Journal of Non-Crystalline Solids 557 (2021) 120652

Contents lists available at ScienceDirect

Journal of Non-Crystalline Solids

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

Structural and optical studies on Dy^{3+} ions doped alkali lead borophosphate glasses for white light applications

P. Arun Jeganatha Joseph [a], K. Maheshvaran [b], I. Arul Rayappan [a,*]

[a] Department of Physics, St. Joseph's College (Autonomous), Affiliated to Bharathidasan University, Tiruchirappalli 620002, India
[b] Department of Physics, Kongu Engineering College, Perundurai, Erode 638060, India

ARTICLE INFO

Keywords:
Melt quenching technique
Borophosphate glasses
Oscillator strength
Emission
White light

ABSTRACT

Dy^{3+} ions doped alkali lead borophosphate glasses with chemical compositions of (45-x) H_3BO_3+20P_2O_5+10Al_2O_3+10PbO+15Li_2CO_3+xDy_2O_3 (where x = 0.0, 0.1, 0.25, 0.50, 1.0 and 2.0 wt%) have been prepared by conventional melt quenching technique and their physical, structural and spectroscopic behavior were studied systematically through XRD, FTIR, SEM with EDAX, optical absorption, luminescence and decay measurements. The density and refractive index increase with increasing of Dy^{3+} ions concentration and accordingly creating more non-bridging oxygen (NBOs) into glass matrix. X-ray diffraction study proves the amorphous nature of the prepared glasses. The FTIR study reveals the presence of BO_4, PO_4 vibrational groups and the bending of B–O–P, P–O–P units. The surface morphology and existence of elements in the prepared glasses have been studied through SEM with EDAX. The absorption spectra exhibit nine peaks with hypersensitive transition corresponding to $^6H_{15/2}\rightarrow{}^6F_{11/2}$ at around 1270 nm. The Judd-Ofelt (JO) theory is used to calculate the calculated oscillator strengths, JO intensity parameters, radiative transition probabilities, stimulated emission cross-section and branching ratio for the present glasses. The JO intensity parameters follow the trend as $\Omega_2>\Omega_6>\Omega_4$. The luminescence spectra of the glass sample displayed three emission peaks with high intensity are centered at 478 nm and 574 nm respectively. These attractive luminescence features of the proposed glasses in the white region verified using CIE 1931 diagram useful for the development of white light applications. The decay measurements of the prepared glasses for the state $^4F_{9/2}$ were measured and exhibits both single and non-exponential behavior.

1. Introduction

Currently, rare earth doped glasses have a great attention for development of photonics applications such as energy converter, sensors and solid-state lighting applications. The precise 4f-4f or 5d-4f narrow emission transition occurs through the shielding of 5s 6p outer electron by the 4f inner electron. This phenomenon is known as shielding effect. The rare earth ions can be doped with either crystalline or amorphous materials. When it is doped with amorphous material, the optical properties are more tunable for the required applications than crystalline [1]. From the various host materials borate has occupied a special place in the glass network due to low melting point, high RE ions solubility, high transparency and large thermal stability [1–3]. Borate glasses encourage the non-radiative process that dominates the absorption and emission due high phonon energy, an addition of phosphate in the network reduces the non-radiative process and hygroscopic nature along with high gain coefficient.

Introduction of modifier (Al_2O_3) in the network enrich the physical and optical properties of the glasses [2]. In addition to that, PbO has the dual nature of glass former as well as modifier that helps to formation of non-bridging oxygens and modified the triangle structural units into the tetragonal units [4]. The alkali element Li_2CO_3 plays vital role in the modification of the structural and optical behaviors of the RE doped glasses [3,4]. These oxides and alkali elements assorted with borophosphate glasses give the new physical and chemical properties with RE ions [1,4–11]. Among the different RE ion, Dy^{3+} has focused by many researchers because of the attractive optical behavior of light emitting in the visible region [12]. Interestingly, the intense emission band arises due to the electric and magnetic dipole moment corresponding to the transitions $^4F_{9/2}\rightarrow{}^6H_{13/2}$ and $^4F_{9/2}\rightarrow{}^6H_{15/2}$ respectively [13–18]. The above emission transitions in the blue and yellow regions yielding the capacity to develop white light.

* Corresponding author.
E-mail address: arulroy@gmail.com (I.A. Rayappan).

https://doi.org/10.1016/j.jnoncrysol.2021.120652
Received 29 September 2020; Received in revised form 31 December 2020; Accepted 4 January 2021
Available online 5 February 2021

Croatica Chemica Acta, Vol. 93 No. 2, 2020.

Original scientific paper

https://doi.org/10.5562/cca3695

A DFT Study on the Efficacy of Linking Agents (Sulfur and Nitrogen) to Connect Trans-azobenzene Sandwiched Between Two Gold Electrodes

C. Karthika ; Department of Physics, Kongu Engineering College (Autonomous), Perundurai, Erode-638 060, Tamil Nadu, India
R. Praveena ; Department of Chemistry, Bannari Amman Institute of Technology (Autonomous), Sathyamangalam Erode-638 401, Tamil Nadu, India
S. Ramachandran ; Department of Physics, Arignar Anna College (Arts & Science), Krishnagiri-635 115, Tamil Nadu, India
K. Sadasivam ; Department of Physics, Bannari Amman Institute of Technology (Autonomous), Sathyamangalam, Erode-638 401, Tamil Nadu, India
G. Salgado ; Facultad de Ciencias Quimicas, Investigador Extramural,Universidad de Concepcion, Chile
P. Muñoz ; Facultad de Ciencias Exactas, Depàrtamento de Quimica, Universidad Andres Bello, Santiago, Chile
L. Gerli ; Departamento de Quimica Ambiental, Universidad Catolica de la Santisima Concepcion, Concepcion, Chile
L. H. Mendoza-Huizar orcid.org/0000-0003-2373-4624 ; Autonomous University of Hidalgo State. Academic Area of Chemistry. Carretera Pachuca-Tulancingo Km. 4.5 Mineral de la Reforma, Hgo., México

Full text: english pdf 12.533 Kb page 147-155 downloads: **267** cite

Abstract

Electronic structure calculations were performed to analyze the effectiveness of linking agents (sulfur and nitrogen) in connecting the trans-azobenzene sandwiched between two gold surfaces (Au-atoms). It was analyzed the dynamics of the load carrier and the electronic structure of the molecular backbone by applying an external electric field (EF), also a detailed structural, frontier orbital and natural bond orbital analysis (NBO) were performed. From the NBO analysis, it was possible to predict the path of charge flow in the molecular system. Electrostatic potential mapping allowed us to visualize the charge redistribution in the molecular system caused by the EF application. Our results indicate that when the nitrogen atom is used as a linking agent, the azo group of molecules may enhance their conductivity.

Keywords

DFT-field application, Moltronics-linking agent, Molecular orbitals, NBO

Hrčak ID:

252017

URI

https://hrcak.srce.hr/252017

Materials Today: Proceedings 43 (2021) 3166–3168

Contents lists available at ScienceDirect

Materials Today: Proceedings

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

Studies on structural and optical properties of Cobalt doped ZnO thin films prepared by Sol-gel spin coating technique

Deepa Rani T [a,*], Sakshi Joshi A [b], Leela S [b]

[a] Kongu Engineering College, Erode, Tamil Nadu, India
[b] Ethiraj College for Women, Chennai, Tamil Nadu, India

ARTICLE INFO

Article history:
Available online 4 March 2021

Keywords:
ZnO
Co
XRD
UV
SEM

ABSTRACT

The Cobalt doped Zinc oxide (CZO) thin films were first prepared by sol–gel method. CZO transparent conductive thin films were deposited on glass substrates using spin coating technique. From XRD graph, the (002) diffraction peak intensity of CZO film decreased with increased doping concentration from 3 to 8 wt%. No extra peaks related to cobalt metal and other oxide phases were detected which illustrates that the obtained films are of single phase. Crystallite size (D) decreases gradually with increase in the Co doping level. The transmission curves of the Co doped ZnO thin films were taken in the wavelength area 300–800 nm. The average value was determined to be 80%. SEM images indicate the uniform distribution of spherical particles without any cracks or pore and exhibits good crystalline quality. It clearly shows that the crystalline decreases as cobalt concentration increases.

Selection and peer-review under responsibility of the scientific committee of Cutting-edge Research in Material Science and Chemistry (CRMSC-2021).

1. Introduction

Zinc oxide (ZnO) belonging to an II-IV metal oxide semiconductor is an interesting material for short wavelength optoelectronic applications owing to its wide band gap 3.37 eV, large bond strength, large exciton binding energy (60 MeV) at room temperature, non-toxic, and abundant in nature [1]. Because of these properties, ZnO thin films are integrated in optoelectronic applications, where they improve the optical absorption property [2]. ZnO has been considered as an alternative photocatalysts to TiO2 because it is highly active towards photo induced redox reaction, bio-compatible in nature, environment friendly and also exhibits high absorption efficiency [3]. ZnO has fascinated great interests because of their potential applications in optics and optoelectronic devices such as ultraviolet (UV) photodetectors, light emitting diodes (LEDs), Laser diodes (LDs), catalysts, gas sensors, and transparent conducting electrodes [4]. ZnO thin film is prepared using various techniques such as spray pyrolysis, radiofrequency (RF) sputtering, sol–gel spin coating, pulse laser deposition (PLD), chemical vapor deposition (CVD), and molecular beam epitaxy (MBE). The sol–gel spin coating method is low cost in compared with others and promising one to prepare components with uniform films, high yield and easy to control the film deposition, generated [5,6]. The adhesion of the film to the substrate is strong in sol–gel method [6]. Doping of ZnO thin films enhances both optical and electrical properties [7].The interest has been extensively grown to study metal iondoped ZnO rather than pure zinc oxide. The electronic structure of the material can be modified with doping leads to increase the generation of excitonspair particularly important for applications in light-induced phenomena [8].The transition metal doped ZnO forms a promising candidate material for the field of Spintronic application. In thin film form, when doped with Co2+, it generates a significant alteration in the band gap of ZnO [9]. The excellent optical properties of ZnO and the possibility of band gap engineering through transition metal ions (TM = Co; Mn; Ni ...) doping strongly encourages the exploration of the magneto-optical properties of the TM-doped ZnO system [6]. Also, doping is important to improve the photocatalytic efficiency of ZnO by retarding the recombination rate of charge carriers [3]. In particular, Co doped ZnO thin films exhibit high electron mobility, good optical transparency and high electrical conductivity [10].In this research work, Co doped ZnO thin films were prepared by sol–gel spin coating method on glass substrates and the structural and optical properties were investigated.

