded to make it conductor or semiconductor which are key materials used in electronic and optoelectronic devices. The reduction of GO indicates the increase of sp² contents and materials tend to transform from insulating GO to conducting graphene structure [12]. Ag nanoparticles (AgNPs) have been widely used to fab-

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Research Article

Molecular docking studies of *Chenopodium album* Linn with Lanosterol synthase enzyme

Jupudi Vasantha Madhuri*

Geethanjali College of Engineering and Technology, Cheeryal, Hyderabad- 501301 (Telangana), India

LNS Prakash Goteti

Tech Mahindra Limited, Hyderabad- 500043 Telangana), India

*Corresponding author. Email: jvmadhuri.fe@gcet.edu.in

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Abstract

Cardiovascular diseases (CVD) are the major cause of death among people across the globe. Hypercholesterolemia is one of the major contributing factors for CVD. Molecules that bind with Lanosterol synthase enzyme, can be potential drug targets. Statin group of compounds like Simvastatin, cerivastatin, Atorvastatin etc., used for treating hypercholesterolemia have side effects and hence there is a growing demand for plant derived flavonoids. This work focusses on studying the compounds quercetin-3-O-(2",6"-di-O- α -L-rhamnopyranosyl)- β -D-glucopyranoside, kaempferol-3-O-(2",6"-di-O- α -L-rhamnopyranosyl)- β -D-glucopyranoside, rutin; quercetin-3-O- β -D-glucopyranoside (iso quercetin); and kaempferol-3-O- β -D-glucopyranoside (Astragaloin) present in *Chenopodium album* Linn to inhibit Lanosterol synthase. Bioactivity score, drug likeness character was assessed *in silico*. Based on bioactivity spectrum, it is observed that the molecules are biologically active and the probability of these compounds to be biologically active is ranging from 0.784 to 0.992, suggesting that these compounds are effective for treating hypercholesterolemia. In the molecular docking studies, the compounds binding affinity score was in agreement that the molecules have the potential to be used as an alternative to the statin group of compounds in treating cholesterol.

Keywords: Bioactivity, *Chenopodium album*, Hypercholesterolemia, Lanosterol synthase enzyme, Molecular docking

INTRODUCTION

Ethnomedicinal plants remain largely unexplored and there is a good scope for researchers and food processors to bring out these economical, easily grown plants to the mainstream food basket (Pala *et al.*, 2019., Salmerón-Manzano Esther *et al.*, 2020). *Chenopodium album* Linn, is one such plant with good nutritive value (fibre, fatty acids and minerals). In India, it is called as Bathua and it belongs to Amaranthaceae family and *Chenopodium* genus (Bajwa Ali *et al.*, 2019). *C. Album* is rich in flavonoids that play an important role in its pharmacological and therapeutic properties. Flavonoids are phenolic compounds possessing a wide spectrum of biological activities and are studied for anti-cancer and reducing the risk of cardiovascular diseases caused by oxidative stress (AlexanderVictor *et al.*, 2016, Thilakavathy Thangasamy *et al.*, 2009). *C. Album* has been found to possess the bioflavonoids, Quercetin and Kaempferol derivatives (Gohar and Elmazar 1997,

Cuttillo *et al.*, 2006, Laghari *et al.*, 2011) Hypercholesterolemia is considered as one of the factors for coronary heart diseases. Chemically synthesised drugs used to treat hypercholesterolemia contain statin group that on prolonged use causes muscle weakness, memory loss and inhibits coenzyme Q10 important for electron transfer in mitochondria (Wagstaff *et al.*, 2003, Jamolowicz Al *et al.*, 2015). In this context, it is highly relevant to focus on plant derived flavonoids that are effective in treating hypercholesterolemia. Lanosterol synthase, also known as lanosterol cyclase, is a microsomal enzyme and a target for drugs lowering cholesterol (Telford *et al.*, 2005, Vanessa *et al.*, 2018). The potential anti-cholesteremic drug binds to the active sites of the Lanosterol synthase enzyme and inhibits it. To establish a plant derived flavonoid as a potential bioactive compound, it is important that we screen it theoretically and know its pharmacological and binding properties. In the present work, we carried out *in-silico* calculation

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Effect of BaTiO₃ phase on frequency dispersion characteristics of Mg_{0.48}Cu_{0.12}Zn_{0.4}Fe₂O₄ + BaTiO₃ nanocomposites

M. Kanaka Durga^{a,*}, P. Raju^b

^a Vignana Bharathi Institute of Technology, Aushapur, Ghatkesar, Hyderabad 501301, India

^b Geethanjali College of Engineering and Technology, RR Dist, Telangana 501301, India

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Keywords:

Nanocomposites
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ABSTRACT

Multiferroic nanocomposites of ferrite and ferroelectric phases with systematically varying composition (100-x) Mg_{0.48}Cu_{0.12}Zn_{0.4}Fe₂O₄ + xBaTiO₃ (MCZBT) (where, x = 0, 20, 40, 50, 60, 80, 100 mol%) were prepared for the first time by mechanical milling and sintering method. The presence of ferrite and ferroelectric phases in nanocomposite samples were confirmed by X-ray diffraction (XRD) while microstructural characterization was carried out by scanning electron microscopy (SEM). The average grain size, from SEM, was found to be in the range 80 nm for ferrite and 86 nm for BaTiO₃ nanopowders. The complex permittivity and the complex permeability variations as a function of frequency in the range 100 kHz – 1.8 GHz, were investigated using LCR meter and Impedance analyzer. The resonance and relaxation phenomena were observed by all the samples around 1.18 GHz from the permittivity studies. From the studies of microwave absorbing properties in X-band (8–12 GHz) frequency region, it was found that the minimum reflection loss of –24.61 dB with bandwidth of 3.38 GHz was obtained by sample with 20% ferroelectric phase. The studies on reflection loss and transmission loss indicated that the effective absorption of incident microwave was found to be above 80% and the composite sample with 80% of ferroelectric phase absorbed more than 91% of the incident wave. The results suggested that the present sample materials can be used for making microwave shielding devises for EMI applications.

1. Introduction

Multiferroic composite materials that display coexistence of ferroelectric and ferromagnetic responses attracted the current interest due to their magnetic and dielectric properties that are appropriate for several novel device applications such as high frequency Multi Layer Chip Inductor (MLCI) applications, electromagnetic interference (EMI) filters and sensors etc [1,2]. Dielectric and magnetic property studies and their dependence on composition and structure of nanocomposites lay the foundation for developing the new materials with pre-determined properties since the interrelationship of properties of filler and matrix phases of composites help in the design of devices for applications. The frequency dispersion characteristics of ferrite and ferroelectric composites are deciding parameters while using these materials as microwave absorbers and EMI shielding materials in various applications [3,4]. The advanced technological developments in the field of telecommunications and several industrial sectors demand not only effective EMI shields but also materials that satisfy certain requirements for each engineered design such as light weight, corrosion

resistant, flexibility, processing easiness, tunable morphology, and inexpensiveness [5]. Another priority is developing radar absorbing materials for military stealth applications in X-band (8–12 GHz) frequency region. A significant research has been done over recent years on microwave absorption performance of various nanomaterials [6,7]. However, these absorbing materials cannot satisfy all requirements simultaneously, such as absorption, wide bandwidth, light weight, etc. [8].

In the current work ferrite ferroelectric nanocomposites are selected to synthesize and study properties, the reason being due to the fact that spinel ferrites and perovskite ferroelectrics show good phase compatibility through magnetoelectric coupling and the interconnectivity of the phases can be controlled by their relative amount and processing methods. Moreover, there exists good lattice match between perovskite ferroelectric, BaTiO₃ (lattice constant, a ≈ 4.03 Å) and spinel ferrite (lattice constant, a ≈ 8.33 Å), with ferrite lattice constant close to twice the perovskite lattice constant, which is expected to have excellent wetting between two phases resulting in strong interface adhesion in composites [9]. Due to their excellent dielectric and magnetic

* Corresponding author.

