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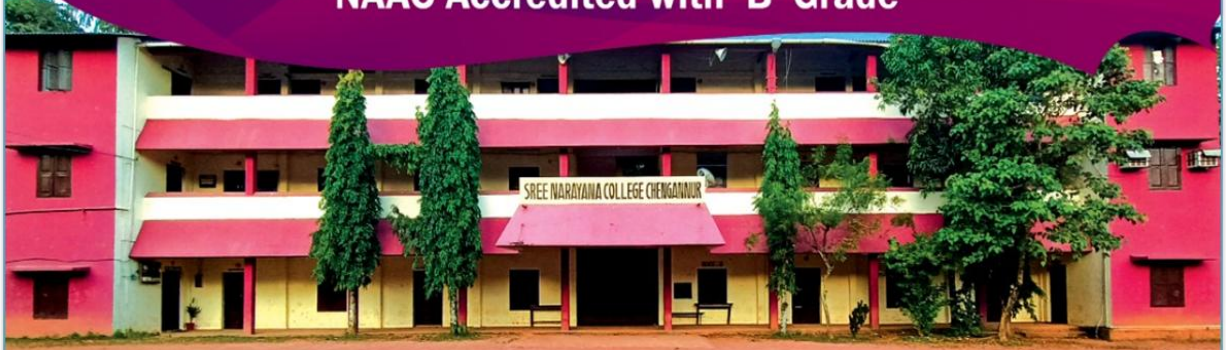

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Effect of Sm^{3+} ions doping on the structural and optical properties, Judd-Ofelt and radiative parameters of ZnS phosphor materials

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HIGHLIGHTS

- Hexagonal structured undoped and Sm^{3+} doped ZnS phosphor were prepared.
- The positive value of bonding parameter reveals its covalent nature.
- Judd-Ofelt analysis were performed and trend observed is $\Omega_2>\Omega_4>\Omega_6$.
- $x = 0.03$ in $Zn_{1-x}Sm_xS$ show maximum emission with life time 1.661 ms.
- The prepared phosphor could be an excellent candidate for photonic displays.

ARTICLE INFO

Keywords:
ZnS:Sm^{3+}
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CIE chromaticity
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ABSTRACT

Undoped ZnS and Sm^{3+} doped with varying concentration of ZnS phosphor materials were synthesized via low temperature solid state reaction method. The samples were investigated for the influence of different concentrations of Sm^{3+} ions on their structural and spectroscopic properties. The presence of various absorption bands in UV–Vis–NIR spectra revealed the transition from ground state to different excited states of Sm^{3+} ions. The Judd-Ofelt (JO) analyses were evaluated to identify the structure and the bonding around the Sm^{3+} ions. The high value of Ω_2 intensity parameter reveals that the site symmetry is lower. The parameters such as radiative transition probabilities, radiative lifetime, branching ratio, stimulated emission cross-sections and the optical gain parameters are also evaluated. The PL spectra shows five high intensity emission bands centered at 567 nm, 590 nm, 619 nm, 641 nm and 667 nm corresponding to $^4G_{5/2}\rightarrow{}^6H_j$ (j = 5/2, 7/2,9/2, 11/2, 13/2) transitions and showed optimum for concentration at $x = 0.03$ in $Zn_{1-x}S$. The quantum yield of the prepared optimal phosphor using integrating sphere method was found to be 10.08%. This indicates that the materials synthesized may be favorable for the applications of laser and other optical devices.

1. Introduction

Nanocrystalline semiconductor phosphors have a wide range of applications in areas such as optical display devices, optical storage, sensors, optical communications etc. due to their size dependent optical properties [1]. In semiconductor phosphoes, zinc sulfide (ZnS) can be widely used commercially for blue or green emission. But to get red emission, Y_2O_2S phosphor is essential, which is very expensive [2]. Group II-VI compounds emit sharp line spectra, and these lines are enhanced when doped with rare earth metals as activators [3]. Among group II-VI compounds, zinc sulfide is an excellent blue light emitter with wide direct band gap energy of 3.67eV. It is a non-toxic semiconductor material. It exhibits strong absorption band and broad luminescence that originate from defect states. The intensity of luminescence and the emission peak of semiconductor can be tuned by adding the appropriate activator [4]. ZnS allows the activator ions to greatly influence the intensity and the emission peaks, due to the wide band gap. ZnS is considered as a potential candidate in the research community because of its excellent unique characteristics when doped with transition metal ions or rare earth ions [3]. The emission from ZnS excites the rare earth ions if there is an overlapping of luminescence band of ZnS with the absorption peak of rare earth ions. This will enhance the

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Folic acid grafted aminated zeolitic imidazolate framework (ZIF-8) as pH responsive drug carrier for targeted delivery of curcumin

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Show more

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Abstract

Smart drug delivery systems responding to pH gradient between physiological conditions and acidic conditions in tumor cells are very crucial for treating cancer. This article describes the process of developing, zeolitic imidazolate framework (ZIF-8) based novel pH responsive drug carrier for the targeted delivery of curcumin (CUR). To enable folic acid (FA) conjugation the surface of ZIF-8 was modified through amination. The so developed CUR loaded folic acid grafted aminated ZIF-8 (CUR@FA-g-AZIF-8) were characterized with UV–Visible, FT-IR, PXRD, SEM, TGA, TEM and BET analysis. It shows high drug loading efficiency and good chemical stability. *In vitro* drug release studies of CUR from folic acid grafted aminated ZIF-8 (FA-g- AZIF-8) shows three times higher efficiency in acidic pH (5) than in normal physiological conditions (pH 7.4). The potential cytotoxicity was evaluated by MTT assay on HeLa cells, CUR@FA-g-AZIF-8 shows 76.8% cytotoxicity. The results show that FA-g-AZIF-8 is a promising drug carrier for targeted drug delivery.

Graphical abstract

Schematic representation of folate receptors mediated pH responsive drug delivery action for efficient anti-tumor therapy.

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Influence of rare earth substitution on structure, photoluminescence emission properties and Judd-Ofelt analysis of ZnS:Eu^{3+} red phosphors

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ABSTRACT

A series of Eu^{3+} doped ZnS red emitting phosphors were synthesized by conventional low temperature solid state reaction technique. The structural and spectroscopic characteristics of the prepared materials were examined by theoretical and experimental methods. The XRD results confirm the formation of hexagonal structured ZnS material. Similar morphology is obtained from TEM and SEM analysis and the particle size and grain size were calculated. The compositional analysis using EDS confirms the atomic percentage present in the materials. The optical band gap energy of the samples varied from 3.59 to 3.43 eV. The PL emission under excitation 390 nm has greater emission intensity at concentration $x = 0.1$ in $Zn_{(1-x)}S$: xEu^{3+} material. The intense red emission (614 nm) for concentration $x = 0.1$ have CIE coordinates (0.6090, 0.3905) with color purity 90.41% and CCT 1629.26 K. The site symmetry of Eu^{3+} ions was explained using PL emission spectra. The intensity parameters Ω_2, Ω_4 and Ω_6, radiative properties like branching ratio (β_R), transition radiative parameter (A_R), stimulated emission cross section σ_e, radiative life time (τ_R) was calculated from Judd-Ofelt theory. The luminescence decay kinetics was analyzed and the life time of material was calculated in millisecond (ms) range. The strong and intense red emission and the improved stimulated emission cross section offer Eu^{3+} doped ZnS material useful for designing optoelectronic device applications.

1. Introduction

The major challenges affecting the global community include energy conservation and environmental management. Active research is going on in materials science to develop environmental friendly high performance devices with good efficiency [1]. Researchers are interested in the development of semiconductor nanophosphors because of their size-dependent optical properties [2]. These size reduced phosphor materials can be tuned to their properties for applications in optoelectronic devices. The unique luminescence characteristics of nanophosphor sulphide semiconductor materials can be changed by reducing dimensions and tuning the band gap [3]. The surface imperfections of nanophosphor particles illustrate their excellent optical properties. This is due to the recombination of excitons on the surface of nanophosphors [4]. The small size of nanophosphors material coated in LED surface offer a solution for saving the energy as well as the material [5].