* Corresponding author.
E-mail address: deeparani@kongu.ac.in (D.R. T).

https://doi.org/10.1016/j.matpr.2021.01.658
2214-7853/
Selection and peer-review under responsibility of the scientific committee of Cutting-edge Research in Material Science and Chemistry (CRMSC-2021).

Physica E 129 (2021) 114665

Contents lists available at ScienceDirect

Physica E: Low-dimensional Systems and Nanostructures

journal homepage: http://www.elsevier.com/locate/physe

Room temperature ferromagnetic behavior of nickel-doped zinc oxide dilute magnetic semiconductor for spintronics applications

D. Anbuselvan [a], S. Nilavazhagan [a], A. Santhanam [a], N. Chidhambaram [a,*], K.V. Gunavathy [b], Tansir Ahamad [c,d], Saad M. Alshehri [c]

[a] Department of Physics, Rajah Serfoji Government College (Autonomous) [Affiliated to Bharathidasan University], Thanjavur, 613 005, Tamil Nadu, India
[b] Department of Physics, Kongu Engineering College, Perundurai, 638060, India
[c] Department of Chemistry, College of Science, King Saud University, P.O. Box 2455, Riyadh, 11451, Saudi Arabia
[d] School of Science and Technology, Glocal University, Saharanpur, India

ARTICLE INFO

Keywords:
Zinc oxide
Co-precipitation
Nickel doping
Room temperature ferromagnetism
Dilute magnetic semiconductor

ABSTRACT

The multifunctional zinc oxide (ZnO) nanoparticles were economically grown through a simple co-precipitation technique. Ni-doped (1, 3, and 5 wt%) ZnO nanoparticles were also grown to comprehend their influence on the ferromagnetic property of the ZnO, especially at room temperature. The structural and surface morphological features of the prepared nanoparticles were studied through X-ray diffraction (XRD) and Scanning electron microscopy (SEM) techniques, respectively. Diffused reflectance, Photoluminescence, and Fourier transform infrared spectroscopic analyses were also carried out to understand the consequence of Ni doping on the ZnO nanostructure. The secondary phase formations such as NiO and NiO_2 elucidate the solid solubility limit of three percent of nickel in the ZnO matrix. Size-strain analysis was performed to evaluate the crystallite size and apparent strain values. An increase in the agglomeration of particles is evidenced by SEM micrographs with an increase in the Ni doping percentage. The bandgap measurements showed a redshift from 3.25 to 3.18 eV for the Ni-doped nanoparticles. Photoluminescence study reveals the existence of lattice defects including interstitials and vacancies in the synthesized nanostructures. The vibrating sample magnetometer studies divulge that 3% Ni-doped ZnO nanoparticles show an intense ferromagnetic property at room temperature. These experimental observations manifested that the Ni-doped ZnO nanoparticles are potential candidates for spintronics device applications.

1. Introduction

The charge of an electron plays a crucial role in the working of semiconductor-based devices and the spin of the electron decides the performance of magnetic devices. When magnetic particles were introduced into the matrix of non-magnetic semiconductors, both the spin and the charge of an electron can be utilized to improve the device's performance. ZnO is one such multifunctional material having diverse applications in the field of optoelectronics to biomedicine [1–7]. This magnetic semiconductor is under rigorous research since the last decade due to its advantageous properties such as high exciton binding energy, thermal conductivity, photostability, refractive index, UV protection, and antibacterial activity as well as a low dielectric constant [8]. The magnetic semiconductor properties can be tailored based on its size and shape [9–11] in addition to the possibility of exhibiting ferromagnetic behavior at room temperature when doped with transition metal ions such as Fe [12], Ni [13], and Co [14]. Usually, ZnO reveals n-type conductivity due to the existence of intrinsic defects such as zinc interstitials and oxygen vacancies [15]. The charge and spin degrees of freedom of ZnO can be manipulated easily by adding suitable dopants. Usually, the transition metal ion replaces the cation in the ZnO matrix altering the electronic structure of the host material. Its prospective application lies in the spintronics field aiding in the manufacture of spin-dependent transistors and light-emitting diodes [16,17], varistors, laser diodes, and sensors. The wider bandgap (3.37 eV) of this material can also be tuned to modify its absorbance property to make it applicable in photocatalytic applications [18]. W. Liu et al.demonstrated that introduction of oxygen into metallic glasses converting them into magnetic semiconductors [19]. They introduced non-magnetic oxygen into a metallic glass to fabricate a $Co_{28.6}Fe_{12.4}Ta_{4.3}B_{8.7}O_{46}$ magnetic

* Corresponding author. Rajah Serfoji Government College (Autonomous), Thanjavur, 613005, Tamil Nadu, India.
E-mail address: nchidambaraselvan@gmail.com (N. Chidhambaram).

https://doi.org/10.1016/j.physe.2021.114665
Received 18 September 2020; Received in revised form 31 December 2020; Accepted 30 January 2021
Available online 4 February 2021

Indian Journal of Chemistry
Vol. 60A, May 2021, pp. 700-704

A DFT approach to analyze charge transfer path through *trans* and *cis* isomers of azobenzene

C Karthika[a], R Praveena[b] & K Sadasivam[c,]*

[a]Department of Physics, Kongu Engineering College (Autonomous), Perundurai, Erode, Tamil Nadu 638 060, India

[b]Department of Chemistry & [c]Department of Physics, Bannari Amman Institute of Technology (Autonomous), Sathyamangalam, Erode, Tamil Nadu 638 401, India

*E-mail: dftsada@gmail.com

Received 19 October 2020; revised and accepted 15 December 2020

The influence of external electrical field (EF) over the *trans* and *cis* isomers of azobenzene is investigated upto molecular orbital level with the aid of density functional theory. The frontier molecular orbital analysis and electrostatic potential (ESP) mapping are used to figure out the response of the molecules (*trans* and *cis* isomers of azobenzene) to the applied EF. The variation in dipole moment gives the extent of polarization in the molecule due to EF. With the aid of natural bond orbital analysis (NBO) the possible charge transfer path through the molecule can be predicted. ESP and NBO analysis clearly shows that drastic charge redistribution takes place for the EF strength of 0.15 V/Å. Hence the EF strength above 0.15 V/Å can be considered as threshold filed strength for organic molecular conductance. All these theoretical investigations provide a basic knowledge about the influence of molecular conformation over the conductivity of a molecule in the presence of EF.

Keywords: DFT, Azobenzene, Molecular orbitals, Charge distribution, NBO

During the past decade, an interdisciplinary group of physicists, chemists and engineers are performing a series of experimental and theoretical studies in molecular electronics to measure and control the charge transport through a single molecule[1-3]. Compared to experimental studies, theoretical investigations give an insight into the electronic structure of molecules which paves the way for the better understanding of the molecule's behaviour under various circumstances[4-6]. In this aspect density functional theory (DFT) is widely employed to find out the electron transport through single molecule sandwiched between two electrodes through a linking agent[7-9].

In this article *trans* and *cis* isomers of azobenzene, the simplest structure among azo- group, is considered for the study. Azo-compounds are well known for their photo-switching between *trans* and *cis* conformations in ultra violet range which makes it suitable to be used in molecular photoelectric switches, electrical data storage devices and logical devices with appropriate fictionalization[10-14]. Actual molecular circuits are established through chemical bonds without any macroscopic interface. But in most of the experimental methods like STM and AFM a single molecule is precisely positioned in between a metal substrate and a metal tip for measuring the electrical conductance of the molecule. Thus, it is necessary to represent such metal-molecule connection in theoretical study also. In this aspect, *trans* and *cis* isomers of azobenzene are connected to gold atoms (Au) through the linking agent nitrogen N. The purpose of including linking agent is to enhance the connection between the metal (Au) and organic molecule. This extended *trans* and *cis* isomers of azobenzene (with N and Au atoms) are named as M-I and M-II, respectively.

The study mainly focuses on the response of M-I and M-II to the applied electric field (EF). The information obtained from these analyses will be useful to tune azo-group of molecules for various applications in molecular electronics. Also the extent of the effect of molecular conformation over the electrical conductivity of a molecule is analyzed.