E-mail address: mallavarapudurga@gmail.com (M. Kanaka Durga).

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PRINCIPAL
Geethanjali College of Engineering and Technology
(Autonomous)
Chowdri (V), Kossare (H), Medchal Dist. (T.S.) - 501 301

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20-21
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IMPACT OF THERMAL RADIATION AND CHEMICAL REACTION ON MHD HEAT AND MASS TRANSFER CASSON NANOFUID FLOW PAST A STRETCHING SHEET IN PRESENCE OF HEAT SOURCE/SINK

Nalivela Nagi Reddy¹, Vempati Srinivasa Rao² and B. Ravindra Reddy³¹Department of Mathematics, Geethanjali College of Engineering and Technology, Hyderabad, Telangana, India²Department of Mathematics, Anurag University, Hyderabad, Telangana, India³Department of Mathematics, JNTUH College of Engineering Hyderabad, Hyderabad, IndiaE-Mail: nagireddynalivela@gmail.com

ABSTRACT

The purpose of present study is to analyse the influence of chemical reaction on MHD Casson nanofluid flow on an elongating sheet taken into the account of radiation and heat absorption/generation. The governing nonlinear PDE's are changed into a nonlinear ODE's by using similarity transformations. The converted equations are solved using numerical technique is notable as Keller box method. The consequence of heat source/sink, Prandtl number, Casson parameter, magnetic field, Brownian motion, thermophoresis, thermal radiation and chemical reaction parameters on velocity, temperature, and concentration profiles are depicted and elucidate in physical terms. A resemblance with previously issued results shown a perfect agreement. Numerical values of physical quantities, such as velocity gradient, heat transfer rate and the mass transfer rate are arranged in tabular form.

Keywords: thermal radiation, heat source/ sink, stretching sheet, casson nanofluid, MHD, chemical reaction.

INTRODUCTION

The study of nanofluids have fascinated because of its remarkable applications in industry such as solar cells, electronics, solar stills, communication, solar cooling systems, computing technologies, solar collectors, optical devices, water heaters, lasers, absorption refrigeration systems, and medicine, synthesis of various solar devices because of their higher properties over the conventional fluids. A nanofluid, consisting of a base fluid and nanoparticles, is a modern division of heat transfer fluids. The utilization of supplement is an approach to intensify the performance of heat transfer in base fluids. The heat conductance of conventional heat transfer fluids does not encounter the demands of modern cooling rate. Nanofluids are suspensions of ultrafine-grained solid particles (nanoparticles) and it improves the convective heat transfer and heat conductivity in common fluids. Choi and Eastman [1] analysed the increased thermal conductivity of nanoparticle fluids. S. K. Das *et al.* [2] investigated the Heat Transfer in Nanofluids. Natural convective heat and mass transfer nanofluid boundary layer flow through a vertical plate with convective boundary condition was studied by Aziz and W.A. Khan [3]. D. Srinivasacharya and Ontela Surender [4] examined the non-similar solution by considering double stratification on natural convection heat transfer of a nanofluid in a porous saturated medium over a vertical plate. Elsheikh *et al.* [5] studied the various applications in solar energy with nanofluids.

Magnetohydrodynamic (MHD) nanofluids perform an important part in several manufacturing procedures such as in hybrid fuel generation, modulator, economy fuel in modern power generation plants, gratings, coolant in continuous metallurgical sheets, fiber filters, vehicle cooling, loud speakers, plastic sheet extrusion and

processes of polymers, and magnetic cells, etc. Rizwan Ul Haq *et al.* [6] analysed the magneto-hydrodynamic stagnation point Nanofluid flow in presence of radiation on a stretching sheet with slip conditions. A.S. Dogonchi *et al.* [7] discussed heat transfer and thermal radiation MHD nanofluid flow between parallel plates. A. Kamran *et al.* [8] observed Magneto-hydrodynamic Casson Nanofluid with velocity slip and Joule heating. Jawad Raza *et al.*, [9] investigated MHD heat and mass transfer Nanofluid flow past a nonlinear permeable stretching sheet with multiple slips. Saeed Islam *et al.* [10] examined the influence of thermal radiation and hall current between two surfaces on MHD micropolar non-Newtonian hybrid Nanofluid flow.

Thermal radiation plays an important role in dissipating heat from the surface. It has applications in manufacturing industries such as chopper, space vehicles, reliable equipment design, satellites, atomic furnaces, missiles, space technology and procedures related to high temperature. Yanala Dharmendar Reddy *et al.*, [11] analyzed thermal radiation and suction effects on MHD Nanofluid boundary layer flow on a non-linear stretching sheet. Kothandapani and J. Prakash [12] observed peristaltic transport in a tapered asymmetric channel of a Williamson Nanofluid in the presence of thermal radiation. C.Sulochana *et al.* [13] analysed effects of solet and suction/blowing on MHD stagnation point flow of a radiative Carreau nanofluid on a stretching surface. Yap Bing Kho *et al.*, [14] investigated impact of radiation on MHD heat and mass transfer Casson Nanofluid flow on a porous stretching sheet. Jawad Raza [15] discussed impact of radiation and velocity slip on magnetohydrodynamic stagnation point flow of Casson fluid with convective boundary conditions through a linear elongated sheet.

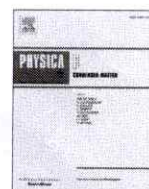


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Molecular interaction studies of hydrogen-bonded N-Methyl-2-Pyrrolidone /Ethanol binary mixtures by dielectric relaxation spectroscopy and their temperature dependence

V. Manjula^{a,b}, T. Vamshi Prasad^c, K.C. James Raju^{d,**}, T. Vishwam^{a,*}

^a Department of Physics, GITAM (Deemed to be University) -Hyderabad, Rudraram, Patancheru (M), TS, 502329, India

^b Department of Physics, Geethanjali College of Engineering and Technology, Hyderabad, Telangana, 501301, India

^c Department of Physics, Jawaharlal Nehru Technological University- Hyderabad, Hyderabad, 500 085, India

^d School of Physics, University of Hyderabad, Hyderabad, Telangana, 500046, India

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ABSTRACT

Complex permittivity of the binary mixtures of N-Methyl-2-Pyrrolidone (NMP) with Ethanol (ETH) has been studied in the microwave frequency range at various temperatures. The binary liquid system NMP-ETH is selected to interpret the effect of carbonyl (-C=O) group of NMP and hydroxyl group (-OH) of ETH on the volumetric, thermal and dielectric properties. The dipole moment (μ) and relaxation time (τ) is evaluated from Higasi's method and Havriliak-Negami equation. The excess molar volume (V_m^E), excess permittivity (ϵ^E), excess refractive index (n_D^E), excess inverse relaxation time ($1/\tau^E$) are fitted with the Redlich-Kister equation. The results obtained from Polarizable Continuum Model (PCM) and Integral Equation Formalism Polarizable Continuum Model (IEFPCM) solvation theories using DFT methods are correlated with the experimentally determined parameters. The molecular association and chemical stability of the system is interpreted in terms of single-point energy, HOMO-LUMO calculations. The existence of a hydrogen bond within the NMP-ETH system is confirmed from the FT-IR, UV-Vis's spectra.