Compared to other II-VI group semiconductor materials, ZnS is the most suitable host material for rare earth doping because it has better chemical stability with a wider direct band gap energy (Eg = 3.67 eV) at room temperature. It is used as a phosphor material in electroluminescent (EL) devices, Light emitting diodes (LEDs), p-type conductors, field emitters, solar cells, flat panel displays, IR windows, sensors, photo catalysis, lasers, nanogenerators etc. [6]. Therefore, ZnS was chosen as the host material for doping to enhance its optical properties. Under ambient conditions, ZnS exists in two phases: Sphalerite (Cubic) with lattice parameters $a = b = c = 5.41$ Å, *Space group* $F4-3m$ and Wurtzite (Hexagonal) with that of $a = b = 3.82$ Å, $c = 6.26$ Å, *Space group* $= P6_3mc$[7]. This small difference in the arrangement of the atoms creates large differences in the band structures and the optical properties of the systems. The hexagonal phase shows better optical properties than the cubic phase [8]. The hexagonal ZnS has a stronger blue emission than cubic ZnS, which is the thermally unstable phase. This may be due to the distribution of Zn^{2+} ions and the interatomic distance between them, since hexagonal is much closer than the cubic.

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ORIGINAL RESEARCH ARTICLE

Optoelectronic Characteristics of In_2S_3-CNT Nanocomposite Thin Films for Photodetector Application

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The present study reports the synthesis of photosensitive carbon nanotube (CNT) intercalated indium sulphide (In_2S_3) nanocomposite thin films by using chemical bath deposition coupled with the spin coating technique. The impact of incorporation of CNT in In_2S_3 thin films is compared with that of pure In_2S_3 films and is discussed in detail by evaluating their structural, compositional, morphological, optical and photocurrent measurements. Structural and compositional analyses such as x-ray diffraction, x-ray photoelectron spectroscopy, Energy dispersive spectroscopy and Raman measurements ensure the successful integration of CNTs within the In_2S_3 thin films. Remarkable variation in morphology from mesh fractal structure to spider web structure due to the intercalation of CNTs is observed in the scanning electron micrograph. Roughness and thickness of as-synthesized samples are determined by atomic force microscopy. The excellent conducting nature of CNTs induces an appreciable enhancement of conductivity (resistance decreased from 31.5 GΩ to 15.1 GΩ) in In_2S_3-CNT nanocomposite thin films with respect to that of pure films, and is estimated from I–V analysis. Photosensitivity, responsivity, detectivity and noise equivalent power of these films are measured to explore their suitability as a photodetectors. Photocurrent responses at room temperature of the In_2S_3-CNT nanocomposite thin films exhibit around 14 times better photosensitivity than that of pure films. Optical absorption studies indicate the reduction in optical bandgap (2.38–2.29 eV) due to the incorporation of CNT. Our results suggest that the In_2S_3-CNT nanocomposite thin film can be considered as a good choice for room temperature photodetector applications.

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DNA-assisted synthesis of nanoceria, its size dependent structural and optical properties for optoelectronic applications

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Abstract. Cerium oxide (CeO_{2-x}) nanoparticles or nanoceria were synthesized by the chemical co-precipitation method using cerium nitrate hexahydrate and ammonium carbonate as starting materials and deoxyribonucleic acid (DNA) as a capping agent. The structural and optical characterization of the prepared nanoparticles was studied in depth by X-ray diffraction (XRD), high resolution transmission electron microscopy (HRTEM), Fourier transform infrared spectroscopy, Raman spectroscopy, UV–visible absorption and diffuse reflectance spectroscopy. The average crystallite size and lattice parameters of the cerium oxide nanoparticles at different calcination temperatures were studied using XRD analysis. The average crystallite size was found to be 6 nm and the size increases with calcination temperature. The polycrystalline nature and the size of the particles obtained are in close agreement with HRTEM and Raman analysis. The optical band gaps of all samples were measured by Tauc plot which showed a blue shift with a decrease in size due to the quantum confinement effect. The optical absorption spectrum of the synthesized nanoparticles showed the absorption of UVA, UVB and UVC light, and the variation in structural and optical properties with size makes them suitable for the optoelectronic application. To the best of our knowledge, this is the first report on using DNA in the synthesis of nanostructured ceria.

Keywords. Nanostructured ceria; chemical co-precipitation; capping agent; DNA; optical studies.

1. Introduction

Cerium oxide, commonly known as ceria, is considered as a promising rare-earth oxide material due to its unique ability to toggle between Ce^{3+} and Ce^{4+} oxidation states depending on the oxygen partial pressure in the surrounding atmosphere. As a result, ceria can easily form nonstoichiometric compositions CeO_{2-x} with $0 < x < 0.5$ without changing the crystal structure. Generally, cerium oxide has a cubic fluorite structure with space group $Fm3m$ [1]. It consists of a face-centred cubic unit cell of cerium cations with oxygen anions occupying the tetrahedral interstitial sites. The activity of cerium oxide particles increases when the size is shrunk down to nano-regime [2]. However, to enhance the properties of nanomaterials and thereby meet the need of different applications, it is very essential to decrease the size and thus to increase the active surface area of nanoparticles. In recent years, much effort has been focused on the development of new routes for the synthesis of nanoceria due to the range of applications in science and technology such as gas sensors, solar cells, high storage capacitor devices, fuel cells and UV filters [3–8]. Different synthetic methods are available for the fabrication of cerium oxide nanoparticles such as sol–gel, sonochemical, hydrothermal, chemical precipitation, combustion and pulsed laser deposition methods [9–13]. For various applications, large-scale manufacturing of nano-powders needs to be cost effective, eco-friendlier and should not be too complex. Therefore, the chemical co-precipitation method is more attractive compared to others. As a better choice, the most fascinating biomaterial known to humans, deoxyribonucleic acid (DNA), has been used as a biological capping agent for the present study to obtain nanoparticles of very low dimensions with less aggregation. The use of capping agents prevents the growth of the particle by effectively shielding the surface of the nuclei as soon as they are formed. It prevents them from coming into direct contact with solution. Often, molecules with longer chains are used as capping agents. DNA is a polymer that carries genetic code of all living beings and it acts as a good capping agent as well as a template for nanomaterials using its double-helix nature [14]. So far, materials such as silver, gold, copper, palladium, platinum, carbon nanotubes and nickel oxide have been fabricated on the DNA template [14–17]. Moreover, there are no reports on the synthesis and characterization of nanoceria using DNA-assisted chemical co-precipitation. The structural features and optical properties of nanoceria have been studied in depth by using different characterization techniques such as X-ray diffraction (XRD), high-resolution transmission electron microscopy (HRTEM), Fourier transform infrared (FTIR), Raman and UV–visible spectroscopy.

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Hesperidin mediated synthesis, structure and optical emission analysis on nanocrystalline CuO

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ABSTRACT

Nanocrystalline Copper (II) oxide was synthesized through hesperidin mediated phytochemical reduction method and post annealed at 600 °C for 4 hrs. Various analytical results obtained after characteristic measurements such as XRD, FESEM, UV–visible spectroscopy and Photoluminescence studies have been discussed. The crystallographic plane reflections obtained in X-ray diffraction pattern was found to be analogous with the monoclinic end centered phase of copper (II) oxide with Halder-Wagner crystallite size 18 nm. The formation of spherical grains via agglomerated crystallites was apparent from the surface morphology obtained through FESEM images. Tauc' plot of UV–visible spectrum employing Kubelka-Munk function provided a direct optical band gap of 1.61 eV. The photoluminescence spectrum using 280 nm optimal excitation wavelength and the related CIE plot revealed that the optical emission occurs at blue region as indicated by the chromaticity coordinates.

Selection and peer-review under responsibility of the scientific committee of the International Conference on Energy and Environment.

1. Introduction

Metal oxide nanoparticles are the widely interested candidates in the contemporary research on materials syntheses, crystallography and optical emission studies. Simple transition metal oxides with high quality crystalline behavior have been established as direct band gap materials [1–3] and hence being considered as appropriate candidates for optoelectronic device applications. At present, the complex alloying of III/V or IV/VI group elements with appropriate doping technique is commercially used for making direct band gap materials [4]. This is often cumbersome that the band gap tuning remains difficult in such materials. The advent of direct band gap behavior in simple transition metal oxides opened up much attention towards their applications in optoelectronic device applications. Interestingly, the nanocrystalline regime in such oxides could further incorporate the tuning behavior in the band gap by varying the crystallite size. Among simple metal oxides, copper (II) oxides are widely explored due to their combined electrical, optical and magnetic properties [5,6]. Many number of studies have been reported elsewhere related to the syntheses, crystallographic structure and optical analyses on nanocrystalline CuO through various synthesis techniques such as inter diffusion process [7], hydrothermal route [8], vapour phase approach [9], sonochemical method [10], microwave assisted hydrothermal method [11], phytochemical mediated synthesis [3,6] etc. Among these, phytochemical mediated synthesis technique is comparatively novel and less expensive [12].