Materials and Methods

Computational details

All the calculations are carried out as implemented in Gaussian 09 software package[15] through DFT[16] with B3LYP hybrid functional. Since heavy atoms

coatings

MDPI

Article

Structural, Magnetic and Gas Sensing Activity of Pure and Cr Doped In_2O_3 Thin Films Grown by Pulsed Laser Deposition

Kamatam Hari Prasad [1,2,*], Karuppiah Deva Arun Kumar [3], Paolo Mele [3,*], Arulanandam Jegatha Christy [4], Kugalur Venkidusamy Gunavathy [5], Sultan Alomairy [6] and Mohammed Sultan Al-Buriahi [7]

1 Department of Physics, Institute of Aeronautical Engineering, Dundigal, Hyderabad 500043, India
2 Department of Physics, Pondicherry University, Puducherry 605014, India
3 College of Engineering, Shibaura Institute of Technology, Saitama 337-8570, Japan; i048267@shibaura-it.ac.jp
4 Department of Physics, Jayaraj Annapackiam College for Women, Periyakulam, Theni 625601, India; jegathachristy@gmail.com
5 Department of Physics, Kongu Engineering College, Perundurai 638060, India; gunavathy@kongu.ac.in
6 Department of Physics, College of Science, Taif University, P.O. Box 11099, Taif 21944, Saudi Arabia; s.alomairy@tu.edu.sa
7 Department of Physics, Sakarya University, 54100 Sakarya, Turkey; mohammed.al-buriahi@ogr.sakarya.edu.tr
* Correspondence: hariprasad.kamatam@gmail.com (K.H.P.); pmele@shibaura-it.ac.jp (P.M.)

Abstract: Pure In_2O_3 and 6% Cr-doped In_2O_3 thin films were prepared on a silicon (Si) substrate by pulsed laser deposition technique. The obtained In_2O_3/In_2O_3:Cr thin films structural, morphological, optical, magnetic and gas sensing properties were briefly investigated. The X-ray diffraction results confirmed that the grown thin films are in single-phase cubic bixbyte structure with space group *Ia*-3. The SEM analysis showed the formation of agglomerated spherical shape morphology with the decreased average grain size for Cr doped In_2O_3 thin film compared to pure In_2O_3 film. It is observed that the Cr doped In_2O_3 thin film shows the lower band gap energy and that the corresponding transmittance is around 80%. The X-ray photoelectron spectroscopy measurements revealed that the presence of oxygen vacancy in the doped In_2O_3 film. These oxygen defects could play a significant role to enhance the sensing performance towards chemical species. In the magnetic hysteresis loop, it is clear that the prepared films confirm the ferromagnetic behaviour and the maximum saturation value of 39 emu/cc for Cr doped In_2O_3 film. NH_3 gas sensing studies was also carried out at room temperature for both pure and Cr doped In_2O_3 films, and the obtained higher sensitivity is 182% for Cr doped In_2O_3, which is about nine times higher than for the pure In_2O_3 film due to the presence of defects on the doped film surface.

Keywords: In_2O_3/In_2O_3:Cr thin films; XPS; magnetization property; NH_3 sensor

Citation: Prasad, K.H.; Deva Arun Kumar, K.; Mele, P.; Christy, A.J.; Gunavathy, K.V.; Alomairy, S.; Al-Buriahi, M.S. Structural, Magnetic and Gas Sensing Activity of Pure and Cr Doped In_2O_3 Thin Films Grown by Pulsed Laser Deposition. *Coatings* **2021**, *11*, 588. https://doi.org/10.3390/coatings11050588

Academic Editor: Joe Sakai

Received: 18 April 2021
Accepted: 14 May 2021
Published: 17 May 2021

1. Introduction

High carrier mobility with the magnetic property of transparent metal oxides attracts as a miniature robust device for spintronic applications. This class of materials is called diluted magnetic metal oxide semiconductors (DMOS) [1]. These magnetic semiconductors could lead to unite the electrical manipulation of magnetic states and the magnetic adjustment of electrical signals that could result in devices such as bipolar transistors, spin resonant diodes, spin field effect transistors, magnetic semiconductor tunnel junction devices, magnetic bipolar junction diodes, and transistors, etc. [2–8]. If carrier-mediated magnetization can be induced in transparent semiconducting oxides such as In_2O_3, ZnO, TiO_2, etc., it is predicted that such DMOS will exhibit coupling among electrical, optical, and magnetic properties, further boosting the prospects of devices emanating from such materials. Among various transparent conducting oxide materials, In_2O_3, ZnO and SnO_2 are multipurpose materials with a wide range of applications in optoelectronics, solar cells, gas sensors, etc. [9–13], due to the interstitial defects of oxygen and other state defects.

Ionics (2021) 27:3443–3459
https://doi.org/10.1007/s11581-021-04106-w

ORIGINAL PAPER

Impact of ammonium formate (AF) and ethylene carbonate (EC) on the structural, electrical, transport and electrochemical properties of pectin-based biopolymer membranes

M. Muthukrishnan[1] · C. Shanthi[1] · S. Selvasekarapandian[2,3] · G. Shanthi[4] · L. Sampathkumar[5] · T. Maheshwari[6]

Received: 4 March 2021 / Revised: 26 April 2021 / Accepted: 16 May 2021 / Published online: 28 May 2021

Abstract

Ion conducting, biopolymer membranes (BPMs) based on pectin as host polymer, ammonium formate (AF) as proton donor salt and ethylene carbonate (EC) as plasticizer are prepared using a simple solution cast method. "Doping AF in host polymer increases the ionic conductivity up to $(2.74 \pm 0.15) \times 10^{-4}$ S cm^{-1} at the ambient temperature and incorporation of EC in to the polymer salt complex further enhances the conductivity to a maximum of $(3.6 \pm 0.21) \times 10^{-3}$ S cm^{-1}." Improvement in ionic conductivity owing to increased amorphous content of BPMs was investigated via X-ray diffraction (XRD) analysis. The interaction of AF and EC with the polymer host is analysed using Fourier transform infrared (FTIR) spectroscopy. The activation energy and regression values are calculated for prepared samples. The transport properties are determined using both the deconvoluted FTIR spectra and the transfer number measurement (TNM) technique, as well as the results are compared and correlated with the ionic conductivity of the BPMs. Using the highest conductive BPM, the primary proton battery was fabricated and the operation was explored and suggested as an alternative research direction for the lower current density applications with improved eco-friendly nature.

Keywords Biopolymer membranes · Plasticizer · Diffusion coefficient · Transference number · Deconvolution

Introduction

The increase in the world's population and economy, with rapid urbanization, will lead to a significant increase in energy consumption in the coming years. The transformation to a renewable energy system would have very positive economic impacts in the near future [1]. One such transition is the use of biopolymers derived from renewable resources for electrochemical applications. Biopolymers gain popularity due to their non-toxic, eco-friendly, biodegradable and biocompatible nature. Biopolymer electrolytes are synthesized by dissolving salts in biopolymers of high molecular weight. In recent years, based on biopolymers such as agar–agar [2], cellulose acetate [3], iota-carrageenan [4], kappa-carrageenan [5], chitosan [6], gelatine [7], dextran [8], carboxy methyl cellulose [9], starch [10], natural rubber [11], ion-conducting electrolytes for various applications have been reported. Over the past two decades, biopolymer membranes conducting lithium ions have been intensively studied. However, the smaller proton radius promotes the intercalation on the electrode contact surface, resulting in better performance for electrochemical applications, suggesting the proton-conducting biopolymer membrane as an alternative option for lithium-ion batteries [12].

In our current research, pectin was chosen as polymer host from the available biopolymers for the preparation of the proton-conducting polymer membrane for electrochemical applications. Pectin is a kind of biopolymer not commonly studied in the area of polymer electrolytes. It is a

✉ M. Muthukrishnan
mmkn80@gmail.com

[1] Department of Physics, Sona College of Technology, Salem 636005, India

[2] Materials Research Center, Coimbatore 641045, India

[3] Department of Physics, Bharathiar University, Coimbatore 641046, India

[4] Department of Chemistry, Sona College of Technology, Salem 636005, India

[5] Department of Physics, Builders Engineering College, Kangayam 638108, India

[6] Department of Physics, Kongu Engineering College, Perundurai 638060, India

Journal of Molecular Structure 1247 (2022) 131277

Contents lists available at ScienceDirect

Journal of Molecular Structure

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

Structural, spectroscopic (IR, Raman, and NMR), quantum chemical, and molecular docking analysis of (E)-2-(2,5-dimethoxybenzylidene)hydrazinecarbothioamide and its dimers

D. Shobana [a], S. Sudha [a,*], D. Ramarajan [a], Nikola Ristivojević [b], Aleksandra Rakić [b], Dušan Dimić [b]

[a] Department of Physics, Kongu Engineering College, Perundurai, Tamil Nadu 638060, India
[b] Faculty of Physical Chemistry, University of Belgrade, Studentski trg 12-16, Belgrade 11000, Serbia

ARTICLE INFO

Article history:
Received 22 June 2021
Revised 22 July 2021
Accepted 8 August 2021
Available online 11 August 2021

Keywords:
DFT
QTAIM
Thiosemicarbazide
Polo-like Kinase 1
Raman

ABSTRACT

Thiosemicarbazides are an important class of compounds with pronounced biological activities. In this contribution, the crystallographic structure of (E)-2-(2,5-dimethoxybenzylidene)hydrazinecarbothioamide (DBH) was described, and further spectroscopic studies (IR, Raman, ^{1}H, and ^{13}C NMR) studies were performed. Several density functional theory functionals (B3LYP, CAM-B3LYP, APFD, PBEPBE, M05-2X, and M06-2X) in conjunction with 6-311++G(d,p) were applied for the optimization of the structure. The highest resemblance to the crystallographic structure was obtained for structure optimized at M05-2X/6-311++G(d,p) level of theory. This structure was further used for the prediction of IR, Raman, and NMR spectra. The detailed vibrational and NMR analysis, with the most prominent bands assigned, proved that the experimental and theoretical spectra match well and that the obtained level of theory was suitable for the description of structure. Special emphasis was put on the analysis of dimers of **DBH** and water/DMSO-**DBH** structures to examine specific interactions. Natural Bond Orbital (NBO) and Quantum Atoms in Molecules (QTAIM) theories were applied for the quantification of the strength of these interactions. The most active positions were outlined through the calculation of the Fukui functions. A molecular docking study of DBH was performed towards Polo-like Kinase 1 (PLK1) to investigate the potential antitumor activity and the results were compared to volasertib. Specific interactions and binding affinities of monomers and dimers of **DBH** were discussed.