1. Introduction

Dielectric Relaxation Spectroscopy (DRS) is one of the prominent methods to explore the molecular structure in the liquid systems by determining the relaxation dynamics of the molecules, dipole moment, and interfacial polarization properties [1–8]. The investigation of molecular interactions in the liquid binary systems is one of the challenging tasks and their change in properties with respective frequency and temperature is very much useful in practical engineering and technological applications [9–15]. The investigation of dielectric relaxation properties of the different solute and solvent systems in the broader frequency range (10 μ Hz- 300 GHz) describes the strength of the molecular interaction, the existence of multimers in the mixtures, the alignment of the dipoles, and their conduction mechanism. The theoretical and experimental studies on the dielectric studies of complex fluids such as aqueous proteins/tissues in an alcohol medium, liquid mixtures are interdisciplinary and increasing demand in the research

field [15–24]. It provides relevant information for the applications of binary liquid mixture systems in the field of pharmaceutical, petrochemical, nuclear, and green industry [25–37].

NMP is an adaptable water-soluble polar aprotic solvent. Due to its multifunctional properties, it is used as a drug solubilizer, penetration enhancer in humans and animals. Also, it is used as a good solvent for many engineering and pharmaceutical utilization by its larger boiling point, lower freezing point, and easy to operate. Ethanol is also one of the good solvents and it has many useful properties that allow it to be used by a range of different industries such as beverage, pharmaceutical, medical, and fuel industry [27–29,38–41]. There are several research papers are available on the frequency-dependent dielectric studies of ethanol with different liquid compounds at various temperatures in the recent past [42–56]. The majority of the dielectric studies on ethanol include calculating the dielectric relaxation time in a different solvent medium at various temperatures and also fluctuations of hydrogen bond networks in the different liquid medium. Further, computational

* Corresponding author.

** Corresponding author.

E-mail addresses: kcjersp@uohyd.ac.in (K.C.J. Raju), vtalloju@gitam.edu (T. Vishwam).

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Study of Microstructure and Thermal Properties of PbTiO₃ Based Glass Ceramics

J. Shankar^{1*}, P. Raju¹, A. Shiva Kumar¹, J. Anjaiah¹, G. Neeraja Rani¹ and V. K. Deshpande²

¹Geethanjali College of Engineering and Technology, Hyderabad-501301, India

²Vishveswaraya National Institute of Technology, Nagpur, 440010, India

*Corresponding author: jshankar001@gmail.com

Abstract: Glass samples with composition (35- X) B₂O₃ - (40 +X) PbO - 25 TiO₂ (where X= 0, 2.5, 5, 7.5 and 10 mol %) were prepared using conventional quenching technique. These glass samples were converted to glass ceramics by following two stage heat treatment schedules. The density (ρ) values of glass ceramic samples are higher than those of corresponding glass samples. It was observed that there was good correlation between the density and Coefficient of Thermal Expansion (CTE) results of the glass-ceramics. The XRD results in the glass ceramics revealed the formation of tetragonal lead titanate (PbTiO₃) as a major crystalline phase and lead borate (PbB₂O₄) as minor crystalline phase. The microstructure of glass ceramic samples contains nano crystallites of lead titanate embedded in a borate glass matrix.

INTRODUCTION

PbTiO₃ (PT) is a tetragonal perovskite with a c/a ratio of 1.063 at room temperature, which is the largest known for lead-based perovskite compounds. Single crystal data have shown that the large ionic displacements in PT lead to a particularly large spontaneous polarization ($>53 \mu\text{C}/\text{cm}^2$) and strain (c/a ratio = 1.06) at room temperature [1]. PT exhibits large pyroelectric coefficients and low relative permittivity (~ 100 -200). However, these excellent properties are not yet fully realised in bulk polycrystalline samples due to difficulty in fabricating undoped PT. PbTiO₃ ceramics when prepared by conventional route generally have micro cracks and fracture on cooling below T_c as a result of the large spontaneous strain generated when the structure changes from cubic to tetragonal.

Glass ceramics are the polycrystalline materials prepared by the controlled crystallization of glasses. A wide variety of applications of these versatile materials have been developed as a result of their many outstanding properties and the distinct advantages of the glass ceramic method, in certain circumstances, over conventional ceramic processing routes. Of particular importance in many applications is the high uniformity of the microstructures of glass ceramics, the absence of porosity and the minor changes in volume during the conversion of glass into glass ceramic [2].

Ferroelectric crystalline phases investigated include SrTiO₃[3-4], BaTiO₃[5-6], LiTaO₃[7], LiNbO₃[8], PbTiO₃[9-11] and (Pb,Sr,Ba)Nb₂O₆[12]. The ferroelectric and dielectric properties of glass-ceramics mainly determined by major crystalline phase and the residual glass or secondary phase(s). However, the excellent adjustability of the composition and microstructure of glass-ceramics promises some advantages of high-permittivity glass-ceramics over the crystalline ferroelectric ceramics (viz. adjustable thermal expansion, dielectric properties, and processing temperature). They also offer the benefit of process compatibility with ceramic substrates and metallized components. Therefore, high-permittivity glass ceramic materials are candidates for capacitors, hybrid circuits, electro-optic, and cryogenic applications [13-14].

In this paper microstructure and thermal properties of PbTiO₃ based Glass Ceramics of (35- X) B₂O₃ - (40 +X) PbO - 25 TiO₂ has been reported.

20-21 (13)

Quenching Effect of co-dopant Pr³⁺ on Red Emitting Yttrium Vanadate Phosphor Doped with Eu(III)

G. Neeraja Rani^{a*}, J. Shankar^a, P. Raju^a, J. Anjaiah^a, B. Mamatha^a and N.H. Ayachit^b

^aDepartment of Physics, Geethanjali College of Engineering and Technology, Cheeryal, Hyderabad, India

^bDepartment of Physics, Rani Channamma University, Belagavi, India

*Corresponding author: neerajarani@gmail.com

Abstract: Y_{1-x}VO₄: Eu_{x-y}³⁺: Pr_y³⁺ with x = 6 mole % and y = 0, 2, 3, 4, 5, 6, mole % phosphors have been prepared by solid state reaction. The dopant Eu³⁺ concentration was optimized along with the co-dopant Pr³⁺ concentration in the yttrium vanadate host lattice with the help of photoluminescence (PL) spectra. The phosphors have displayed red color under UV source. Pr³⁺ acts as quencher and quenching effect of co-dopant Pr³⁺ on Red Emitting Yttrium Vanadate Phosphor Doped with Eu(III) using luminescence Studies on Y_{1-x}VO₄: Eu_{x-y}³⁺: Pr_y³⁺ systems are presented in detail in this paper. The emission intensities were determined and the relative fluorescence intensities have been estimated. The richness of the red color is verified by determining the chromaticity coordinates (X, Y) from the CIE standard charts.

INTRODUCTION

The crystal field of the monazite characteristics makes YVO₄ a very attractive laser material with dopants Eu³⁺, Tm³⁺, Tb³⁺, Er³⁺, Ho³⁺, Ce³⁺ and Pr³⁺ [1-14]. Of these Red Emitting Yttrium Vanadate Phosphor doped with Eu(III) is found to be very attractive potential laser material. YVO₄ is an important host lattice for phosphors [5-6] due to its application in TV screens and high pressure mercury vapor (hpmc) lamps. Among the rare earth ions, praseodymium (Pr³⁺) has drawn the attention of several researchers due to the capability of emitting efficiently [15]. Examples Pr³⁺ as a sensitizer, which enhances the excitation resulting in transfer of energy to dopants through a non-radiative process and Pr³⁺ as quencher which quenches emission of energy of dopants through non-radiative relaxation of the system are available in literature i.e. in some hosts it demonstrates energy transfer between Pr³⁺ and dopants [16-24] while in some other hosts it demonstrates a lack of energy transfer between it and dopants [25,26]. Photo luminescent (PL) properties of Pr³⁺ co-doped phosphors especially in crystalline hosts have been reported by many researchers [16-29].