However, one of the major tribulations with this green approach is the difficulties in separating the exact phytochemical reductant from the mixture of plant extract, which often leads to poor yield of high quality crystalline products. In order to overcome this crisis, a high purity phytochemical, namely hesperidin, capable of acting as effective reductants were utilized to directly substitute for complex plant extracts (Fig. 1).

Hesperidin is a bioflavonoid, which was first separated in 1828 from the inner section of orange peels [13]. Profuse quantity of Hesperidin is found in citrus fruits such as orange, lemon, grapes etc. Depending on species, parts, geographic sites of cultivation and processing procedures, the content of hesperidin varies greatly in citrus fruits [13]. In this context, this paper disuses the characteristic studies on CuO nanocrystallites synthesized through commercially available hesperidin as phytochemical mediator.

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Preparation and evaluation of alginate nanoparticles prepared by green method for drug delivery applications

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ABSTRACT

Nanosized natural polymers have attained considerable attention in drug delivery applications due to their high encapsulation efficiency, non-toxic nature, sustained and targeted drug delivery. Here we have synthesized Rifampicin loaded alginate nanoparticles by green method. Physicochemical characterization of the nanoparticles was assessed using Transmission electron microscopy, Fourier transform infrared spectroscopy, Dynamic light scattering and X-ray diffraction technique. The swelling and in vitro drug release showed that the framework experiences pH-dependent swelling and release of Rifampicin. Rifampicin has lower release in acid medium and higher release in intestinal condition. Moreover, in view of the drug release results, the release kinetics and transport mechanisms were investigated and discussed. In vitro cytotoxicity assay demonstrated that the nanoparticles were non-toxic in nature. The acute oral toxicity study of the synthesized nanoparticles was done in Wistar albino rats. No systemic toxicity was observed after oral administration of nanoparticles. The present study demonstrated the potential of using alginate nanoparticles synthesized by a green method for drug delivery applications.

1. Introduction

Nowadays the benefits and potential advantages which can be obtained from drug delivery systems using natural and synthetic polymers has gained a wide interest [1–6]. Natural polymers are considered as preferable drug carriers over synthetic materials because they possess several unique advantages such as hydrophilicity, biocompatibility and nontoxicity [7,8]. Among the different natural polymers, alginate (ALG) stands as one of the most advantageous biopolymers due to its low cost and easy availability [9]. The majority of the alginate particles portrayed in literature have micrometer dimension [10–13].

Nano sized drug delivery systems have numerous advantages such as targeted delivery, enhanced bioavailability, sustained drug release, improved patient compliance and reduced side effects [14]. The surface characteristics and particle size of nanoparticles can be easily tailored by varying the composition of polymers, drugs and other additives used in the formulation [15–17]. Particle size also assumes a pivotal part in intestinal uptake and in vivo distribution [18–20]. Panyam and his coworkers demonstrated that the particles below 100 nm were appeared to offer 15 to 250 fold cellular uptake than the micro particles using rat model study [21].The considerably high surface area of nanoparticles also guarantees significant payload [22–24].

Although, many methods for the preparation of alginate nanoparticles has been reported in the literature, including polyelectrolyte complexation, emulsification/internal gelation, solvent evaporation/diffusion and solvent-casting methods; however they have some limitations, such as porosity, difficult to reproduce, precipitation during the evaporation and use of volatile organic solvents [25]. Green chemistry principles could be adequately connected to the generation of ALG nanoparticles in a more secure and greener manner by avoiding organic solvents [26].Our group had developed a green method for the synthesis of highly stable, non-aggregate ALG nanoparticles of size above 100 nm using honey and demonstrated the potential of utilizing it for water purification [27–29]. In the present work, attempts were made to modify these nanoparticles suitable for drug delivery applications. Since particle size has a crucial role for drug delivery application, the preparation method was modified with the application of probe sonication. It was found that the high energy of probe sonication during the preparation stage of nanoparticles produced particles of smaller size [30].

Honey, an ancient pharmaceutical ingredient, rich in carbohydrate, has fantastic antioxidant, antibacterial, antifungal and anti-inflammatory properties. Ayurvedic medicine of India use honey

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Chrysin mediated synthesis, crystallographic structure and optical emission characteristics of ZnO nanoparticles

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ABSTRACT

ZnO nanoparticles were synthesized through chrysin mediated phytochemical reduction mechanism. pH of the reaction mixture was kept proximate to 9 and the reaction was carried out at room temperature. The powdered sample obtained was annealed at 600 °C for four hours. X-ray diffraction pattern analysis revealed the formation of nanocrystalline hexagonal primitive lattice phase of zinc (II) oxide with crystallite size equal to16 nm as estimated from Debye-Scherrer equation. The coalescence resulted from annealing the sample which led to the formation of needle like grains of edge to edge crystallites aggregate was evidenced from FESEM images, with grain size equivalent to crystallite size calculated from x-ray diffraction analysis. Tauc' plot of uv–visible spectrum employing Kubelka-Munk function provided a direct optical band gap of 3.27 eV. The photoluminescence spectrum using 280 nm optimal excitation wavelength and the related color coordinates estimated from chromaticity diagram revealed that the optical emission in the sample occurs at blue region in the visible spectrum.

Selection and peer-review under responsibility of the scientific committee of the International Conference on Energy and Environment.

1. Introduction

Zinc (II) oxide (ZnO) nanoparticles have been attracted intense attention over the years, especially because of their photocatalytic [1], optoelectronic device [2] and solar cell [3] applications. The high efficiency, low cost and non-toxicity altogether brought this semiconducting material as a promising candidate for device fabrication in connection with light harnessing [4]. Due to the interesting physical properties, for instance the larger absorption coefficient, high carrier mobility and high chemical stability, ZnO has been listed as a well known gas sensing material as well [4]. In analogy with our earlier reports [5–8] on phytochemical mediated synthesis of various semiconducting transition metal oxide nanostructures such as Fe_2O_3 [5,6], Mn_3O_4 [7] CuO [8], an attempt has been made to synthesis ZnO nanostructures using phytochemical mediated reduction method.

Chrysin has been used as phytochemical mediator. Fig. 1 shows the molecular structure formula of the natural flavonoid chrysin (5,7-dihydroxy – 2 –phenyl – 4H – chromen – 4 - one) [9]. Recently, chrysin has been identified as a potential candidate for inhibiting aromatase and human immune deficiency virus activation [9]. It has also been demonstrated as having superior anti inflammatory effects and has shown capability as antioxidants [9]. The chemo preventive activity of chrysin was explored for utility in cancer treatment in a variety of human and rat cells [9]. Natural existence of chrysin is found to be rich in honey and propolis [10]. In this context, this paper reports the detailed analysis on crystallographic structure, morphological features, band gap evaluation and emission characteristics of ZnO nanostructures synthesized through chrysin mediated chemical reduction method.

2. Experimental

The precursor salt, zinc sulfate hepta hydrate ($ZnSO_4{\cdot}7H_2O$) was purchased from Merck Life Science Pvt. Ltd. and used without further purification. Aqueous solution of 0.1 M precursor was mixed with 0.0125 M alkaline solution of Chrysin dissolved in 1 M NaOH solution by keeping 2:3 vol ratio. The mixture was stirred at room temperature for 1 hr and the pH was regularly tested and maintained at 7 to 8. The change in color to a pale yellowish during the course of reaction was indicative of the reduction reaction

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RESEARCH Open Access

Theoretical and experimental studies on theophylline release from hydrophilic alginate nanoparticles

Deepa Thomas[1,4], Vinish V. Nair[2], M. S. Latha[3,4*] and K. Kurien Thomas[1]

Abstract

Background: Mathematical modelling may be able to reduce the number of in vitro experiments and provide an insight into the elementary physical and chemical mechanisms that regulate the rate and degree of drug release. The aim of the present examination was to develop a simple mathematical model to portray drug release from the alginate-type hydrophilic matrix, taking into account the Fickian diffusion of drug and swelling of the matrix using theophylline as the model drug.

Results: The nanoparticles show a remarkable swelling in the simulated intestinal fluid. The theoretical drug release values were validated with experimental values by considering diffusion and diffusion with swelling. The experimental value fitted well with the theoretical value predicted based on diffusion. It was found that after 3 h, the entire drug release followed a pure diffusion transport.

Conclusions: The numerical model was found to be sufficiently accurate in guessing the drug release from the alginate matrix. The developed model could be extended to quantitatively prognosticate the drug release from hydrophilic spherical matrices.