1. Introduction

Hydrazides are the significant starting material for a broad range of derivatives exploitable as surfactants and in pharmaceutical products. Hydrazides became more attractive to the leading theorists and experimenters because of their biological importance especially in enzyme and medicinal chemistry. Moreover, the molecular structure of hydrazides, which includes multifunctional groups such as an amine, amide, and a long alkyl chain, results in a chemically reactive molecule that may promote numerous organic synthesis reactions.

The thiosemicarbazide $H_2N–NH–C(=S)–NH_2$ and its S-alkylated derivatives are encouraging units for synthesizing new polyfunctional organic compounds with a variety of analytical and biological properties, including antibacterial, antifungal, anticonvulsant, biocidal, and antitumor activities [1–3]. Thiosemicarbazide is an especially fascinating scaffold because it allows more probable photochemical isomerization than hydrazines [4]. Because of their unusual properties, thiosemicarbazide-based derivatives are of great importance in scientific development, especially due to the formation of transition metal complexes with interesting biological activity [3,5]. They have a wide range of applications in structural chemistry. The Schiff bases have a higher inhibitory efficiency than amines and aldehydes since they have an imine functional group (-C=N-) [6].

Till now, the crystal structure of 2,5-Dimethoxybenzaldehyde thiosemicarbazone was reported by Fun et al. [7]. Synthesis, crystal structure, and characterization of (E)-2-(2,4-dimethoxybenzylidene)hydrazinecarbothioamide and (E)-2-(2,5-dimethoxybenzylidene)hydrazinecarbothioamide were done by Khalaji et al. [8]. The same compound showed high activity

* Corresponding author.
E-mail address: physicist.sudha@gmail.com (S. Sudha).

https://doi.org/10.1016/j.molstruc.2021.131277
0022-2860/

Optik - International Journal for Light and Electron Optics 247 (2021) 167869

Contents lists available at ScienceDirect

Optik

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

Structural, spectral, optical and Z-Scan budding studies of (*E*)-N′-(4-bromobenzylidene)-4-fluorobenzohydrazide

N. Latha [a], S. Sudha [b], D. Ramarajan [b], Barathi Diravidamani [a,*,1]

[a] PG and Research Department of Physics, N.K.R. Government Arts College for Women, Namakkal 637 001, Tamil Nadu, India
[b] Department of Physics, Kongu Engineering College, Perundurai 638 060, Tamil Nadu, India

ARTICLE INFO

Keywords:
BBFBH
FTIR
NMR
UV
Z-scan
DFT

ABSTRACT

A Schiff base third-order nonlinear optical material (*E*)-N′-(4-bromobenzylidene)− 4-fluorobenzohydrazide (BBFBH) was synthesized. It was characterized by victimization chemical analysis techniques like Fourier Transform Infrared (FTIR), Nuclear Magnetic Resonance (NMR), Ultra-Violet (UV) spectra and Z-scan. The molecular structure of hydrazide derivative $C_{14}H_{10}BrFN_2O$ has been studied with Gaussian 09 using density functional theory. The experimental and theoretical FTIR spectral peaks were analyzed and compared. The absorption in the Ultra-Violet region makes the material to be suitable for optical activity. The static first-order hyperpolarizability (β_0) were calculated and compared with carbamide. The molecule's potential and compatibility in optical limiting applications are revealed by Z-scan investigations.

1. Introduction

Organic nonlinear optical (NLO) materials are important in a variety of optical applications. Schiff bases are the most convenient approach to make NLO materials. Schiff base organic materials [1] are attracted extensive interest from different study fields such as physics and chemistry due to their optical nonlinearity which makes them demanded materials for optoelectronic properties [2], optical communication [3], electro-optical applications [4]. Also, NLO materials are used for extremely fast optical switching and modulation [5]. The z-scan approach is widely used experimental technique for nonlinear susceptibilities of various materials that are intensity-dependent like organometals [6], metal crystals [7] nano-particles [8], organic materials [9].

Hydrazides are identified as a tunable compound of Schiff base NLO material [10]. Albayati et al. also reported benzohydrazide derivative [11]. Ramesh Babu et al. [12] synthesized and reported the structural characterization of another benzohydrazide material. A low first-order hyperpolarizability value was pronounced by Abed [13]. Arunagiri et al. [14] have reported the synthesis, crystal structure and vibrational spectra analyses, DFT computations, electronic properties and Hirshfeld analysis of (E)=4-Bromo-N′-(2, 4-dihydroxybenzylidene)benzohydrazide. The nonlinear optical property of this material has been proved by Z-scan analysis in this research work. Other benzohydrazide derivatives were also shown to be excellent NLO materials [15,16]. The synthesis of hydrazide derivative with high molecular hyperpolarizabilities exhibit several considerable NLO properties. The Z-scan technique is the simplest methodology for determining third-order optical nonlinearity. So, the literature survey reveals that the hydrazide derivatives are good candidate for NLO applications.

* Corresponding author.
E-mail address: barathi.rammohan@gmail.com (B. Diravidamani).
[1] ORCID ID: http://orcid org/0000-0003-1965-084X.

https://doi.org/10.1016/j.ijleo.2021.167869
Received 28 June 2021; Received in revised form 14 August 2021; Accepted 21 August 2021
Available online 27 August 2021

Physica Scripta

PAPER

Optimization of the optoelectronic properties of copper zinc tin sulfide thin films for solar photovoltaic applications

RECEIVED
30 March 2021

REVISED
14 July 2021

ACCEPTED FOR PUBLICATION
21 July 2021

PUBLISHED
12 October 2021

K V Gunavathy[1], A M S Arulanantham[2], Aslam Khan[3], C S A Raj[4], Ahmed M El-Toni[3], Muhammad A Shar[3], Anees A Ansari[3] and S AlFaify[5]

[1] Thin Film Research Centre, Kongu Engineering College, Perundurai, 638060, India
[2] Department of Physics, St. Joseph College of Arts and Science, Vaikalipatti, 627808, India
[3] King Abdullah Institute for Nanotechnology, King Saud University, Riyadh, 11451, Saudi Arabia
[4] PG & Research Department of Physics, Arul Anandar College, Karumathur, 625514, India
[5] Advanced Functional Materials and Optoelectronics Laboratory (AFMOL), Department of Physics College of Science, King Khalid University, Abha, 61413, Saudi Arabia

E-mail: aslamkhan@ksu.edu.sa

Keywords: solar cell, Cu2ZnSnS4 thin film, nebulizer assisted spray pyrolysis, precursor variation, optoelectronic properties

Abstract

Copper Zinc Tin Sulfide (CZTS), a successful contender for environmentallybenign thin film photovoltaics was successfully prepared on soda-lime glass substrates through an economically feasible nebulizer assisted spray pyrolysis technique. Further, a solar cell structure withn-CdS/p-CZTSheterojunction was fabricated to study the performance of the nebulizer sprayed CZTS absorber layer using different precursor solutions for copper such as copper acetate, copper chloride, and copper nitrate. Investigations were done to ascertain the influence of different copper precursors on the optoelectronic properties of CZTS thin films by systematically analyzing their characteristics determined by using different analytical techniques. X-ray diffraction studies show a preferential orientation along (112) plane for the deposited kesterite film. The obtained film thickness and crystallite size were found to be 507 nm and 8 nm, respectively, for the film derived from copper nitrate based spray solution. AFM morphological analysis also confirmed a higher particle size for copper nitrate based CZTS film whose band gap was found to be 1.50 eV. The absorption characteristic was also in the favor of nitrate form of the copper precursor which shows a higher absorption value in the visible region than the rest of the samples. Its carrier concentration was found to be 8.06×10^{17} cm^{-3} which is 4 times higher than the rest of the films and mobility was found to be of the order of 12.3 $cm^2 V^{-1} s^{-1}$. The open circuit voltage, short circuit current, fill factor, and efficiency of copper nitrate based CZTS solar cell structure was found to be better and is determined to be 0.27 V, 2.51 mA cm^{-2}, 24.3%, and 0.165%.