The YVO₄ crystal is tetragonal, belonging to space group D_{4h}. The dopant rare earth ion substitutes on Y³⁺ ion sites the local site symmetry will be D_{2d} and it is surrounded by eight O²⁻ ions [30,31]. The information on the red luminescence under ultraviolet excitation of rare earth vanadate was first reported by Van Uitert et al [32]. Europium doping gives red emission in YVO₄ with four main groups of emission lines of peaks at 700nm, 655nm, 621nm and 595nm and has been assigned to ⁵D₀ → ⁷F₄, ⁵D₀ → ⁷F₃, ⁵D₀ → ⁷F₂ and ⁵D₀ → ⁷F₁ transitions respectively, for Eu³⁺ ion. The luminescent properties and the crystallographic data on all rare earth vanadates are available in literature [30,31]. The development by Levine and Palila [33] of europium activated yttrium orthovanadate as a highly efficient red emitting cathodoluminescent phosphor and its adoption for color television aroused interest in other lanthanide activated orthovanadates. Bixner et al [34] investigated Ca₃(VO₄)₂ and found it to be moderately efficient as a host of Eu, but simultaneously inferior to YVO₄. The systems more efficient than Ca₃(VO₄)₂ based on were described by Palila et al. [33], who showed that the exciting energies are absorbed by the VO₄³⁻ ions and is transferred to activators.

In the present work an attempt has been made to vary the concentration of Pr³⁺ and study the efficiency of red emitting YVO₄: Eu³⁺: Pr³⁺ phosphor. Initially, Eu³⁺ concentration in the lattice was optimized at 6 mole % with the help of PL studies and this composition has been taken further to study the effect of Pr³⁺ as co dopant. Prepared powder phosphors were characterized by XRD and PL spectra. The results are reported and discussed in this article.

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Enhanced electrical properties of $\text{Sr}(\text{Bi}_{3.9}\text{La}_{0.1})(\text{Ti}_{3.975}\text{Zr}_{0.025})\text{O}_{15}$ ceramic with the doping of Nd

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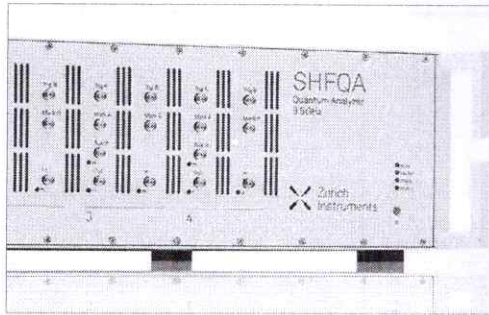
B. Mamatha, K. Ashok, G. Neeraja Rani, and A. R. James



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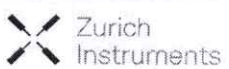


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(67)



WEB 2.0 TOOLS: USE OF KAHOOT TO REDUCE THE SPELLING MISTAKES AMONG B.TECH LEARNERS OF COMMUNICATIVE ENGLISH

G. Latha Suhasini* & Dr. Diksha Dhar**

* PhD Scholar, Department of English, School of Humanities & Sciences, KL (Deemed to be University), Hyderabad, Telangana

** Assistant Professor, Department of English, School of Humanities & Sciences, KL (Deemed to be University), Hyderabad, Telangana

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Abstract:

BTech learners of Communicative English are inclined towards technology and hardly focus on spellings in their writing. Today, students are called as netizens or net generations (Educause.edu, 2016) due to their over usage of web tools. My paper explores strategies to reduce spelling mistakes in BTech learners of Communicative English by introducing games using Kahoot, in the class. In the empirical design approach, the questions framed by the teacher would help the learner identify the correct spelling through game based learning. Though the learners face technical challenges, learning through games is very interesting.

Key Words: Net Generation, Kahoot, Undergraduates of Engineering, Spellings

Hypothesis:

The Engineering undergraduates who are interested in anything with internet would learn correct spelling through game based e-learning.

Introduction:

Most of the teachers find it challenging to teach spellings to students at undergraduate level. Due to heterogeneous educational background, many students are unable to spell the words right in their academic writing. This has affected their career growth. As technical students are inclined towards technology, teaching-learning process using web 2.0 tools becomes more compatible. Introducing Quizzes through Kahoot which is a game based LMS motivates and engages students and a positive impact develops in the learning process in them.

Rabail Tahir in his research investigated the effect of using Kahoot in his classroom. He focused on learning performance, classroom dynamics, students' and teachers' attitudes and perceptions, and student anxiety. Through his qualitative and quantitative research with 93 students, he found Kahoot to have a positive effect in teaching and learning process. He felt technical hitches, time stress and fear of losing the game were the challenges the students faced.

The method is to design a game based questionnaire where students would respond using the Kahoot! Kahoot! is a game-based student response system (GSRS) where the classroom is temporarily transformed into a game show where the teacher is the game show host, and the students are the contenders (Wang, 2015)¹. The teacher frames some quiz questions and creates the game using Kahoot! The students would respond to them. Some conceptual questions that would test their retention and spelling ability will be asked in the game as a quiz. The students have an option to redo their wrong questions. In this process the students identify their mistakes and learn the correct spelling. Kahoot! The game-based application is very interesting and easy to create and motivating to play games in the classroom. Multiple choice questions or true or false type questions can be asked using Kahoot. The background music while playing the game not only triggers enthusiasm in students but also keeps them alert throughout the game. This enhances students' concentration and keeps them focused on what they are supposed to do. Above all, playing games break the monotony of the traditional classroom and makes a learner centred class. The results would be based on score of every individual. It would be number of questions answered correctly in the given time. Based on the score the ability of the student would be analysed and the teacher would plan further quizzes based on the responses.

Samples/Population:

40 students of III year Mechanical Engineering of whom only 19 could participate.

Method:

To test the spellings, I have framed 10 questions on the topic Presentation skills. The questions were to review the lesson and also to test the spelling ability in the learner. Four options were given to answer each question. Three of the four options had wrong spelling that would sound similar. The learner needs to comprehend the question, recollect the answer and identify the answer with its correct spelling. Of 40 students in the class only 19 could participate as few did not have an extra device to play, few had problem with the connectivity and few others had no technical knowledge. Of 19 participants only 17 were able to answer as the other two could not match the speed of the game as the game has fixed time to answer each question. This gave

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A simple rule of thumb for the explanation of d-orbital splitting in complexes

R. Sanjeev¹, V. Jagannadham² and R.Veda Vrath³

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Abstract

In chemistry at pre-university level and freshman engineering (non-chemistry discipline) classrooms at universities in India, the splitting of the energy levels of d-orbitals in complexes is an important concept to be learnt, but is not explicitly explained in the standard books used. In the standard books such as 'Concise Inorganic Chemistry' by J.D. Lee and 'Theoretical Inorganic Chemistry' by Marion Clyde Jr. Day and Joel Selbin, they have explained the splitting of d-orbitals in octahedral, tetrahedral, square planar etc., complexes very well. The same is the case with the latest pre-university NCERT chemistry textbook (Volume I) written for the Indian audience. The reason why the energy levels of certain d-orbitals are above the barycenter and why some are below the barycenter, however, is not explained explicitly in any of the books (including the latest books). This short communication outlines a simple rule of thumb that allows this phenomenon to be explained to students. Further, an important graph in the standard books is plotted, but the trend of the curve is not explained. This simple rule is also helpful in explaining this graph and the chemical phenomenon represented.

Keywords

D-orbitals, lowering of energy, gain of energy, attraction, repulsion.