Keywords: Matrix, Diffusion, Swelling, Modelling

Background

During the last decades, drug delivery systems have received considerable attention [1–4]. These systems are intended to offer controlled administration of the pharmaceutical compound to keep their concentration within the therapeutic range. Additionally, they help to reduce the number of drug dosages, initial drug concentration, and side effects due to the unspecific systemic distribution of drugs [5–7]. In vitro drug release studies have been considered as a vital component in the pharmaceutical formulation development. Preliminary data obtained from these studies facilitate the design of the system with optimal in vivo performance. In vitro experiments with varying parameters are required to optimize the device design.

Mathematical modelling may be able to reduce the number of in vitro experiments and provide a perception of the underlying physical and chemical mechanisms that govern the rate and degree of drug release [8]. Diffusion characteristics, distribution pattern, and loading of a drug in the matrix affect the kinetics and mechanism of drug release [9]. Drug diffusion is significantly influenced by the topology and swelling nature of the matrix. Upon contact with body fluids, the polymer swells and the active ingredient diffuses through the network meshes [10]. The diffusional mass transport assumes a critical part for overcoming the key hindrances, such as mucosa in the gastrointestinal tract [11].

The mathematical model suggested by Higuchi in 1961 based on diffusion mechanism was the first to describe drug release from a matrix system [12]. It may be able to explain the drug release from various pharmaceutical dosage forms [13]. Numerous other models were also formulated to describe the release mechanisms from various polymeric drug delivery systems and most of them involve

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Synthesis of Nanocurcumin-alginate Conjugate and Its Characterization by XRD, IR, UV-Vis Andraman Spectroscopy

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ABSTRACT

The compounds which extracted from spices and herbs exhibit antiviral, anti-fungal and anti-cancerous effects having potential pharmacological uses. Curcumin, a component of turmeric, which has been used as a food additive and a coloring material in India and other Asian countries due to its potential medicinal properties. Earlier reports suggest that application of curcumin in foods is limited because of its low bioavailability and its high degradation in acid and alkaline medium. In this study the effect of stabilization of both free curcumin and nano curcumin–alginate conjugate in honey was studied by UV–Vis absorption, IR, vibrational spectroscopy (Raman)and XRD. Curcumin is degraded in acid and alkaline medium is highly stable with the nano formulation. From this work it was deduced that in presence of surfactant honey curcumin-alginate inhibits the formation of small sub-products. This work reveals the complexation of curcumin with alginate in presence of surfactant honey was demonstrated to protect this molecule from the degradation. UV–Vis, FTIR XRD and Raman spectroscopy were important to determine the nature of the structural modifications.

Keywords: Curcumin, UV-Vis, FTIR, XRD and Raman Spectroscopy.

INTRODUCTION

Curcumin is a bright yellow chemical produced by plants of the ginger family (Zingiberaceae). It is the principal curcuminoids in herbal supplement, cosmetics ingredient, food flavoring, and food colouring[1]. Although curcumin has been used widely in *Ayurvedic* medicine, its potential medicinal properties are till unproven and are an area of active investigating field. Chemically, curcumin is a diarylheptanoid with two methoxide and hydroxyl groups, belonging to the group of curcuminoids, which are natural phenols responsible for turmeric's yellow color. It is a tautomeric compound existing in enolic form in organic solvents and as a keto form in water (Figure. 2).[2]

COMPUTATIONAL INVESTIGATIONS ON STRUCTURAL AND FUNCTIONAL IMPACT OF SNP IN PARKINSON'S DISEASE ASSOCIATED WITH HUMAN MONOAMINE OXIDASE-B (MAO-B)

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Abstract

Single nucleotide polymorphism (SNP) is type of mutation and one of the major factor in determining susceptibility of an individual to a particular disease and response to the action of a drug. Thus mapping the structural and functional effects of SNP is the most important step in drug research and development in the context of personalized medicine. Parkinson's disease is a neurodegenerative disorder affecting central nervous system (CNS) usually associated with aging. The symptoms of this disease includes nervous coordination problems like difficulty in walking, swallowing, chewing, slowness of movement and speaking along with other emotional problems like depression. The inhibition of metabolic enzyme monoamine oxidase B (MAO-B) is a key step to suppress the progression of the disease. The three dimensional crystal structure of the MAO-B was taken from Protein Data Bank (PDB ID: 4CRT). Gene name of the enzyme were selected using Kyoto encyclopedia of genes and genomes (KEGG) database. Single Nucleotide Polymorphism (SNP) data were retrieved from dbSNP database. SIFT and Polyphen-2 were used complementary for selecting 'high confidence non synonymous SNP (nsSNP) based on sequence based and structure based approaches respectively. The nsSNP which were found to be damaging using both SIFT and PolyPhen-2 score analysis were further evaluated for their stability using IMutant-2.0. The functional impact of deleterious and damaging SNP were studied by modelling the homology modelling the protein using SWISS MODEL. The effect of the standard drug Zelapar was analysed in both mutated and native proteins using molecular docking studies. Results revealed that almost all the mutated proteins had a significantly lesser interaction with the drug compared to the native protein.

Keywords: Homology modeling, Parkinson's disease, MAO-B, Single nucleotide polymorphism

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ORIGINAL PAPER

Plasmon Based Cellulose Nano Fibril–PVA Film for Effective Ultra Violet Radiation Blocking

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Abstract
Recent years have witnessed significant interest in biodegradable and transparent ultraviolet (UV) protecting films from renewable resources. In the present paper, preparation, characterization and evaluation of UV radiation blocking capability of transparent and flexible cellulose nano fibril (CNF)–poly vinyl alcohol (PVA) films are described. Synthesized films exhibited good transparency in the visible region and UV blocking ability. Addition of plasmonic silver ($\sim$ 22 nm) to the films lead to complete blocking of UV radiations. Synthesized films were highly stable for a long exposure to intense sunlight. The defined methods show a straightforward procedure for the fabrication of environment friendly UV-radiation blocking films for industrial/commercial/textile applications.

Keywords Composites · Cellulose · Nano fibril · UV blocking films

Introduction

Most of the living things and products needed for human life are highly affected by ultra violet radiations (UV). Coating/packaging is the only way to minimize the effect of UV radiations. Due to these, recent years have witnessed much increased interest in the development of UV protecting films. Currently, UV absorbers and inorganic photoactive compounds are the two classes widely available in the market as UV protectors. Polymers and their hybrid forms are also promising materials as UV protecting agents due to their facile processability, recyclability, and economical attractiveness [1, 2]. Most of the polymers presently available are less effective in offering complete protection from UV radiations. Majority of the polymers/hybrids allow UV radiations to pass through, which eventually affects the desired properties of materials/products. To overcome these matters, development of films which are transparent in the visible range, and effective in blocking electromagnetic radiations below 400 nm demands wide application in industries particularly in packaging industry and in textile industry. In recent past, researchers were in search of new materials having dependable properties. Performance of a large number of systems viz; polymers, polymer-organic dyes, ZnO-doped polymers, TiO_2 incorporated hybrid systems etc., were evaluated for increased performance [3]. Unfortunately dyes are not environment friendly and will degrade during exposure to ultraviolet radiation/sunlight. Also, it was observed that increase in concentration beyond a particular level of ZnO, TiO_2 etc. significantly affects transparency of films [1, 2].

Last few years have witnessed much increased interest in research on nano sized cellulose viz; cellulose nano fibrils (CNFs) and cellulose nano crystals (CNCs) as new class of functional materials with wide potentials [4, 5]. Interesting properties, eco friendliness, nano dimensions,

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A STUDY ON BEACH TOURISM AND ITS OVERALL DEVELOPMENT – A SPECIAL REFERENCE TO BEACHES IN TRIVANDRUM DISTRICT

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ABSTRACT
The travel industry seems, by all accounts, to be an industry that anybody can get it. The travel industry in Kerala is being advanced as a monetary improvement procedure for country networks dependent on contentions of its immediate and backhanded advantages. The travel industry advertisers, in any case, don't promptly recognize the ecological effects and the subsequent social costs that the neighbourhood networks will endure when they bring the travel industry into their zone. There is no uncertainty that travel industry, alluded to as 'the world's biggest industry', is a major business. Amid the recent decades, numerous nations in this world have left in the travel industry situated strategies. The travel industry is the movement of people making a trip to and remaining in spots outside their typical condition for recreation and different purposes. In the modem days, the travel industry is additionally a monetary movement. It lands position openings and win outside trade. The travel industry is a procedure including visitors, places they visit and exercises they include into. Beach the travel industry, subsequently, is the travel industry offered as a powerful influence for the beach front condition and its common and social assets. It happens along the beach and in the water quickly contiguous the beach lines. In this investigation, the term beach front district includes not just the locale situated near the ocean, yet additionally its expansions through the substantial arrangement of estuaries and backwaters far into the inland of Kerala. Attributable to the convicts of interests of the partners of this business, the contention for and against the travel industry improvement in immature and least creating countries is probably going to proceed. It is viewed as proper in this setting to assess the status of India's travel industry. Tourists involve a critical position in the travel industry since they are the customers of the travel industry items. Thusly, the perspectives on the visitors are expected to improve the travel industry. It will likewise support the monetary improvement. A huge number of sightseers visit India since it unimaginably has the most various assortments of beaches anyplace on the planet. Peaceful backwaters and tidal ponds, bayous and unpleasant magma shook oceans, marine estuaries with fish, slamming surf, fine brilliant sand or palm bordered beaches profound India has them all.