1. Introduction

Recent advances in thin film fabrication technology have resulted in the production of many commercially viable thin films having diverse applications from nanotechnology to space missions. It is more remarkable in the field of photovoltaic conversion of energy. The best performing thin film solar cells are based on CIGS or CdTe [1, 2] whose constituents are either rare and costly or toxic. So the major concern in solar thin film technology is to produce an absorber that is cheap and ecofriendly. Due to the similar structure and bandgap like CIGS and its excellent visible light absorption, CZTS is an emerging absorber material belonging to the chalcogenide family [3–5]. In addition, due to its isoelectronic structure, much extensively studied chalcopyrite fabrication technologies can be used to prepare this quaternary compound semiconductor. The advantage of CZTS is its earth abundance and non-toxic nature which makes it cheap, besides its favorable characteristics such as high absorption coefficient around the visible region and its optimal direct tunable bandgap lying around 1.5 eV [6]. The Shockley–Queisser theoretical limit predicts the highest efficiency of around 33% for a

J Mater Sci: Mater Electron (2021) 32:25493–25506

Influence of carrier gas pressure on the characteristics of nebulizer-sprayed Cu_2ZnSnS_4 absorber thin films

K. V. Gunavathy[1,*], A. M. S. Arulanantham[2], K. Tamilarasan[1], C. Rangasami[1], M. Malathi[1], Mohd Shkir[3,4], and S. AlFaify[3,4]

[1]*Thin Film Research Centre, Kongu Engineering College, Perundurai 638060, India*
[2]*Department of Physics, St. Joseph College of Arts and Science, Vaikalipatti 627808, India*
[3]*Research Centre for Advanced Materials Science (RCAMS), King Khalid University, Abha 61413, Saudi Arabia*
[4]*Advanced Functional Materials and Optoelectronic Laboratory (AFMOL), Department of Physics, Faculty of Science, King Khalid University, Abha 61413, Saudi Arabia*

Received: 10 June 2021
Accepted: 9 September 2021
Published online: 24 September 2021

ABSTRACT

The current work reports the synthesis of the Earth-abundant Copper Zinc Tin Sulfide (CZTS) absorber thin films at low temperature through modified spray pyrolysis technique without high-temperature annealing. The impact of carrier gas pressure during the synthesis of this potential solar absorbing material in the form of thin film is studied within the range of 0.10 to 0.20 Pa at a substrate temperature of 350°C to understand the variation in its inherent characteristics. The deposited films were analyzed subsequently using X-ray diffraction, Raman spectroscopy, Scanning electron microscopy, Energy dispersive X-ray spectroscopy, Atomic force microscopy, and a UV–Vis spectrophotometer. The influence of the carrier gas pressure on the electrical property of the deposited films is also studied by analyzing its I–V characteristics. Structural and morphological analysis exhibits the formation of highly crystalline CZTS absorber film with good adherence on SLG substrate. The Raman analysis establishes the kesterite structure and the phase purity in the grown CZTS films except 0.15 Pa sample which shows the presence of a trace of Cu_2S binary phase. The grain size as well as roughness of the deposited films is observed to increase with the gas pressure up to 0.15 Pa and decreased thereafter. The band gap of the film is found to decrease from 1.42 to 1.30 eV under the testing limits. The I–V characteristics of the deposited film at 0.15 Pa show higher current value than the rest of the samples. Apart from the study of influence of carrier gas pressure, this study also confirms the usage of the modified nebulizer-assisted spray pyrolysis technique as one of the economical fabrication methods for mass production of nontoxic CZTS absorber thin films that can be used in the development of environment-friendly low-cost solar cells.

Address correspondence to E-mail: gunavathy.kec@gmail.com

https://doi.org/10.1007/s10854-021-07014-x

Indian J Phys
https://doi.org/10.1007/s12648-021-02215-w

ORIGINAL PAPER

Concentration dependence of white light generation in Dy^{3+}-doped lithium-fluoroborophosphate glasses

V A Raj[1,3], K Maheshvaran[2] and I A Rayappan[3]*

[1]Department of Physics, Bishop Heber College (Autonomous), Affiliated To Bharathidasan University, Tiruchirappalli 620017, India

[2]Department of Physics, Kongu Engineering College, Perundurai, Erode 638060, India

[3]Department of Physics, St. Joseph's College (Autonomous), Affiliated To Bharathidasan University, Tiruchirappalli 620002, India

Received: 14 March 2021 / Accepted: 25 September 2021

Abstract: A new series of Dy^{3+}-doped lithium-fluoroborophosphate glasses have been prepared by conventional melt-quenching technique and explored by XRD, FTIR, optical absorption, photoluminescence and decay spectral measurements . XRD results confirm the amorphous nature of the prepared glass. The physical properties were calculated with density and refractive index measurements. FTIR spectra reveal the various stretching and bending vibration of borate (BO_3 and BO_4) and also phosphate (PO_4) networks. The absorption spectra exhibit nine absorption peaks from the ground state $^6H_{15/2}$ to various excited states. Using absorption spectra ligand field environment around the Dy^{3+} ions, Judd–Ofelt parameters, optical band gap and Urbach's energy were calculated and reported. The JO theory has been applied to calculate the oscillator strengths and to evaluate the radiative properties of the emission transitions of Dy^{3+} ions in the prepared glasses. The luminescence spectra exhibit three transitions $^4F_{9/2} \rightarrow {}^6H_J$ (J = 9/2, 11/2, 13/2) at 483 nm (blue), 574 nm (yellow) and 663 nm (red), respectively. The Inokuti–Hirayama (IH) model (S = 6) fits well with non-exponential decay curves and indicates dipole–dipole interaction between donor and acceptor Dy^{3+} ions through cross-relaxation. The (x, y) coordinates and CCT values of the prepared glasses are found to be near the white light region representing the suitability of synthesized glasses for solid-state lighting applications.

Keywords: Melt-quenching technique; Rare earth; Absorption; Photoluminescence; CIE diagram; Fluoroborophosphate glasses

1. Introduction

Over a period of time, rare earth (RE) ions-doped materials have achieved a remarkable importance in the field of research because of the unique transitions between 4f-4f levels shielded by the outermost shells. The glasses are the best optical materials for RE ion doping as compared to ceramics and phosphors because of good RE ions solubility and good chemical, mechanical and thermal stability [1–5]. These properties attracted the researchers to prepare and investigate RE ions-doped glasses. Among the various glass network formers, borate glasses are more interesting because of their physical, optical and structural properties, along with modifiers like alkali metal oxides [6–8]. The addition of phosphate into the borate (B_2O_3) glass forms a cross-linked P-O-B bonds which enhances the mechanical and thermal stability, chemical durability and increase in glass-forming ability [9, 10]. There has been a good interest in synthesis and investigation of Dy^{3+}-doped B_2O_3–P_2O_5 glasses, for the applications in diversified fields like solid-state lighting and lasers, IR to visible up converts, field emission display and non-linear optical devices.

In borate network, addition of network modifiers in certain compositions increases the degree of polymerization, converting boron coordination from BO_3 to BO_4, resulting increase of non-bridging oxygen's. Whereas in phosphate network, the modifiers lead to depolymerization by breaking P-O-P bridges and creating non-bridging oxygen's. The mixture of these two network formers, B_2O_3–P_2O_5, allows considerable modifications of the host structure by controlling volume nucleation, resulting a higher disorder. The network modifiers are playing vital role in forming hypersensitive transition with high

*Corresponding author, E-mail: arulroy@gmail.com

Published online: 26 October 2021

Journal of Molecular Structure 1250 (2022) 131856

Contents lists available at ScienceDirect

Journal of Molecular Structure

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

Synthesis, crystal structure, spectral characterization and Hirshfeld surface analysis of (E)-N′-(3-ethoxy-4-hydroxybenzylidene)-4-fluorobenzohydrazide single-crystal – a novel NLO active material

D. Shobana [a], S. Sudha [a,*], D. Ramarajan [a], D. Dimić [b]

[a] Department of Physics, Kongu Engineering College, Perundurai, Erode, Tamil Nadu 638 060, India
[b] Faculty of Physical Chemistry, University of Belgrade, Studentski trg 12-16, Belgrade 11000, Serbia

ARTICLE INFO

Article history:
Received 12 October 2021
Accepted 31 October 2021
Available online 2 November 2021

Keywords:
XRD
FTIR
NBO
Z-scan
Hirshfeld surface analysis
3E4H4FB

ABSTRACT

(E)-N′-(3-ethoxy-4-hydroxybenzylidene)-4-fluorobenzohydrazide (3E4H4FB) single crystal was obtained by recrystallization method. Single-crystal X-ray diffraction analysis revealed the crystalline structure, packing, and molecular geometry features of the prepared crystal. The structural parameters such as bond distances and angles of 3E4H4FB crystal were discussed. The B3LYP/6-311G(d,p) level of theory was used to do optimize the structure, and the computed results reveal that the optimized geometry can perfectly replicate the crystal structure. The inter- and intramolecular hydrogen bonding interactions were also interpreted. Hirshfeld surface analysis was used to elucidate and quantify the intermolecular interactions between the molecules in the crystal structure. FTIR analysis was applied to identify the characteristic functional groups of the synthesized crystal. Natural bond orbital (NBO) and Quantum Theory of Atoms in Molecules (QTAIM) analyzes of the molecule were also used to quantify interactions present in the molecule. The excitation wavelengths, oscillator strengths, and excitation energies were determined by the TD-DFT calculations and compared to the experimental wavelengths. The charge transfer within the molecule was explained by the frontier molecular orbital analysis. Nonlinear optical (NLO) properties were calculated to predict the electric dipole moment and first-order hyperpolarizability of the compound. The static third-order susceptibility value was measured by the Z-scan technique. Finally, the ecotoxicity impact of the novel NLO material was assessed towards fish, daphnia, and green algae.

1. Introduction

Researchers are drawn to organic materials in their search for technologically important materials because of their delocalized electronic structure. Organic molecules with electron donor and acceptor groups have a π-conjugated system, which makes these materials suitable for nonlinear optical (NLO) application [1]. Attempts to design and synthesize Schiff bases and their complexes have been made for decades to employ these molecules in diverse fields of research. Schiff bases are prepared by forming an azomethine or imine (–CH=N–) group by condensation of a primary amine with an aldehyde or ketone. The carboxyl (C=O) group is substituted with the C=N-R group in a Schiff base, which is a nitrogen analog of an aldehyde or ketone. Schiff bases are used as good chelating agents due to their relative ease of synthesis, synthetic flexibility, and the specific property of the C=N group. Due to the broad spectrum of applications, Schiff bases have been employed in organic dyes catalysts, liquid crystals and also used as intermediates for several bioactive compounds [2]. Due to the presence of delocalized electron clouds between donor and acceptor groups, Schiff bases demonstrate unique hyperpolarizabilities as characteristics of interest [3].