Una simple regla para la explicación de la división del orbital d en complejos

Resumen

En las aulas de química a nivel preuniversitario y de ingeniería (disciplina no química) de primer año en universidades de la India, la división de los niveles de energía de los orbitales d en complejos es un concepto importante que debe aprenderse, pero no se explica explícitamente en los libros estándar usados. En los libros estándar como 'Química inorgánica concisa' de J.D. Lee y 'Química inorgánica teórica' de Marion Clyde Jr. Day y Joel Selbin, han explicado la división de los orbitales d en octaédricos, tetraédricos, planos cuadrados, etc., complejos muy bien. Lo mismo ocurre con el último libro de texto de química preuniversitario NCERT (Volumen I) escrito para la audiencia india. La razón por la que los niveles de energía de ciertos orbitales d están por encima del baricentro y por qué algunos están por debajo del baricentro, sin embargo, no se explica en ninguno de los libros (incluidos los últimos libros). Esta breve comunicación describe una simple regla empírica que permite explicar este fenómeno a los estudiantes. Además, se traza un gráfico importante en los libros estándar, pero no se explica la tendencia de la curva. Esta sencilla regla también es útil para explicar este gráfico y el fenómeno químico representado.

Palabras clave

D-orbitales, disminución de energía, ganancia de energía, atracción, repulsión.

¹Departamento de Química, Geethanjali Colegio de Ingeniería y Tecnología, Cheeryal-501301, Telangana, India. orcid: <https://orcid.org/0000-0002-6117-7112>

²Departamento de Química, Universidad de Osmania, Hyderabad-500007, India. orcid: <https://orcid.org/0000-0001-9152-7729>. Email: jagannadham1950@yahoo.com

³Departamento de Química, Colegio J.N. Gupta, Charminar, Hyderabad-500002, Telangana, India. Correo: vedavrath@rediffmail.com

20-21-19



Structural and microwave behavior of Dy³⁺-substituted Ni_{0.5}Zn_{0.5}Dy_xFe_{2-x}O₄ ferrites

P. Neelima^{1,2}, T. Ramesh^{3,*}, P. Raju⁴, and S. R. Murthy¹

¹Department of Physics, Osmania University, Hyderabad, India

²Department of Physics, St. Peter's Engineering College, Hyderabad, India

³Department of Physics, BVRIT Hyderabad College of Engineering for Women, Hyderabad, India

⁴Department of Physics, Geethanjali College of Engineering and Technology, Hyderabad, India

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ABSTRACT

The enhancement of microwave absorbing properties in dysprosium ion (Dy³⁺)-substituted nickel-zinc ferrites (Ni_{0.5}Zn_{0.5}Dy_xFe_{2-x}O₄; x = 0.00, 0.01, 0.03, 0.05, 0.07 and 0.09) has been investigated in this work. The ferrite powders were synthesized by microwave-hydrothermal method and then powders were densified at 900 °C for 40 min using microwave furnace. The samples' structural and morphological properties were studied using X-ray diffraction and scanning electron microscopy (SEM), respectively. The structural result confirms the spinel phase under low Dy³⁺ content, like the pure Ni-Zn ferrite, while a secondary phase of DyFeO₃ appears after the content of Dy³⁺ exceeds a certain limit (x > 0.07). Morphological analysis from the SEM images reveals the formation of spherical grains of the samples. DC resistivity of the samples has been measured using two-probe method. Magnetic hysteresis data confirm the soft magnetic nature of the samples. The vector network analyzer results show that adjusting the content of Dy³⁺ is significant in changing the magneto-dielectric properties and microwave absorption capacity of the materials. The composition x = 0.07 sample showed a reflection coefficient of - 33.24 dB at the frequency and bandwidth of 10.31 GHz and 2.59 GHz for an absorber thickness of 2.5 mm for losses less than - 10 dB. This acquired result indicates that the investigated samples could be used as a microwave absorber application in X-band.

1 Introduction

Spinel ferrites are the most attractive magnetic oxides due to their diversified fundamental and technical applications [1–3]. The general formula of the spinel ferrites is MFe₂O₄, where M represents the divalent

metal cation like Ni, Co, Zn, Mg and Mn. The unit cell of these ferrites has a cubic symmetry and contains eight formula units of MFe₂O₄. The relatively large-sized oxygen ions form a face-centered cubic structure and each cubic unit cell consists of '64' tetrahedral (A) sites and '32' octahedral (B) sites; out of these

Address correspondence to E-mail: rameshouphysics@gmail.com

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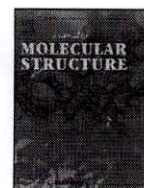
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Influence of hydrogen bond networks in Glycerol / N-Methyl-2-Pyrrolidone mixtures studied by dielectric relaxation spectroscopy

V Manjula^{a,b}, T. Vamshi Prasad^c, K Balakrishna^a, K. C. James Raju^{d,*}, T Vishwam^{a,*}^a Department of Physics and Chemistry, GITAM (Deemed to be University), Hyderabad, Rudraram, Patancheru (M), Telangana, 502329, India^b Department of Physics, Geethanjali College of Engineering and Technology, Hyderabad, Telangana 501301, India^c Department of Physics, Jawaharlal Nehru Technological University, Hyderabad, Hyderabad, 500 085, India^d School of Physics, University of Hyderabad, Hyderabad, Telangana 500046, India

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ABSTRACT

In this paper, we report the dielectric permittivity of the Glycerol (Gly) with N-Methyl-2-Pyrrolidone (NMP) binary mixtures in the microwave frequency region at different temperatures. The dipole moments of Gly, NMP and their equimolar binary mixtures are calculated by using Higasi's method in the temperature range 298.15K-323.15K. The dielectric relaxation spectra of the binary mixtures are calculated using Cole-Cole and Cole-Davidson equation and shows an unsymmetrical relaxation behaviour. The excess parameters of volume, permittivity, refractive index, polarization and relaxation times are fitted with Redlich-Kister polynomial equation. The molecular association and their hydrogen bond interactions between the components in the mixture are discussed in terms of Kirkwood correlation g^{eff} factor and excess Helmholtz energy (ΔF^E) equation. The mean molecular polarizability (α_M) of the individual and their binary mixture are calculated using Lippincott δ -function potential model and compared with the LeFevre method of polarizability values. The enthalpy of activation ΔH^* , entropy of activation ΔS^* and Gibbs free energy of activation ΔG^* are also evaluated and the results are discussed in terms of the orientation of the dipoles. The presence of hydrogen bonding between Gly and NMP is confirmed from the FT-IR spectra.

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1. Introduction

The non-destructive characterization of biological samples/liquids, polymers and gels have stimulated the use of dielectric relaxation spectroscopy (DRS) at a broader frequency range at different temperatures [1]. The DRS is one of the sensitive methods to interpret the structural dynamics, molecular association and orientation of the dipoles in the liquid medium [2]. The dielectric relaxation spectroscopy is well suited for to observe the changes in the electrical properties when liquids mix up at different concentrations and also the hydrated studies of proteins/gels with the change in temperature. Therefore, temperature-dependent dielectric relaxation studies of liquid mixtures are of growing interest [3–9]. The investigation of dielectric permittivity of the mixtures by varying concentration of liquid samples helps to ascertain the structure of the complexes formed in the solution

[10–15]. The presence of the hydrogen bond between components present in the mixtures that affect the dielectric permittivity, polarization and its relaxation behaviour properties. The understanding the nature of hydrogen bond remains a complex task due to the type of bonds and components present in the given liquid system [16–22]. The dielectric permittivity studies of hydrogen-bonded polar liquids/polymer nanocomposite materials at broader frequency region are very much interesting and these results are quite useful in the field of biological, medical, and shielding applications [23–32].

Glycerol is a simple polyol compound; due to its antimicrobial and antiviral properties, it is extensively used in wound and burn treatments, effective marker to measure liver diseases, the sweetener in the food industry and as a humectant in pharmaceutical formulations [33–39]. NMP is a good polar solvent with magnificient properties. It is having a wide range of applications due to its higher boiling point, lower freezing point and ease of handling [40,41]. It is used as a solvent for engineering polymers, coating resins, paint stripping, oven cleaners, automotive and industrial cleaner formulations. The dielectric permittivity of the Glyc-

* Corresponding authors.