Keywords: Beach, Travel, Tourism.

1. INTRODUCTION

The beach is the limit among land and ocean. The advancement of the travel industry has been personally connected with the sea beach. Individuals needed to escape from the drudgery of day by day life and appreciate the incredible marvels of nature along the beach. India is lucky in having a long beach line of 6100 km from West Bengal to Gujarat limited by the Arabian Sea, the Bay of Bengal, and the Indian Ocean. The beaches, sea beaches, estuaries and deltas of the streams all through the beach district offer chances to create the travel industry and financial advancement. The travel industry assumes a noteworthy job in the nations like China, England, Germany, Hong Kong, Thailand, and United States. They are drawing in more visitors and producing tremendous income in regard of remote trade. Before, the travel industry was restricted due to the non-accessibility of frameworks like transport and correspondence, yet in the present time, the general populations are living in the time of Science and Technology. The improvement of air, ocean, street transport and partnered foundations like lodgings, beach, resorts and human services focuses have been in charge of the advancement of the travel industry around the globe. Numerous nations have come to understand that worldwide the travel industry is one of the quickly developing businesses of the world. It has additionally turned into the fundamental area of the economy of any country.

More than the development in the piece of the overall industry which is as yet pitiful in a worldwide setting, the state has been recognized just like a goal with the most astounding potential. This finding has been over and over affirmed by movement middle people both with in India and in the conventional producing markets of Europe. In this manner the broadly acknowledged end is that for Kerala the travel industry could be a most dominant motor that could move the state's economy. Truth be told on the off chance that we are sincerely dissect the restrictions and shortcoming of huge numbers of our other monetary segments, we will understand that we have couple of options, being bio-innovation and data innovation the two of which we presently can't seem to create. India isn't a nation however a landmass to the extent the vacation destinations are concerned. For no nation on the planet can flaunt so differed an atmosphere, so unique wide open spaces thus rich legacy. India

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A COMPARATIVE STUDY ON THE GOVERNMENT SUPPORT TO ALLOPATHIC AND AYURVEDIC MEDICAL TOURISM PROVIDERS IN KERALA

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ABSTRACT

Travel and the tourism industry is the biggest service industry in India and the second most astounding remote trade worker, representing almost nine percent of the aggregate work in the nation. A noteworthy and progressively forthcoming fragment of this is the multibillion dollar medicinal and wellbeing the travel industry which has recorded astounding development in the ongoing years. A few highlights, for example, financially savvy and propelled social insurance frameworks, accessibility of specific and gifted human services experts, and expanding ubiquity of customary mending frameworks and elective drug, have all situated India as a positive goal for wellbeing and medicinal services in the worldwide situation. This article is an endeavor to disentangle the issues and prospects in restorative the travel industry and an examination on the degree of government bolster that therapeutic the travel industry is at present benefiting. Medicinal the travel industry is additionally seen as an interim of holidaying, and it covers wide scope of medical and human services administrations. The legislature can help in the general advancement of a nation as a medicinal the travel industry goal through visa assistance, exchange fairs association and support and promoting endeavors by its consular workplaces abroad, or assistance of inbound cross-outskirt development of therapeutic experts.

KEYWORDS: Medical Tourism, Government, Allopathic, Ayurveda.

1 INTRODUCTION

In Medical travel people were known to have crossed fringes to exploit fixes like hot showers, famous chemists, or incredible prophets performing wonderful treatments. Be that as it may, while beforehand, the bearing and stream of medicinal explorers has been, by and large, from poorer to cutting edge nations where refined restorative methods were all the more promptly

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A Study on Medical Tourism Providers and Social and Political Risks in Kerala

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ABSTRACT

The study intends to survey the social and political performing artists for medical and the travel industry in Kerala from the medical tourism providers' point of view. Medicinal Tourism has changed varying backgrounds. Independent of the age and sexual orientation factors, the industry reinforces the economy of the nation and tops off the trade hold of the country. It is a path through which the nation ventures itself to world. Interest for Medical service is expanding because of Continuous increment in Population and future. Most recent innovation and aptitude learning is added favourable position to nation. Consequently it winds up important to ponder the new measurements in the travel industry that can procure remote trade and produce work by giving incredible administration. In the present globalized world there is need of persistent learning and execution of new thoughts like medicinal the travel industry by wellbeing industry. Medical and the travel industry is moderately more established idea however nations comprehended the significance of this idea presently aftereffect of which Medical Tourism is developing quickly. Real favourable position of India according to as Medical Tourism concern is that India offers top class medical facilities at standard with any of the western nations. Indian clinics are having great framework, exclusive Medical facilities, well qualified doctors and very important competitive cost of treatment. The main focus can be on expanding the quantity of medicinal tourists just as keeping up and upgrading the nature of social insurance administrations at sensible expenses and furthermore guaranteeing moral issues.

Keywords: Medical Tourism, Social, Political, Kerala.

INTRODUCTION:

The fast development in the travel industry business can be ascribed to increment in disposables, enhanced offices, weight on urban families, enhanced network to vacationer goals, and so forth. There is high need and extension to draw in these guests to the different vacationer goals in Kerala. Because of increment in number of Medical travelers number of private hospitals offering administrations to these patients increments naturally. Vital thing for these private doctor's facilities to pull in patients from abroad is a quality "authentications" and few of these hospitals get such endorsements from bodies that give them to clinics in the country. Essential thing to include this is a portion of the doctor's facilities in India have significantly higher quality administrations than the clinics in the country. The Medical the travel industry of India is one of the biggest administration segment businesses which produce immense totals of cash and later on time it is required to gain significantly more. In next five years. Indian Medical Tourism business can contribute 25% to GDP. India is developing as favored goal by remote patients over the globe because of different reasons. Training framework in India is extremely solid and India has made vast upgrades in advanced education. Important in Ayurvedic medication, India has included preferred standpoint over different nations. In most recent ten years proficiency

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Identification of Antimastits Componenets in *Boerhavia diffusa* as an Inhibitor of *Staphalococus aureus* Monofunctional Glycosyltransferase, Causing *Bovine mastitis* (An Insilico Approach)

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ABSTRACT

Bovine mastitis is an infection of cattle leading to a huge reduction in milk production that causes severe economic loss in dairy industry across the world. Causative of the disease includes bacteria, virus and non-bacterial pathogens. Among these, *Staphalococus aureus* is the common cause of mastitis and is highly resistant to the most routinely used antibiotics. So current antibiotic therapy has shown limited efficacy. The crude extract of locally available medicinal plant *Boerhavia diffusa* is used traditionally against mastitis and is found to be highly effective. The objective of the study is the identification of the phytochemicals in *Boeravia diffusa* responsible for the antimastitis activity by insilico docking analysis using Schrodinger Suit v 9.2. 20 phytochemicals in *Boerhavia diffusa* were selected for docking studies based on ADMET properties. The high resolution crystal structure of the target receptor protein of *Staphalococus aureus* was retrieved from PDB. Structure of the phytochemicals and the most commonly used antibiotic against *Bovine mastitis* were selected from PUB CHEM NCBI. The phytochemicals, Boeravinone A, B, C, D, E and F from *Boehravia diffusa* showed good docking scores and better interaction with the active sites of the target proteins used for the evaluation than the most commonly used commercially available drug. Results of this study are important for the designing of novel drugs for the treatment of mastitis.

Keywords: *Staphalococus aureus* monofunctional glycosyltransferase, *Bovine mastitis*, Docking, *Boerhavia diffusa*, Qik prop.