The hydrazones have the formula >C=N–N, which makes them nucleophilic and electrophilic. The nitrogen atom in the hydrazone moiety is nucleophilic, whereas the carbon atom is both nucleophilic and electrophilic. The nucleophilic and electrophilic behavior of hydrazones strengthens their efficacy in organic chemistry and drug designing networks [4]. Benzohydrazide derivative crystals have good third-order nonlinear optical properties. Benzohydrazide derivatives also have antibacterial and antitubercular properties, making them possible prostate cancer inhibitors [5], and also have antifungal and antiproliferative activities.

* Corresponding author.
E-mail address: physicist.sudha@gmail.com (S. Sudha).

https://doi.org/10.1016/j.molstruc.2021.131856
0022-2860/

ScienceDirect

Journal of the Indian Chemical Society
Volume 99, Issue 2, February 2022, 100342

Structure, surface analysis and bioactivity of Mn doped zinc oxide nanoparticles

P. Pachamuthu [a], A. Pricilla Jeyakumari [b], N. Srinivasan [c], R. Chandrasekaran [d], K. Revathi [e], P. Karuppannan [f]

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https://doi.org/10.1016/j.jics.2022.100342

Highlights

- Undoped and Mn (5 atomic % & 10 atomic %) doped zinc oxide nanoparticles were prepared by the soft chemical method.
- The nanoparticles were characterized using XRD, SEM, EDAX, UV–Vis, FT-IR, and room temperature PL Analysis.
- Antimicrobial activity of prepared nanoparticles were tested against both gram positive and gram negative human pathogens.
- The antioxidant potential of prepared nanoparticles was estimated using Phosphomolybdate and DPPH assay.
- The MTT assay was used for cytotoxicity evaluation of prepared nanoparticles against breast cancer cell line MDAMB231.

Abstract

Undoped zinc oxide nanoparticles and Mn (5 atomic % & 10 atomic %) doped zinc oxide nanoparticles were prepared by soft chemical method. Antibacterial, antioxidant and anticancer activities in breast cancer cell line MDAMB231 of prepared nanoparticles were investigated. The nanoparticles were characterized using XRD, SEM, EDAX, UV–Vis, FT-IR, and room temperature PL Analysis. Antimicrobial activity was tested against both gram positive and gram negative human pathogens. The antioxidant potential of prepared nanoparticles was estimated using Phosphomolybdate and DPPH assay. The MTT assay was used for cytotoxicity evaluation of prepared

J Mater Sci: Mater Electron (2022) 33:10814–10827

Influence of heat treatment on the optoelectronic performance of electrodeposited CdSe thin films

A. M. S. Arulanantham[1], M. Maria Stephy[1], K. V. Gunavathy[2,*], N. Sundaramurthy[3], P. Mohanraj[4], and Ehab El Sayed Massoud[5,6,7]

[1] *Department of Physics, St. Joseph College of Arts and Science, Vaikalipatti 627808, India*
[2] *Thin Film Research Centre, Kongu Engineering College, Perundurai 638060, India*
[3] *Department of Physics, Annamalai University, Chidambaram 608002, India*
[4] *Department of Physics, Pondicherry University, Pondicherry 605014, India*
[5] *Biology Department, Faculty of Science and Arts in Dhahran Al Janoub, King Khalid University, Abha, Kingdom of Saudi Arabia*
[6] *Research Center for Advanced Materials Science (RCAMS), King Khalid University, Abha, Kingdom of Saudi Arabia*
[7] *Agriculture Research Centre, Soil, Water and Environment Research Institute, Giza, Egypt*

Received: 14 January 2022
Accepted: 8 March 2022
Published online: 22 March 2022

ABSTRACT

In this work, a thin film of Cadmium selenide is deposited on fluorine tin oxide-coated glass substrate through a simplified 2-electrode electrodeposition technique. The performance of the as-deposited films is compared with its annealed counterparts at two different temperatures of 250 °C and 350 °C in air. The impacts of annealing on different physical characteristics of the prepared films were investigated with the help of an X-ray diffractometer (XRD), scanning electron microscopy, and UV–Vis spectrometer. Studies on the photoresponse characteristics of the deposited films were also carried out. Structural a nalysis was done to determine the lattice parameters, size of the crystallite, dislocation density, and microstrain, utilizing the data from XRD analysis which exhibits a predominant orientation of CdSe films along (002) direction and showed the presence of hexagonal nanocrystalline phase. Morphological analysis shows larger grains for 350 °C-annealed sample than the as-grown and the 250 °C-annealed sample. The analysis of the optical property confirms a higher absorption in the visible region and shows a band gap of 1.65 eV at the annealing temperature of 350 °C. The photoresponse characteristic recorded a responsivity of 109 × 10^{-2} A/W, detectivity of 192 × 10^{8} Jones, and an external quantum efficiency of 253% for the same sample which is annealed at higher temperature. The calculated rise time and decay time from the transient current characteristics at different incident power intensities were found to be 4.4 s and 5.1 s, respectively. The I–V characterization curve of the 350 °C-annealed CdSe sample affirms a good photocurrent response demonstrating that the heat treatment on the electrodeposited CdSe films improves its photodetecting capability that can be exploited for photodetector device applications.

Address correspondence to E-mail: gunavathy.kec@gmail.com

https://doi.org/10.1007/s10854-022-08062-7

Journal of Molecular Structure 1253 (2022) 132259

Contents lists available at ScienceDirect

Journal of Molecular Structure

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

Structural, spectroscopic, quantum chemical, and molecular docking investigation of (E)-N'-(2,5-dimethoxybenzylidene)picolinohydrazide

Eswaran Kavitha[a], Devarajan Ramarajan[b], Aleksandra Rakić[c], Dušan Dimić[c,*], Shanmugam Sudha[b,*], Putta Narasimhan Nirmala[d]

[a] Department of Physics, N.K.R. Govt Arts College for Women, Namakkal 637001, Tamil Nadu, India
[b] Department of Physics, Kongu Engineering College, Perundurai 638060, Tamil Nadu, India
[c] University of Belgrade, Faculty of Physical Chemistry, Studentski trg 12-16, Belgrade 11000, Serbia
[d] Department of Physics, Sri Meenakshi Govt Arts College for Women (A), Madurai 625002, Tamil Nadu, India

ARTICLE INFO

Article history:
Received 21 November 2021
Revised 14 December 2021
Accepted 20 December 2021
Available online 22 December 2021

Keywords:
XRD
Vibrational spectra
NMR
QTAIM
Z-scan
DBP

ABSTRACT

Schiff bases and hydrazides are groups of compounds with important biological activities. In this contribution, (E)-N'-(2,5-dimethoxybenzylidene)picolinohydrazide (**DBP**) was synthesized and characterized by X-ray crystallography, IR, Raman, UV–vis and NMR spectroscopies. The Hirshfeld surface analysis was performed to investigate the interactions within the crystal package. The structure of **DBP** was optimized by several functionals (B3LYP, CAM-B3LYP, B3PW91, M05-2X, and M06-2X) in conjunction with the 6-311++G(d,p) basis set. The suitable level of theory was determined based on the comparison between experimental and theoretical bond lengths and angles (M06-2X/6-311++G(d,p)). The Natural Bond Orbital (NBO) and Quantum Theory of Atoms in Molecules (QTAIM) approaches were used for the quantification of the interaction strengths within a structure. The experimental IR and Raman peaks were assigned based on the calculated one, with the aid of the Potential Energy Distribution (PED) analysis. The ^{1}H and ^{13}C NMR signals were also assigned when compared to the calculated ones. The reproducibility of the experimental results proved that a suitable level of theory was obtained. The experimental UV–vis spectra consisted of a wide peak between 200 and 450 nm, while the most prominent theoretical transitions were located at 324, 231, and 213 nm. The nonlinear optical (NLO) studies Z-scan experiment allowed the determination of the nonlinear absorption coefficient and nonlinear refractive index, thus proving that **DBP** can be used as NLO material. Various reactivity descriptors of **DBP** and its analogs were computed and the reactivity was checked towards Cyclin-Dependent Kinase 2 protein, with the influence of structural parameters explained.

1. Introduction

Schiff bases have received much interest in different fields because of their unique properties such as thermal stability, preparative accessibility, biological activities, structural diversity, varied coordination capacity, and catalytic properties [1,2].

Schiff bases are ketone or aldehyde-like compounds with an azomethine (-C=N-) group replacing the carbonyl group. Schiff bases have a wide variety of uses, such as catalysts [3], stabilizers, dyes [4], and organic synthesis intermediates. Furthermore, Schiff bases have a variety of biological functions, involving antiproliferative [5], antioxidant [6], antifungal, antiviral, antibacterial, anti-inflammatory, antimalarial [7], and antipyretic effects, though the exact action mechanisms of these Schiff bases are unknown. The Schiff base molecular structure has been shown to impact the biological activities and therefore, the structural analysis of Schiff base compounds can shed light on the structure-bioactivity relationships [8].

Hydrazides became very attractive to both theoreticians and experimentalists because of their biological importance especially in enzyme and medicinal chemistry [9–11]. Moreover, the molecular structure of hydrazides, which includes multifunctional groups such as an amine, amide, and long alkyl chain, results in a chemically reactive molecule that may promote numerous organic synthesis reactions [9]. The scientific community has continued focusing on the preparation and production of novel derivatives to achieve greater biological applications for these kinds of molecules [12].