E-mail addresses: kcjrsp@uohyd.ac.in (K. C.J. Raju), vtalloju@gitam.edu (T. Vishwam).

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FeF₃ MEDIATED SYNTHESIS OF 3,4-DIHYDRO-3-PYRIDYL-2H-NAPHTHA[2,1-E][1,3]OXAZINE DERIVATIVES

Shashikala K^a, Praveena D^b, Ramesh M^c and Laxminarayana E^{*b}

^aGeethanjali College of Engineering and Technology, (Autonomous) Cheeryal, Keesara, Hyderabad, Telangana

^bSRUniversity, Warangal Urban-506 371, Telangana, India.

^cJawaharlal Nehru Technological University Kakinada, Kakinada, Andhra Pradesh, 533003, India

^dSreenidhi Institute of Science and Technology (Autonomous) Yamnampet, Ghatkesar, Hyderabad Telangana

Email: elxnkits@yahoo.co.in

ABSTRACT

Biologically active 3,4-dihydro-3-substituted-2H-naphtho [2,1-e][1,3]oxazine derivatives were synthesized using environmentally benign and economically feasible Lewis acid FeF₃. They are characterized by FT-IR, HNMR and Mass spectroscopic methods.

INTRODUCTION

1,3-oxazine derivatives, especially, when they were condensed with aromatic rings displayed diverse biological properties, such as antibacterial, anticancer, anti-fungal, analgesic, anticonvulsant and anti-tubercular activities.^{i,ii} Moreover, trifluoromethyl-1,3-oxazine-2-one is highly active against various HIV-1 mutant strains, since, they are non-nucleoside reverse transcriptase inhibitors that have an ability to bind and block HIV reverse transcriptase. Further, naphthoxazine derivatives showed high-level potential for the treatment of Parkinson's disease.^{iii,iv} They were shown to be anti-inflammatory agents. They were also used for treating allergies, ulcers, asthma, diabetes, and arthritis. 1,3-Oxazines have been used as key intermediates in the synthesis of thrombolytic agents, chiral auxiliaries in organic synthesis and liquid crystal devices.^v In a comprehensive survey of literature, it was found that naphth-1,3-oxazine derivatives were conventionally prepared using 2-naphthol, and various substituted aryl and heteroaryl aldehydes in the presence of dry methanolic ammonia. Further, the multi-component condensation of phenols or naphthols with primary amines (or ammonia) and two equivalents of aldehydes led to these target molecules. Similarly, condensation of derivatives of Betti base with aromatic aldehydes led to the formation of the corresponding 1,3-oxazine with varied biological properties.^{vi} Yet another method involves using the condensation reaction of salicylaldehyde with a primary amine, followed by reduction and then cyclization reaction with a suitable aldehyde. The oxazines containing six-membered ring nitrogen and oxygen was constructed by a type of Mannich reaction, in which zirconyl(IV)

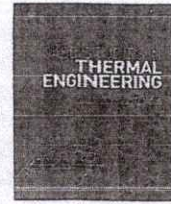
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Chemical reaction impact on MHD natural convection flow through porous medium past an exponentially stretching sheet in presence of heat source/sink and viscous dissipation

Nalivela Nagi Reddy^{a,*}, Vempati Srinivasa Rao^b, B Ravindra Reddy^c

^a Department of Mathematics, Geethanjali College of Engineering and Technology, Hyderabad, Telangana, 501301, India

^b Department of Mathematics, Anurag University, Hyderabad, Telangana, 500088, India

^c Department of Mathematics, JNTUH College of Engineering Hyderabad, Hyderabad, 500085, India

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MHD
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Eckert number
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ABSTRACT

This study investigates the viscous dissipation impact on free convection MHD flow through a porous medium over an exponentially stretching surface in presence of chemical reaction. The basic governing PDEs are converted into non-linear ODE's by using similarity transformations and then using the Keller-box method, numerical solutions are obtained. The flow features of boundary layers along with the bounding surface are identified and analysed using diagrams. It is noted that the increase in the Eckert number, Radiation and Magnetic parameter (M) increases the temperature profiles, while the increase in the chemical reaction parameter, porosity and Schmidt number decreases the concentration profile. To validate the results, a comparative study between the present study and previously published results for a particular case is conducted and good agreement is found between them.

1. Introduction

Engineering and Industrial procedures such as in extrusion processes, the movement of biological fluids, hot rolling, glass-fiber production, the cooling of metallic plates, rubber sheets, the performance of lubricants and paints, wire drawing, melt-spinning, manufacture of plastic, the extrusion of polymers, and aerodynamic plastic sheet extrusion, etc., is needed, has received considerable attention over the last few decades, to research flow on a stretching sheet. Many researchers are researching the movement of fluid over the stretching surface [1–5].

The influence of thermal radiation on convective fluid flows has an abundance of uses in physics and engineering for instance gas-cooled nuclear reactors, gas turbines, propulsion systems, hypersonic flights, space vehicles, solar power engineering, nuclear power plants, and lots of industrial areas, and so on. Several researchers [6–10] are attracted the thermal radiation.

In modern metallurgical and physical procedures, the research of the magnetohydrodynamic (MHD) flow of electrically conductive fluid is actually of great significance as a result of the effect of the magnetic field on the regulation of the boundary layer flow control as well as the effectiveness of numerous systems utilizing electrically conductive fluids. its application in many engineering problems, this kind of flow has attracted the focus of several researchers [11–15] such as plasma studies, geothermal energy extractions, MHD generators, nuclear reactor safety, and furnace structure. Hydromagnetic strategies are employed for the decontamination of

* Corresponding author.

E-mail address: nagireddynalivela@gmail.com (N.N. Reddy).

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An efficient synthesis of novel anti influenza viral and cytotoxic derivatives of 4-oxothiazolidin-3-yl)-3-hydroxyquinoxaline-2-carboxamide

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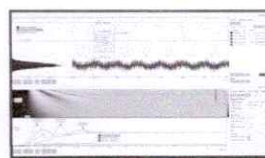
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Review

Recent Trends in Noble Metal Nanoparticles for Colorimetric Chemical Sensing and Micro-Electronic Packaging Applications

Anurag Gautam^{1,*}, Pragya Komal², Prabhat Gautam³, Ashutosh Sharma⁴, Neeraj Kumar⁵ and Jae Pil Jung^{6,*}

- 1 Department of Chemistry, Geethanjali College of Engineering and Technology, Cheeryal, Hyderabad, Telangana 501301, India
 - 2 Department of Biology, Birla Institute of Technology and Science, Pilani-Hyderabad Campus, Jawaharnagar, Shamirpet Mandal, Hyderabad, Telangana 500078, India; pragya@hyderabad.bits-pilani.ac.in
 - 3 Department of Chemistry, CMR Institute of Technology, Bengaluru, Karnataka 560037, India; prabhatgautam28@gmail.com
 - 4 Department of Materials Science and Engineering, Ajou University, 206 Worldcup-ro, Yeongtong-gu, Suwon 16499, Korea; ashu.materials@gmail.com
 - 5 Department of Metallurgical Engineering, SOE, O.P. Jindal University, Raigarh 496109, India; materials3@gmail.com
 - 6 Department of Materials Science and Engineering, University of Seoul, Seoulsiripdae-ro, Dongdaemun-gu, Seoul 02504, Korea
- * Correspondence: ganurag13@gmail.com (A.G.); jujung@uos.ac.kr (J.P.J.)