Vibrational spectra, dielectric properties, conductivity mechanisms and third order nonlinear optical properties of guanidinium 4-aminobenzoate

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ARTICLE INFO

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NLO
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ABSTRACT

The frequency response of dielectric permittivity measurements at temperatures 35 °C and 100 °C suggests enhanced inherent optical quality and few defects in the crystal. The Cole-Cole plot shows the presence of grain and grain boundary, it is found that single relaxation is observed in the crystal. The ac and dc conductivity and dielectric behavior of the grown crystal were systemically investigated as a function of frequency and temperature. The third order nonlinear optical property extensively studied by z-scan technique revealed high third order nonlinearity in the form of self-defocusing and two-photon absorption with saturable absorption. The strong intermolecular charge transfer interaction evident from NBO and AIM studies confirms the NLO property of the material. The detailed vibrational assignments were carried out on the basis of potential energy distribution (PED) analysis and scaled quantum mechanical force field calculation using MOLVIB program. The red shifted NH stretching wavenumbers and the broadening of corresponding bands in the solid state as well as the gas phase spectra, optimized molecular geometry and NBO analysis have confirmed the presence of N-H···O hydrogen bonding in G4AB.

1. Introduction

Organic derivatives comprising of molecules with strong electron donor and acceptor groups are well known to exhibit significant nonlinear optical (NLO) activities due to their electron transfer mechanisms by the intramolecular charge transfer interaction (ICT) processes that are mediated by the push-pull substituent pairs which cause large hyperpolarizabilities to the molecular systems [1]. The extended hydrogen bonding associations can result in the structural asymmetry of the molecular system which is an important requirement for the materials to have NLO applications [2]. Crystallization of ionic salt produce can more cohesive crystalline structures which possess inherently greater thermal stabilities, sufficient mechanical strength and have higher chromophore number densities which are requisites for quadratic NLO effects [3].

The organic complexes of cationic guanidinium based systems have received considerable attention as NLO materials [3–7] due to their capability to form multiple, strong and charge assisted hydrogen bonds with the carboxylate group, phosphate group, nitrate group and polar molecules [8]. The guanidinium cation is formed by the protonation on guanidine which is a strong organic base and the cation is stabilized through the Y-aromaticity by the delocalization of positive charge on the three nitrogen atoms and the central carbon atom within the CN_3 unit. The concept of aromatic domino effect stresses the importance of the aromatic stabilization triggered by protonation [9–15]. 4-aminobenzoic acid is one of the most versatile of the carboxylic acids for co-crystal formation. The acid molecules have the property of establishing molecular self-assembly by extended hydrogen bonding structures through both the carboxylic acid group and the ring-substituted amino group with other molecules and thereby promoting stability to the resulting crystalline structure [16]. The molecular complexes of 4-aminobenzoic acid such as, the coordination polymer $[Zn(C_7H_7NO_2)_2]\cdot H_2O$ [10], Morpholin-4-ium p-aminobenzoate [17] and 2-amino-4-picolinium 4-aminobenzoate [18] have been identified as potential NLO materials. The surface-enhanced Raman spectroscopy of p-aminobenzoic acid with excitation in the visible and near infrared spectral region has been reported by *E.J. Liang* et al. [19]. The growth and physico-chemical properties of gunidinium derivatives such as Guanidinium tetrafluoroborate [20], Guanidinium trichloroacetate [21], Guanidinium 3-nirobenzoate [22] and Guanidinium tosylate [23] have

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Synthesis of Nanocurcumin-alginate Conjugate and Its Characterization by XRD, IR, UV-Vis Andraman Spectroscopy

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ABSTRACT

The compounds which extracted from spices and herbs exhibit antiviral, anti-fungal and anti-cancerous effects having potential pharmacological uses. Curcumin, a component of turmeric, which has been used as a food additive and a coloring material in India and other Asian countries due to its potential medicinal properties. Earlier reports suggest that application of curcumin in foods is limited because of its low bioavailability and its high degradation in acid and alkaline medium. In this study the effect of stabilization of both free curcumin and nano curcumin–alginate conjugate in honey was studied by UV–Vis absorption, IR, vibrational spectroscopy (Raman)and XRD. Curcumin is degraded in acid and alkaline medium is highly stable with the nano formulation. From this work it was deduced that in presence of surfactant honey curcumin-alginate inhibits the formation of small sub-products. This work reveals the complexation of curcumin with alginate in presence of surfactant honey was demonstrated to protect this molecule from the degradation. UV–Vis, FTIR XRD and Raman spectroscopy were important to determine the nature of the structural modifications.

Keywords: Curcumin, UV-Vis, FTIR, XRD and Raman Spectroscopy.

INTRODUCTION

Curcumin is a bright yellow chemical produced by plants of the ginger family (Zingiberaceae). It is the principal curcuminoids in herbal supplement, cosmetics ingredient, food flavoring, and food colouring[1]. Although curcumin has been used widely in *Ayurvedic* medicine, its potential medicinal properties are till unproven and are an area of active investigating field. Chemically, curcumin is a diarylheptanoid with two methoxide and hydroxyl groups, belonging to the group of curcuminoids, which are natural phenols responsible for turmeric's yellow color. It is a tautomeric compound existing in enolic form in organic solvents and as a keto form in water (Figure. 2).[2]

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Zinc-Alginate Beads for the Controlled Release of Rifampicin

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ABSTRACT

The present study describes the preparation of a carrier system based on zinc-alginate beads and to evaluate its potential for the controlled release of rifampicin, the poorly water soluble drug using ionic gelation technique. The surface topology of the developed beads were analyzed by Scanning Electron Microscopy and the crosslinking process was investigated by Fourier Transform. Infrared spectroscopy. The pH dependent swelling properties of the beads were analyzed. Drug entrapment efficiency and *in vitro* drug release studies were also investigated. The *in vitro* cytotoxicity and antibacterial activity were evaluated. Results indicated that the entrapment efficiency improves as the amount of polymer incresed. The developed beads showed a pH dependent swelling behaviour. The sustained release of drug was more prominent in pH 7.4 than 1.2. The MTT assay results proved the cell biocompatibility of the developed beads. The beads showed good antibacterial activity.

Keywords: Alginate, Drug delivery, Rifampicin, Cytotoxicity, Tuberculosis.

INTRODUCTION

Tuberculosis(TB) is a chronic pulmonary disease caused by mycobacterium tuberculosis. Rifampicin (RIF) is one of the effective first line drug for TB and isthe semi synthetic hydrazine derivative of rifampicin B.Major limitations of conventional tuberculosis therapy using RIF tablets are the long duration of treatment with frequent multiple dosage due to its short biological half-life, low stability and low water solubility. The continuous presence of RIF at high concentration above therapeutic range for prolonged period of time is associated with for prolonged effects such as renal failure, hepatotoxicity, fever, thrombocytopenia and antibody formation[1,2]. Development of drug delivery system that release the antimicrobial agent in a slow and sustained manner, could provide maximum therapeutic benefit while minimizing the side effects.

Chapter 4
Cellulose Based Green Adsorbents for Pollutant Removal from Wastewater

Anitha George Varghese, Sherely Annie Paul, and M. S. Latha

Contents

Abstract Water pollution is a major problem affecting people across the world. Heavy metals and dyes are major pollutants that pose potential threat to the health of humans and ecosystems. Several treatment technologies are available to reduce the pollutant concentration in water and wastewater. However, many of these processes are costly, have high energy requirements and generate toxic sludge and wastes that need to be carefully disposed. Addressing these problems invoked the need for green methods that are more efficient, cost effective and environment friendly for water purification. Adsorption is regarded as a green, clean and versatile method for wastewater treatment. Cellulose based materials attained considerable

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Research Article

EVALUATION OF THE ANTIBACTERIAL ACTIVITY OF CALCIUM ALGINATE BEADS MODIFIED WITH ETHANOLIC EXTRACT OF *ADHATODA VASICA* LEAF EXTRACT ON *STAPHYLOCOCCUS AUREUS* AND *ESCHERICHIA COLI*

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ABSTRACT

Objective: The objective of the present study was to investigate the antibacterial activity of calcium alginate (Ca-ALG) loaded with ethanolic extract of *Adhatoda vasica* (*A. vasica*) leaves against *Staphylococcus aureus (S. aureus) and Escherichia coli (E. coli).*

Methods: Ca-ALG beads containing ethanolic extract of *A. vasica* leaves were developed by ionic gelation technique. The prepared Ca-ALG beads were characterized by Fourier-transform infrared (FT-IR) spectroscopy and scanning electron microscopy (SEM). The antibacterial effect of *A. vasica* leaf extract loaded Ca-ALG beads was examined against *S. aureus* and *E. coli.*

Results: FT-IR studies revealed the cross-linking of ALG and calcium ions. The spherical morphology of the beads was designated by SEM. The prepared beads were found to display distinctive growth inhibition against *S. aureus* and *E. coli.*

Conclusion: The antibacterial activity analysis indicated that the prepared beads have good activity against *S. aureus* and *E. coli.* The present study proposes a strategy to enhance antibacterial properties of ALG which are widely used in biomedical applications.