* Corresponding authors.
E-mail addresses: ddimic@ffh.bg.ac.rs (D. Dimić), physicist.sudha@gmail.com (S. Sudha).

https://doi.org/10.1016/j.molstruc.2021.132259
0022-2860/

International Journal of Green Energy ›
Volume 19, 2022 - Issue 3

Research Article

Synthesis and characterization of Dextran, poly (vinyl alcohol) blend biopolymer electrolytes with NH_4NO_3, for electrochemical applications

T. Maheshwari, K. Tamilarasan, S. Selvasekarapandian, R. Chitra & M Muthukrishnan

Pages 314-330 | Received 06 Jan 2021, Accepted 29 May 2021, Published online: 16 Jul 2021

Download citation https://doi.org/10.1080/15435075.2021.1946811 Check for updates

ABSTRACT

New biocompatible biopolymer membranes have been synthesized from naturally occurring bacterial polysaccharide Dextran, which is efficacious versatile polymer known for medicinal applications. In the present study, biodegradable solid polymer electrolytes based on Dextran:Poly vinyl alcohol (PVA) with different composition of ammonium nitrate (NH_4NO_3) are prepared by solution casting technique with double

Physica Scripta

PAPER

Enhancing the photodetection property of CdSe thin films via thermal evaporation technique: role of substrate temperature

RECEIVED
13 March 2022

ACCEPTED FOR PUBLICATION
28 March 2022

PUBLISHED
7 April 2022

S Sathish Kumar[1], S Valanarasu[1,*], K V Gunavathy[2], S Vinoth[3], Kumar Haunsbhavi[4], Devarajan Alagarasan[5], K Deva Arun Kumar[1], Mohd Ubaidullah[6,*], Shoyebmohamad F. Shaikh[6] and Bidhan Pandit[7]

[1] PG and Research Department of Physics, Arul Anandar College, Karumathur, India
[2] Thin Film Research Centre, Kongu Engineering College, Perundurai, 638060, India
[3] Department of Electronics and Communication Engineering, Manakula Vinayagar Institute of Technology, Kalitheerthalkuppam, Puduchcrry—605 107, India
[4] Department of Physics, Jnanabharathi Campus, Bangalore University, Bangalore 560056, India
[5] Department of Physics, Indian Institute of Science, Bengaluru, 560012, India
[6] Department of Chemistry, College of Science, King Saud University, Riyadh 11451, Saudi Arabia
[7] Department of Materials Science and Engineering and Chemical Engineering, Universidad Carlos III de Madrid, Avenida de la Universidad 30, 28911 Leganés, Madrid, Spain
* Authors to whom any correspondence should be addressed.

E-mail: valanroyal@gmail.com **and** mtayyab@ksu.edu.sa

Keywords: CdSe thin films, thermal evaporation technique, photodetector, substrate temperature

Supplementary material for this article is available online

Abstract

The current work investigates the influence of the substrate temperature on the photodetection capability of cadmium selenide (CdSe) thin films deposited through economically viable thermal evaporation technique on glass substrates. The substrate temperature varied from room temperature (30 °C to 250 °C). The existence of a single-phase of hexagonal structured CdSe was established from XRD patterns with dominant peaks along the (002) plane in all the samples. The SEM micrographs show the homogeneous surface of the films without any pinholes. The bandgap of the films was found to vary with the variation in the substrate temperature and the sample fabricated at 200 °C substrate temperature showed a bandgap of 2.00 eV. The light-dependent electrical analysis is also made to reveal the photodetection capability of the deposited CdSe films. The 200°C deposited CdSe film exhibits a higher responsivity of 8.07×10^{-2} A W^{-1} and a maximum detectivity of 6.66×10^{9} Jones. The external quantum efficiency (EQE) was found to rise with the substrate temperature and a maximum value of 18.8% for the 200 °C deposited sample. The observed rise and decay times show a rapid response when the incident light intensity is changed from 1 to 5 mW cm^{-2}.

1. Introduction

Research on metal chalcogenide thin films has increased enormously in the last decade due to their heavy demand in the optoelectronic industries as laser diodes, light emitting diodes [1], and photodetectors [2]. Apart from optoelectronic industries, the narrow bandgap semiconductors such as CdSe and CdS found their applications in the field of photonics as well as nanoelectronics owing to the enhancement in their electrical properties at the nanoscale. In particular, the CdSe thin films were under rigorous research to improve their inherent properties to find their application in devices such as solar cells [3], photoelectrochemical cells [4], thin film transistors [5, 6], radiation detectors, sensors [7, 8], bio labeling probes [9], photoconductors [10] and acoustic optical devices [11].

CdSe is an n-type semiconductor that belongs to group II–VI materials and has a direct bandgap. It is found to exist in Wurtzite (hexagonal), Zinc blende (cubic), or in a mixed hexagonal cubic structure. The bandgap varies according to its structure defining its field of application. It has a larger bandgap of 1.80 eV in the wurtzite

Applied Physics A (2022) 128:364
https://doi.org/10.1007/s00339-022-05491-3

Applied Physics A
Materials Science & Processing

Photosensitivity properties of Eu-doped SnS_2 thin films deposited by cost-effective nebulizer spray pyrolysis technique

A. M. S. Arulanantham[1] · P. Mohan Raj[2] · K. V. Gunavathy[3] · M. Rigana Begam[4] · V. Ganesh[5] · H. Algarni[5]

Received: 19 January 2022 / Accepted: 14 March 2022

Abstract

The current research explores the outcome of europium doping on the structure, morphology, electrical conductivity and optoelectronic characteristics of SnS_2 thin films deposited on glass substrates by nebulizer spray technique. X-ray diffraction analysis substantiates the presence of hexagonal structure in both pure and Eu-doped SnS_2 thin films with the highly preferred orientation diffracted from the plane (002). It shows the intensity of the predominant peak is highest for 2% Eu-doped SnS_2 thin film. From the XRD data, the crystallite size was found to be highest for 2% SnS_2:Eu, and same sample showed a less dislocation density of 0.97×10^{15} lines/m^2 and microstrain of 0.081×10^{-3}/lines^2 m^4. The crystallite size first increases with increasing doping concentration of Eu (0–2%), then decreases for higher concentrations. The SEM and AFM micro images reveal the agglomeration of grains at higher Eu concentration. The compositional analysis through EDAX studies supports the presence of Eu, Sn and S. The SnS_2 optical band gap value is found to vary from 2.70 to 2.91 eV as the Eu doping is increased from 2 to 6%. All the SnS_2 thin film samples manifest a n-type conductivity as authenticated from Hall studies and a low resistivity of 4.34×10^{-1} cm with an elevated carrier concentration of 5.43×10^{17} cm^{-3}, respectively, was observed for SnS_2:Eu (2 wt%). The same sample established a higher responsivity (41.64×10^{-3} AW^{-1}), competent external quantum efficiency (97.24%), and a better detectivity (40.88×10^8 Jones). Hence, the 2% Eu-doped SnS_2 film is recognized to be best suited for the fabrication of high-speed optoelectronic devices. This paper also discusses a putative mechanism for photodetector performance under air and UV radiation.

Keywords Europium-doped SnS_2 · Optical studies · Hall-effect measurement · Photosensitivity

1 Introduction

Metal-based semi-conducting chalcogenide thin films have showed considerable promise in the production of optoelectronic devices, solar cells, thermoelectric, and sensor applications in recent years [1–4]. The physical, chemical, and optoelectronic features of sandwiched metal-based chalcogenide-related materials have been best revealed lately, including excellent transparency, carrier mobility, superior pliability, and high specific surface area. Layered semiconducting transition-metal dichalcogenides such as WS_2, MoS_2, SnS_2, and WSe_2 materials have been reported to have exceptional optical and electrical properties, making them ideal for photo sensing applications [5–8].

SnS_2 is a significant optical semiconductor that can be tuned to exhibit either n-type orp-type conductivity based on the dominance of either tin or sulfur molar concentrations [9]. Depending on the bonding properties of tin with sulfur, the sulfide exists in a number of phases, such as SnS, SnS_2,

✉ A. M. S. Arulanantham
amsarul@gmail.com

1 St. Joseph College of Arts and Science, Vaikalipatti, Tirunelveli 627808, India

2 Department of Physics, Pondicherry University, Pondicherry 605014, India

3 Thin Film Research Centre, Kongu Engineering College, Perundurai 638060, India

4 Department of Physics, School of Science and Humanities, Vel Tech Rangarajan Dr.Sagunthala R&D Institute of Science and Technology, Avadi, Chennai 600062, India

5 Advanced Functional Materials and Optoelectronic Laboratory (AFMOL), Department of Physics, Faculty of Science, King Khalid University, P.O. Box 9004, Abha, Saudi Arabia

Published online: 31 March 2022

Hindawi
Journal of Mathematics
Volume 2022, Article ID 2635564, 8 pages
https://doi.org/10.1155/2022/2635564

Research Article

Assignment Computations Based on C_{exp} Average in Various Ladder Graphs

A.Rajesh Kannan,[1] **P. Manivannan**,[1] **K. Loganathan**,[2,3] **K. Prabu**,[4] **and Sonam Gyeltshen**[5]

[1]*Department of Mathematics, Mepco Schlenk Engineering College, Sivakasi 626005, Tamil Nadu, India*
[2]*Department of Mathematics and Statistics, Manipal University Jaipur, Jaipur 303007, Rajasthan, India*
[3]*Research and Development Wing, Live4Research, Tiruppur 638 106, Tamil Nadu, India*
[4]*Kongu Engineering College, Perundurai, Erode 638060, Tamil Nadu, India*
[5]*Department of Humanities and Management Jigme Namgyel Engineering College, Royal University of Bhutan, Dewathang, Bhutan*

Correspondence should be addressed to K. Loganathan; loganathankaruppusamy304@gmail.com and Sonam Gyeltshen; sonamgyeltshen@jnec.edu.bt

Received 20 February 2022; Revised 29 March 2022; Accepted 7 April 2022; Published 11 May 2022

Academic Editor: M. T. Rahim

This study introduces the C_{exp} average assignments and investigates its properties using various ladder graphs. The ladder graphs can be found in every communication networks. Ladder networks are increasingly being used in everyday life for monitoring and environmental applications such as domestic, military, surveillance, industrial, medical applications, and traffic management. These datasets are afflicted by the average representation of the graph structure. It aids in the visualisation and comprehension of data analysis. The C_{exp} labeling is used in sensor networks, adhoc networks, and other applications. It also efficiently creates a communication network after using noise reduction methods to remove salt and pepper noise.