Abstract: Noble metal NPs are highly attractive candidates because of their unique combination of physical, chemical, mechanical, and structural properties. A lot of developments in this area are still fascinating the materials research community, and are broadly categorized in various sectors such as chemical sensors, biosensors, Förster resonance energy transfer (FRET), and microelectronic applications. The related function and properties of the noble metals in these areas can be further tailored by tuning their chemical, optical, and electronic properties that are influenced by their size, shape, and distribution. The most widely used Au and Ag NPs in dispersed phase below 100 nm exhibit strong color change in the visible range which alters upon aggregation of the NPs. The chemical sensing of the analyte is influenced by these NPs aggregates. In this article, we have summarized the uniqueness of noble metal NPs, their synthesis methods, nucleation and growth process, and their important applications in chemical sensing, microelectronic packaging, and Förster resonance energy transfer.

Keywords: colloid; nanostructure; microelectronic systems; crystalline; hydrothermal; nucleation and growth

1. Introduction

Nanomaterial is defined as a material in which the maximum value of one dimension can be 100 nm, which can be further defined as one billionth of meter or 10^{-9} m [1–6]. It is approximately 10 H or 5 Si atoms in a line. It is continuing to be the most rapidly growing R/D sector in last decades, which is evident from more than several billion dollars of annual investment in this particular field [7,8]. Due to its unique features, nanomaterials and NPs allow them to be used for a wide variety of applications in nanotechnology covering medical science, chemical, bio-network, applied physics, materials, microelectronic and metallurgy science, and engineering. There are lots of investments in the area of medical science, in particular, theragnostics, which refers to two kinds of word therapeutics and diagnostics [9]. It is an advanced technique in which cancer diagnosis and therapy is done simultaneously, for early detection and cure of the cancer [10,11]. To achieve this, some special metals in the periodic table include alkaline to alkaline metallics, rare metallics, and noble metallics used for theragnostics application [12]. Compared to these metals, noble

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20-21-28

Impact of Soret and Dufour on bioconvective flow of nanofluid in porous square cavity

Chandra Shekar Balla¹ | Alluguvelli Ramesh² |
Naikoti Kishan³ | Ahmed Mohamed Rashad⁴

¹Department of Mathematics, Chaitanya Bharathi Institute of Technology, Gandipet, Telangana

²Department of Mathematics, Geethanjali College of Engineering & Technology, Hyderabad, Telangana, India

³Department of Mathematics, Osmania University, Hyderabad, Telangana, India

⁴Department of Mathematics, Faculty of Science, Aswan University, Aswan, Egypt

Correspondence

Ahmed Mohamed Rashad, Department of Mathematics, Aswan University, Faculty of Science, Aswan 81528, Egypt.
Email: am_rashad@yahoo.com

Abstract

This article addresses the bioconvection in a porous cavity associated with Soret and Dufour effects. The bioconvective flow in a porous medium is based on Hillesdon and Pedley's model and is governed by nonlinear partial differential equations. These equations are transformed into a dimensionless form with suitable nondimensional parameters. The finite element method is employed to solve the dimensionless equations. The outcomes of the study are presented by streamlines, temperature distributions, iso-concentrations of solute, nanoparticles, and microorganisms. Furthermore, the tendency of average Nusselt number and average Sherwood number and the influence of Soret parameter, Dufour parameter, Peclet number, and bioconvective Rayleigh number is interpreted. Thermophoresis and Soret number show a strong effect on the concentration of nanoparticles. Brownian motion and thermophoresis exhibit a significant effect on the density distributions of microorganisms. The novelty of the paper is to combine the effects of Soret–Dufour and oxytactic bioconvection. The present study can be useful in the following applications: microbial-enhanced oil recovery, toxin removal, antibiotics, and modeling of microfluidic devices.



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Microwave Assisted Synthesis of 3-Chloro-N-(2-(5-chloro-1-tosyl-1H-benzo [d] Imidazol-2-yl) ethyl)-N-Substituted Quinoxalin-2-Amine Derivatives Using DCQX

K.Shashikala^{1*}, E.Laxminarayana², M.Ramesh³, M.Thirumala Chary⁴

¹ Geethanjali College of Engineering and Technology, Cheeryal(V), Keesara(M), Medchal Dt 501301, (Telangana) India

² Sreenidhi Institute of Science and Technology (Autonomous), Ghatkesaer, Hyderabad 501301, Telangana, India

³ Department of Biotechnology, Jawaharlal Nehru Technological University Kakinada, East Godavari Dt, Andhrapradesh 533003, India

⁴ Jawaharlal Nehru Technological University Hyderabad, Kukatpally, Hyderabad 500085, (Telangana) India
E-mail: kala.shashi2010@gmail.com

Abstract: The microwave assisted synthesis of 3-Chloro-N-(2-(5-chloro-1-tosyl-1H-benzo [d] imidazol-2-yl) ethyl)-N-substituted quinoxalin-2-amine derivatives is described. 2,3-dichloro quinoxaline (DCQX), as a starting compound and propargyl bromide, as an efficient alkylating agent are used in the synthesis of N-substituted quinoxalin-2-amine derivatives. We realized that microwave assisted synthesis is efficiently replacing conventional method of synthesis.

Keywords: 2,3-dichloroquinoxaline, quinoxaline, imidazoles, alkylating agent, microwave assisted synthesis

1. Introduction

There are several reported methods for the synthesis of quinoxaline-2-amine derivatives. Nevertheless, synthesis using 2,3-dichloroquinoxaline (DCQX) with nucleophilic species such as aryl amine has become a feasible substitute because of the presence of two chlorine atoms at C2 and C3 of DCQX. 2,3-dichloroquinoxaline (DCQX) is a reagent, extensively used as a synthetic intermediate in pharmaceutical industry as well as materials science^[1,2]. Furthermore, this reagent is easily prepared from low-cost starting materials and commercially available.

One of the major advantages associated with the reactions of DCQX with nucleophiles is the possibility to control single or double substituted products. This exceptional feature of DCQX makes it significant in the synthesis of specific products that can be used in a variety of applications^[3-7]. Propargyl bromide, an efficient alkylating agent is used for the N-alkylation of aryl amides. It is also used in enyne metathesis of propargylic amines, propargylation of spiro ketones, synthesis of allylic alcohols and enone complexes^[8,9].

The effective approach for the synthesis of quinoxalin-2-amines is the reaction between 1,2-diamines with aldehydes and isocyanides using CeO₂ nanoparticle catalyst. Also 3,4-dihydroquinoxalin-2-amines were synthesized by reactions between 1,2-diamines, ketones and isocyanides^[10].

Reaction between 2,3-dichloro quinoxaline and anilines is a convenient method for the preparation of N-aryl substituted 3-chloroquinoxalin-2-amines, particularly, 2-(N-aryl amino)-3-chloroquinoxalines that are further converted into N-substituted 3-chloro-N-(2-(1-tosyl-1H-benzo [d]-imidazol-2-yl) ethyl) quinoxalin-2-amine^[11]. This method is facilitated by AlCl₃ on forming C-N bond^[1]. These target molecules were found to be potential inhibitors of phosphodiesterase 4 (PDE-4) and have apoptosis inducing properties in an animal model (zebrafish)^[12,13]. Further, the reaction is facilitated in more effective way using an alkylating agent, propargyl bromide.