Keywords: Alginate, *Adhatoda vasica*, Ethanolic extract, Biomedical application, Antibacterial.

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INTRODUCTION

Natural polymers with antibacterial property receive considerable attention in the biomedical field. Usually, metal ions and metal nanoparticles are added to the system to improve its antibacterial activity. Cellular toxicity of such systems restricts its wide applications in the biomedical field [1]. The material utilized for biomedical application should be free of toxic chemicals and biocompatible in nature. The need of environmentally friendly and green antibacterial material intensifies the development of products of plant origin. The use of herbal extracts as therapeutic agents has numerous benefits such as biocompatibility, non-toxic, and eco-friendliness.

Adhatoda vasica (*A. vasica*) is a popular medicinal plant with well-known antibacterial and antitussive activities [2,3]. It is an active ingredient of indigenous medicine for respiratory disorders. The leaf extract of *A. vasica* is used to cure chronic bronchial disorders, phthisis, cough, and asthma [4]. Earlier studies showed that it possesses excellent antibacterial activity [5]. The presence of quinazoline alkaloids such as vasicinone, vasicine, and deoxyvasicine is responsible for its medicinal value. Recent investigations reveal its bronchodilator activity [6].

Alginate (ALG) is a naturally occurring anionic polymer typically obtained from brown seaweed and is water soluble. It has the ability to gel in mild and aqueous conditions in the presence of divalent ions such as Ca^{2+} and Zn^{2+} and trivalent ions such as Al^{3+} and Fe^{3+} which leads to the formation of egg box junctions [7]. The biocompatible and non-toxic nature of ALG finds wide applications in the delivery of bioactive agents such as small chemical drugs and proteins, and cell transplantation [8-11]. ALG is well-known material in the wound management field due to its ability to maintain a moist environment and rich water content [12].

Among different metal cross-linked ALGs, calcium-ALG (Ca-ALG) was superior for wound healing applications. This is due to the unique hemostatic properties of the calcium ion and the ability of the gel to be used as a matrix for the aggregation of platelets and erythrocytes [13]. The porosity of ALG also allows the entrapment of bioactive agents and able to release it on the targeted site in a sustained and controlled manner. Usually, antibiotics such as minocycline, gentamycin, and ofloxacin are used for treating wound infections. The constant administration of these drugs may cause the resistance of the microorganisms to them. Antimicrobial dressings based on natural materials with therapeutic properties are the best solution to overcome this problem. The incorporation of medicinal plant extract into biocompatible polymer provides a unique opportunity for the development of novel therapeutic approaches toward biomedical application.

The aim of the present study is to prepare Ca-ALG beads loaded with ethanolic extract of *A. vasica* leaves by ionic gelation and examine its antibacterial activity against *Staphylococcus aureus (S. aureus) and Escherichia coli (E. coli).* In this work, Ca-ALG beads loaded with ethanolic extract of *A. vasica* leaves were prepared by exploiting the hemostatic properties of ALG, and therapeutic activity of *A. vasica* leaves extract for wound healing and drug delivery applications.

MATERIALS AND METHODS

Materials

The materials used were sodium ALG (medium viscosity≈3500 cps, Sigma-Aldrich, London), calcium chloride dihydrate (Merck, Germany). All the other reagents were of analytical grade and used without further purification. *A. vasica* leaves were freshly collected from the college garden and identified with the help of Dr. Dinesh Raj, Department of Botany, Bishop Moore College, Mavelikara, Kerala.

Preparation of extract

Shade-dried leaves of *A. vasica* were coarsely powdered. About 250 g of this powder was extracted with 1000 ml of 100% ethanol in an ultrasonicated

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Alginate/Chitosan Nanoparticles for Improved Oral Delivery of Rifampicin: Optimization, Characterization and *in vitro* Evaluation

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Alginate/chitosan nanoparticles were synthesized by ionotropic method using natural honey as the stabilizing agent. The nanoparticles were characterized and the potential of these nanoparticles for the controlled oral delivery of antitubercular drug rifampicin was evaluated in terms of entrapment efficiency, swelling behaviour and *in vitro* release of the drug. Carboxyl content and *in vitro* cytotoxicity of the nanoparticles were also evaluated. The swelling and *in vitro* drug release indicates that the system undergoes pH-dependent swelling and release of drug. Drug release was very low in acidic pH and a maximum of only 20 % of the drug was released in 5 h. A sustained release of drug was observed at pH 7.4 and complete release was obtained in 8 h. Kinetics of the drug release was analyzed by fitting the experimental data into Korsmeyer-Peppas equation and show that the mechanism involved in the release was non-Fickian, controlled by a combined mechanism of diffusion and polymer relaxation. This study shows that the obtained nanoparticles can be a potential carrier for the pH controlled oral delivery of rifampicin.

Keywords: Rifampicin, Sodium alginate, Chitosan, Nanoparticle, Honey, Controlled release.

INTRODUCTION

Tuberculosis (TB) caused by *Mycobacterium tuberculosis*, is a chronic communicable and persistent bacterial infection. The current tuberculosis therapy involves the daily administration of combination of antituberculosis drugs for a period of more than 6 months [1]. But due to limited solubility, rapid and premature degradation and low cellular uptake of these drugs, concentration of the drug reached to target site is less than the therapeutic level. The prolonged drug administration often causes several side effects such as nausea, nephrotoxicity, hepatotoxicity, fever and vomiting. This may results in the patients non-compliance and chance for treatment failure [2]. Treatments based on controlled release drug delivery systems using polymeric micro and nanoparticles is one of the best solution for the problems related to the existing tuberculosis therapy. There are various efforts have been made to develop micro and nano polymer [3]. But some of them include complex preparation steps, inconvenient routes of administration and toxicity problems [4]. Oral controlled delivery of rifampicin (RIF) using nano formulation can be improved the efficacy of tuberculosis therapy and the patient comfort. The key factors involved in the selection of carrier in drug delivery application are its size, shape, drug loading and encapsulation efficiency [5]. Nano particulate drug delivery formulations have the potential to improve these factors and also capable to increase the drug solubility. Alginate a water soluble linear polysaccharide, composed of β-D-mannuronic acid and α-L-guluronic acid (G) is extracted from brown seaweed and is widely used for the bio encapsulation of drugs without the risk of mucosal damage. But, low durability, high-diffusion rates resulting from the high porosity and limited mechanical stability were the major drawbacks of alginate based drug delivery system [6]. Chitosan, a natural cationic polymer, has the capacity to interact with anionic bio macromolecules and enhance their loading as holds them tightly. Ribeiro and co-workers could successfully retarded the release of haemoglobin from alginate micro particles by chitosan coating [7]. The studies made by Wittaya-areekul *et al.* [8] and Takka & Gürel [9] revealed that the incorporation of chitosan into alginate micro particles enhances its bioadhessive nature. Oral delivery with alginate nanoparticles coated with chitosan is expected to offer advantages of controlled drug delivery, high drug payload and improved stability. It also ensure protection for encapsulated drugs from acidic environment of gastrointestinal tract and enzyme degradation. The small size of nanoparticles increases

Biosynthesis of Nanostructured Ceria, its Optical and Magnetic Studies for Spintronic Applications

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Abstract. Nano structured ceria or nanoceria of average crystallite size ~ 6 *nm* are synthesized by chemical co precipitation method using cerium nitrate hexa hydrate and sodium hydroxide as starting materials. Onion juice extract is used as biological capping agent. Structural, optical and magnetic properties of prepared samples were investigated by X-ray diffraction (XRD), transmission electron microscopy (TEM), Raman, UV-Visible spectroscopy and vibrating sample magnetometer (VSM) measurements. The increase in the value of optical band gap compared to bulk may be attributed to the quantum confinement and its band gap is well matching with that silicon. In addition to this, it also possess room temperature ferromagnetism. Thus the synthesized nanoceria have the potential to combine both semiconducting and magnetic behavior in a single system for making compatible spintronic devices.