1. Introduction

A graph labeling is the assignment of labels, conventionally indicated by integers, to edges and/or vertices of a graph in the mathematical domain of graph theory. The concept of labeling may be applied to many areas of graph theory, for example, in automata theory and formal language theory. We use [1–5] for notations and nomenclature. We recommend [6] for a thorough examination of graph labeling. Let P_n be a path on n nodes denoted by $u_{1,\mu}$, where $1 \le \mu \le n$, and with $n-1$ lines denoted by $e_{1,\delta}$, where $1 \le \delta \le n-1$, where e_μ is the line joining the vertices $u_{1,\mu}$ and $u_{1,\mu+1}$. On each edge e_δ, erect a ladder with $n-(\mu-1)$ steps including the edge e_μ, for $\mu = 1, 2, 3, \ldots, n-1$. The resulting graph is called the one-sided step graph, and it is denoted by ST_n. Let G_1 and G_2 be any two graphs with p_1 and p_2 vertices, respectively. Then, $G_1 \times G_2$ is the Cartesian product of two graphs. A ladder graph L_n is the graph $P_2 \times P_n$. The graph $G^{\circ}S_m$ is obtained from G by attaching m pendant vertices to each vertex of G. The triangular ladder TL_n, for $n \ge 2$, is a graph obtained from two paths by $u_1, u_2, \ldots u_n$ and $v_1, v_2, \ldots v_n$ by adding the edges $u_\mu v_\mu$, $1 \le \mu \le n$ and $u_\mu v_{\mu+1}$, $1 \le \mu \le n-1$. The slanting ladder SL_n is a graph obtained from two paths $u_1, u_2, \ldots u_n$ and $v_1, v_2, \ldots v_n$ by joining each v_μ, with $u_{\mu+1}$, $1 \le \mu \le n-1$. The graph D_n^* having the vertices $\{a_{\mu,\delta}: 1 \le \mu \le n, \delta = 1, 2, 3, 4\}$ and its edge set is $\{a_{\mu,1}a_{\mu+1,1}, a_{\mu,3}a_{\mu+1,3}: 1 \le \mu \le n-1\} \cup \{a_{\mu,1}a_{\mu,2}, a_{\mu,2}a_{\mu,3}, a_{\mu,3}\ a_{\mu,4}, a_{\mu,4}a_{\mu,1}: 1 \le \mu \le n\}$.

2. Literature Survey

In [7], the authors talked about the F-root square mean labeling for line graph of the path, cycle, star, $P_n{\circ}S_1, P_n{\circ}S_2$, $[P_n; S_1], S(P_n{\circ}S_1)$, ladder, slanting ladder, the crown graph $C_n{\circ}S_1$, and the arbitrary subdivision of S_3. The authors in [8] discussed $(1, 1, 0)$ F-face mean labeling some planar graphs and, in [9], face labelings of type $(1, 1, 1)$ for generalized prism.

Hindawi
Journal of Nanomaterials
Volume 2022, Article ID 5252918, 11 pages
https://doi.org/10.1155/2022/5252918

Research Article

Heat Transfer Analysis on Carboxymethyl Cellulose Water-Based Cross Hybrid Nanofluid Flow with Entropy Generation

F. Ali,[1] **K. Loganathan**,[2,3] **S. Eswaramoorthi**,[4] **K. Prabu**,[5] **A. Zaib**,[1] **and Dinesh Kumar Chaudhary**[6]

[1]*Department of Mathematical Sciences, Federal Urdu University of Arts, Sciences, & Technology, Gulshan-e-Iqbal, Karachi 75300, Pakistan*
[2]*Department of Mathematics and Statistics, Manipal University Jaipur, Jaipur, 303007 Rajasthan, India*
[3]*Research and Development Wing, Live4Research, Tiruppur, 638106 Tamilnadu, India*
[4]*Department of Mathematics, Dr. N.G.P. Arts and Science College, Coimbatore, Tamilnadu, India*
[5]*Department of Physics, Kongu Engineering College, Perundurai, Erode-638060, Tamilnadu, India*
[6]*Department of Physics, Amrit Campus, Tribhuvan University, Kathmandu, Nepal*

Correspondence should be addressed to K. Loganathan; loganathankaruppusamy304@gmail.com and Dinesh Kumar Chaudhary; din.2033@gmail.com

Received 25 December 2021; Revised 15 March 2022; Accepted 2 May 2022; Published 1 June 2022

Academic Editor: Anwar Saeed

The physical phenomena of convective flow of Cross fluid containing carboxymethyl cellulose water over a stretching sheet with convective heating were studied. Cross nanofluid containing Al_2O_3, Cu nanoparticles, and based fluid of CMC water is used. Entropy generation minimization is examined in the current analysis. The system of PDEs is altered into a set of ODEs through suitable conversion. Further, these equations are computed numerically through the MATLAB BVP4c technique. The behavior of governing parameters on the velocity, temperature, entropy generation, and Bejan number is plotted and reported via graphs. It is found that the larger value of unsteady variable reduced the velocity, thermal layer, and entropy production. Surface drag frication of the Al_2O_3 and Cu and Al_2O_3 + Cu is enhanced with the more presence of unsteady parameter. Comparison of current results in a limiting case is obtained with earlier analysis and found an optimum agreement.

1. Introduction

Carboxylmethyl cellulose (CMC) is a water-soluble cellulose derivative [1], and it has many flow properties due to its greater stability and high viscosity. The stability of nanoparticles in CMC escalates the fluid behavior. It is engaged to increase lubricating effects such as polymeric structures [2, 3]. These multifunction aspects of various cellulose derivatives have many industrial and technical applications. To recognize the fluid flow with CMC study, research have been studied [4–6]. Saqib et al. [7] described the natural convective flow of CMC with carbon nanotube using a fractional derivative approach. The effect of slip velocity and non-Newtonian nanofluid contained with 0.5% wt CMC water was discussed by Rahmati et al. [8]. Akinpelu et al. [9] explored the thermophysical metal properties in CMC. MHD flow of Casson nanofluid under heat transfer in CMC over a solid sphere was developed by Alwawi et al. [10].

Nanotechnology has been progressively more fascinated by the researchers because of their efficiency in several industrial processes such as microelectronic, oil emulsion, and molecular emulsion. Nanotechnology has the ability in suspending nanoscale particles $(1 \le 100\text{nm})$ in ordinary fluids, like ethylene glycol, oil, and water. The origin of nanotechnology was initiated by Choi and Eastman [11] in 1995. After, Buongiorno [12] developed a mathematical model of heat transfer with the addition of Brownian motion and thermophoresis effects. Tiwari and Das [13] investigated to examine the solid volume fraction in nanofluids. Devi and Devi [14] reported the numerical simulation of hybrid

Optical and Quantum Electronics (2022) 54:386
https://doi.org/10.1007/s11082-022-03749-x

Study on modulational instability in three-core nonlinear directional saturated coupler with septic nonlinearity

P. Mohanraj[1] · R. Sivakumar[1] · A. M. S. Arulanandham[2] · K. V. Gunavathy[3]

Received: 16 October 2021 / Accepted: 15 April 2022

Abstract
In this work, we examine the modulation instability (MI) in a three-core oppositely directed saturated coupler with a negative refractive material channel. Further, the MI is deliberately studied with a non-Kerr nonlinear effect using septic nonlinearity. Using a standard linear stability method, we solved the modified nonlinear Schrodinger equation and obtained the MI gain spectrum with analytical results. It clearly shows that the forward to backward propagating wave power, nonlinear saturation, pump power, and optical nonlinearity play a vital role in the MI of a three-core nonlinear directional coupler. The septic nonlinearity plays a major role in both two and three-core couplers with the negative indexed material channel. The septic nonlinearity can suppress the MI gain and bandwidth in a normal dispersion regime alone in the two-core coupler. In the anomalous dispersion regime, the generation of MI is utterly different from the normal dispersion case since the septic nonlinearity can increase the gain and the bandwidth of the MI spectrum. In a three-core coupler, the nonlinear septic effect suppresses the MI gain and width in a normal (anomalous) dispersion regime in contrast to the two cores oppositely directed saturated coupler. Normally, the saturable nonlinearity simultaneously suppresses the MI gain and bandwidth in both normal and anomalous dispersion regimes. Hence, it can significantly change the instability region in the presence of septic nonlinearity. Thus, we present a new path to manipulate and generate the MI and solitons or solitary waves in three-core nonlinear directional couplers with NIM channel and septic nonlinearity.

Keywords Nonlinear saturation · Modulational instability (MI) · Oppositely directional coupler (ODC) · Negative-index material (NIM) · Septic nonlinearity

✉ P. Mohanraj
mohanrajsphysics@gmail.com

[1] Department of Physics, Pondicherry University, Puducherry, India

[2] St.Joseph College of Arts and Sciences, Vaikalipatti, Tirunelveli, Tamilnadu, India

[3] Department of Physics, Kongu Engineering College, Perundurai 638060, India

Published online: 05 June 2022