2. Results and discussions

All the compounds were synthesized using microwave irradiation. The synthesis of new compounds is described according to synthetic Figure 1. Compound 2 was synthesized from the starting materials, 2,3-dichloroquinoxaline (DCQX) and aniline, substituted at 4th position. Then compound 2 is irradiated with an alkylating agent, propargyl bromide in presence potassium carbonate and DMF to acquire compound 3. The final compound 3-Chloro-N-(2(5-chloro-1-tosyl-1H-benzo [d] imidazol-2-yl) ethyl)-N-substituted quinoxalin-2-amine (4) is obtained, when compound 3 was reacted with a

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Comparison of Substituent Effects in Benzenes (XC₅H₅C), Pyridines (XC₅H₄N) and Phosphorines (XC₅H₄P) and their Protonated Species

R. Sanjeev¹, V. Jagannadham^{2*}

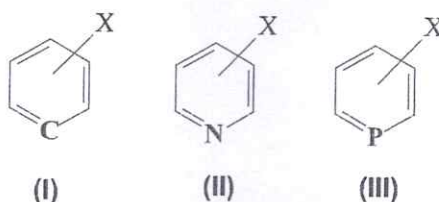
¹Department of Chemistry, Geethanjali College of Engineering and Technology Cheeryal-501301, Telangana, India

²Department of Chemistry, Osmania University, Hyderabad-500007, India

*Corresponding author: jagannadham1950@yahoo.com

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Abstract Collection of interesting and stimulative data led us to construct Hammett plots for different properties like proton affinities, gas phase basicities, solvation free energies of free and protonated benzenes (I), pyridines (II) and phosphorines (III), and for pK_a values of protonated pyridines and phosphorines. Trends in Hammett reaction constants (ρ) for all these processes were discussed.



Keywords: benzenes, pyridines, phosphorines, pK_a, proton affinities, gas phase basicities, solvation free energies

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1. Introduction

Acuity of work in chemical education and chemical research that took a shape from literature reported data on several chemical and physical aspects like phase transition temperatures, dipole moments, surface tensions, attenuation effect, associative and non-associative behavior of liquids, stability and lifetimes of reactive intermediates, LFER, effect of hybridization of carbon on Hammett (ρ) and Taft (ρ*) reaction constants, prediction of pK_a values of unstable arenium ions and benzenes, from our group has been ever increasing in recent times [1-63]. In the present work to go a step ahead we have tried the comparison of substituent effects on pK_a, proton affinities, gas phase basicities, solvation free energies in benzenes (C₅H₆C), pyridines (C₅H₅N) and phosphorines (C₅H₅P) and their protonated species.

2. Methods

All the linear correlations were done using the KaleidaGraph software, Reading, PA, USA. All chemical

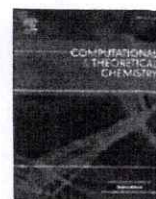
structures were drawn using chemdraw software. All Hammett σ values are from reference 64.

3. Discussion

Hammett reactions constants (ρ) and pK_a data of arenium, pyridinium and phosphorinium ions are given in Table 1. The corresponding plots are shown in Figure 1, Figure 2 and Figure 3.

Since the Hammett ρ can not be determined for the dissociation equilibriums of arenium ions XC₆H₆⁺ ⇌ XC₆H₅ + H⁺ as they are highly unstable, an alternate and lucid method was adopted by us based on the attenuation effect [26]. Figure 1 shows the determination of the Hammett ρ for the dissociation equilibriums of arenium ions XC₆H₆⁺ ⇌ XC₆H₅ + H⁺ from the study of attenuation effect of methylene group (-CH₂-) on the dissociation equilibriums of anilinium ions, benzyl ammonium ions and 2-phenylethyl ammonium ions [26] and using the Andrew Williams' empirical equation ρ = m1⁽²⁻ⁱ⁾ [65] where m1 is an arbitrary constant "i" is the number of atoms between ionizable proton and the ring carbon.

20-21-8



Application of Hammett equation to hydrogen bond interactions of benzoic acid in chloroform/water system and explanation for non-linear Hammett relation to partition coefficients for the same system



Sanjeev Rachuru^a, Adam A. Skelton^{b,*}, Jagannadham Vandanapu^{c,*}

^a Department of Chemistry, Geethanjali College of Engineering and Technology, Cheeryal 501301, India

^b Department of Pharmacy, School of Health Science, University of Kwazulu Natal, Durban, South Africa

^c Department of Chemistry, Osmania University, Hyderabad 500007, India

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ABSTRACT

It is well known that benzoic acid distributes itself between chloroform and water. The partition coefficients (K_p) of seven different benzoic acids in chloroform/water are documented in the literature. Plausible hydrogen bonded structures of these seven benzoic acids with the two immiscible solvents were envisaged and the DFT calculation for these hydrogen bonds were carried out. Further, the conformity of Hammett relation to the hydrogen bond interactions was assessed. Application of Hammett equation to the hydrogen bonding of distribution of different *para*-substituted benzoic acids to these immiscible solvents is done for the first time. Further, an explanation for non-linear plot of partition coefficients $\log K_p$ of *para*-substituted benzoic acids in chloroform-water system versus Hammett σ value has been explained for the first time.

1. Introduction

Partition or distribution coefficients has a wide range of applications in the fields of pharmacology [1–3], pharmacokinetics [4–6], pharmacodynamics [7–9], environmental science [10,11], agrochemical research [12], metallurgy [13] and consumer product development [14]. Octanol is believed to have the lipophilic character of the biological membranes. The *n*-octanol/water [15] partitioning system resembles the lipid membrane/water systems in the body. Hence most of the partition studies appearing in the literature were carried out in octanol/water system. Over the last century numerous studies on partition of organic solutes have appeared in literature. To quote them is beyond the scope of this article as they run in several hundreds.

It is a well-established fact that Hammett [16,17] and Taft [18–21] equations are good mechanistic tools in physical-organic chemistry [16–21]. We have carried out several studies in our laboratory with regard to their application. Non-Linear Taft Relationship is applied to surface tensions of aliphatic acids: Inter-molecular hydrogen bonding versus intra-molecular hydrogen bonding [22], Non-Linear Taft Polar Free energy Relationships (TPER), reactions of *N*-substituted benzyl amines with benzyl bromide [23], dipole moments and melting points and their unsolved miracles on the application of Hammett equation [24] and application of non-linear Hammett relationship to surface

tensions and dipole moments in estimating the associative behavior of phenols [25]. It is known that benzoic acid distributes itself between chloroform and water. We have considered the distribution of seven *para*-substituted benzoic acids. In the present study we envisaged the plausible hydrogen bonded structures (Scheme 1) and found the interaction energies in them. Further, we assessed the conformity of Hammett relationship to these interactions. To comprehend Hammett equation, let us suppose a reaction is performed on a substrate molecule [26] that can be represented as XGY where Y is the site of the reaction, X a variable substituent and G is a skeleton group to which X and Y (in our Scheme 1, X = OH, OCH₃, CH₃, H, Cl, Br and NO₂, Y is hydrogen bonding between COOH moiety of substituted benzoic acid and solvents, G is C₆H₄) are attached and we observe that changing X from H to CH₃, results in the change in the rate of reaction. The change in the rate of the reaction might be due to factors like mesomeric effect or inductive effect of the substituent X. The first attempt of quantitative treatment of X on the reaction site was given by Hammett. For the cases of meta and *para*-XC₆H₄Y, Hammett set up the equation $\log(k/k_0) = \sigma\rho$ and this equation is known as Hammett equation. Here k_0 is the rate or equilibrium constant for X = H, k the rate or equilibrium constant for group X, ρ is a constant known as Hammett reaction constant for a given reaction under a given set of conditions, and σ is a constant known as Hammett substituent constant. Hammett substituent constant σ reflects

* Corresponding authors.

E-mail addresses: rachuru1sanjeev1@rediffmail.com (S. Rachuru), skelton@ukzn.ac.za (A.A. Skelton), jagannadham1950@yahoo.com (J. Vandanapu).

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Investigation on natural convective flow of ethylene glycol nanofluid containing nanoparticles Fe_3O_4 in a porous cavity with radiation

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Ramesh Alluguvelli, Chandra Shekar Balla, Lavanya Bandari, and Kishan Naikoti



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