Keywords: Nanoceria, chemical co- precipitation, Onion juice extract, RTFM

INTRODUCTION

Diluted magnetic semiconductors are currently being explored with a strong drive due to their unique property of exploiting spin of the carriers in addition to or in the place of the charge for creating new functional devices. This removes the difficulties in injecting spins into nonmagnetic semiconductors which are used in the conventional spintronic devices [1]. Spintronic devices can be used as magnetic high density data storage devices, spin based switches, transistors, diodes, modulators, etc. [2] To be commercially useful, spintronic devices have to work at room temperature and be compatible with existing semiconductor based electronic devices. Among them, nanostructured cerium oxide has attracted much attention due to its interesting characteristics such as it possess a stable cubic fluorite structure far from the stoichiometric proportion of oxygen [3]. It is one of the most important rare earth oxides which are endowed with high dielectric constant and is used as a buffer layer for silicon on insulator devices and as a high k-dielectric material in capacitors [4]. These unique and novel properties make cerium oxide a good matrix to develop compatible spintronic devices.

The properties of nano materials can be enhanced by decreasing the size and thereby increasing the active surface area. In recent years, much effort have been done for the development of new routes for the fabrication of nanostructured ceria due to wide range of applications in science and technology The large-scale manufacture need to be cost effective, simple and more eco-friendly. So chemical co-precipitation method using biological capping agent is more attractive compared to other synthesis routes such as sol-gel, sonochemical, hydrothermal, combustion and pulsed laser deposition methods [5, 6, 7].

EXPERIMENTAL

The materials used were analytical grade Cerium (III) nitrate hexa hydrate ($Ce(NO_3)_3.6H_2O$) and sodium hydroxide (NaOH) were purchased from Merck, India and were used without further purification. Cerium oxide nanoparticles were synthesized by chemical co precipitation method by taking 0.1M aqueous solution of cerium nitrate hexa hydrate and 0.4M Sodium hydroxide as starting materials and onion juice extract as capping agent. Upon adding the solutions,

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Identification of Antimastits Componenets in *Boerhavia diffusa* as an Inhibitor of *Staphalococus aureus* Monofunctional Glycosyltransferase, Causing *Bovine mastitis* (An Insilico Approach)

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ABSTRACT

Bovine mastitis is an infection of cattle leading to a huge reduction in milk production that causes severe economic loss in dairy industry across the world. Causative of the disease includes bacteria, virus and non-bacterial pathogens. Among these, *Staphalococus aureus* is the common cause of mastitis and is highly resistant to the most routinely used antibiotics. So current antibiotic therapy has shown limited efficacy. The crude extract of locally available medicinal plant *Boerhavia diffusa* is used traditionally against mastitis and is found to be highly effective. The objective of the study is the identification of the phytochemicals in *Boeravia diffusa* responsible for the antimastitis activity by insilico docking analysis using Schrodinger Suit v 9.2. 20 phytochemicals in *Boerhavia diffusa* were selected for docking studies based on ADMET properties. The high resolution crystal structure of the target receptor protein of *Staphalococus aureus* was retrieved from PDB. Structure of the phytochemicals and the most commonly used antibiotic against *Bovine mastitis* were selected from PUB CHEM NCBI. The phytochemicals, Boeravinone A, B, C, D, E and F from *Boehravia diffusa* showed good docking scores and better interaction with the active sites of the target proteins used for the evaluation than the most commonly used commercially available drug. Results of this study are important for the designing of novel drugs for the treatment of mastitis.

Keywords: *Staphalococus aureus* monofunctional glycosyltransferase, *Bovine mastitis*, Docking, *Boerhavia diffusa*, Qik prop.

Dendrimers: General Aspects, Applications and Structural Exploitations as Prodrug/ Drug-delivery Vehicles in Current Medicine

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In Silico Identification of the Antimastitis Components in Allium cepa

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Abstract

Bovine mastitis is a pathogenic inflammation to the mammary gland of cattle results in huge reduction of milk production. Antibiotics are used for the treatment of mastitis. Limitted cfficacy of the antibiotic treatment is a threat to the diary industry. Farmers of South Kerala use the crude extract of Allium cepa for the treatment of mastitis and is found to be highly effective. Present study focus on the identification of the antimastitis components in Allium cepa which can perform efficient docking interaction with the target protein (PDB ID: 1JIL) of *Staphalococus aureus* bacteria using Schrodinger suit v 9.2. The phytochemicals, Myricetin, Quercetin-4'-glucoside and Quercetin-3-glucoside in Allium cepa are identified as the antimastitis components. The results of the study are helpful in developing novel drugs for the treatment of mastitis.

Keywords: Bovine mastitis; Docking; *Staphalococus aureus*; Target protein

Introduction

Bovine mastitis is associated with the presence of infectious agents as bacteria, Bovine Herpes virus, non bacterial pathogens like mycoplasmas, fungi, yeast and chalmydia [1,2]. Among these, Staphalococus aureus bacterial infections are most common. Transfer complex protein (PDB ID:1JIL) [3] is an excellent drug target in Staphalococus auerus. Inhibition of which results in bacterial cell lysis. Allium cepa is a biennial plant, a good source of nutrients. Various phytochemicals present in the plant are responsible for its therapeutic potential [4]. 20 phytochemicals in Allium cepa were selected for the docking study based on ADMET properties predicted by Qik prop option.

Methodology

Bioinformatics analysis

Preparation of Protein: Crystal structure of the target proteins of Staphalococus aureus transfer complex protein was obtained from RCSB Protein Data Bank (PDB ID: 31JIL). Automatically imported PDB files from the RCSB PDB website to the Maestro working interface [5-7]. Subsequently the protein was optimized and minimized.

Ligand preparation

Twenty phytochemicals present in Allium cepa were selected to find out the inhibitory activity towards the target protein. The structure of the phytochemicals and commonly used commercially available antibiotic Pirlimycin hydrochloride were downloaded from pub chem in the (.sdf) format. These ligands were subjected to ligand preparation using the ligand preparation wizard (ligprep) of Schrodinger software in the Maestro interface 12 [6,7].

Docking Studies

The compounds were screened by Schrodinger docking software to study inhibitors of the target protein. Grid generation was done using the centroid of workspace ligand R0 48-8071. The rigid receptor docking using the Glide program was carried out against the target protein with the set of ligands. The mode of docking was selected as XP (Extra precision) for a high docking accuracy. The glide docking was carried out for the minimised protein [6-8]

ADMET properties prediction

The bioactive compounds from Allium Cepa were checked for their ADMET properties using Qik prop module [8,9]. QikProp helped in analyzing the pharmacokinetics and pharmacodynamics of the ligand by accessing the drug likeness.

Results and Discussion

(Range of properties - Molecular weigh less than 500, Hydrogen bond donor 0-6, Hydrogen bond acceptor 2-20 and QP logP(o/w) -2 - 6.5), From the results obtained it has been understood that the phytochemicals Myricetin, Quercetin-4'glucoside and Quercetin-3-glucoside are responsible for

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Research Article

DOCKING STUDY ON MYCOBACTERIUM TUBERCULOSIS WITH PHYTOCHEMICALS OF ACALYPHA INDICA

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Mycobacterium tuberculosis, Molecular docking, Acalypha indica, 4RHU, 1W30, 1N2B.

ABSTRACT

Considering the world- wide TB issues, there is an earnest need to develop moderately economical new medications to treat this destructive infection. Natural products isolated from plants have assumed a vital part in revelation of medications against irresistible ailments. In the present study, thirty ligand molecules which were present in the plant Acalypha indica were docked with the selected target proteins of Mycobacterium viz. 4RHU, 1W30, 2A7S, 1N2B, 1F0N. Among them Potassium Brevifolincarboxylate had a significant inhibitory activity with 1N2B protein forming bonds at a very low energy value, thus forming a stable complex. The other active compounds were found to be beta-Glucogallin and Caffeic Acid. The active substances from the extracts of Acalypha indica which exhibited promising activities is reported for the first time. These can serve as promising candidates to develop new drugs to combat M. tuberculosis.

INTRODUCTION

Microbial diseases are a developing issue in contemporary drug, yet just a couple of antimicrobial agents are utilized as a part of clinical practice. Mycobacterium tuberculosis (MTB) is a pathogenic bacterial species in the genus Mycobacterium and the causative agent of most instances of tuberculosis (Ryan K.J. *et al*., 2004). Tuberculosis (TB), a lung contamination and is one of the infectious and dangerous maladies which have added to the troubles of the humankind. The primary explanation behind across the board of this sickness is the populace development, rise of multi- drug resistant TB strains, budgetary weight in the growing nations and unsuccessful endeavor to orchestrate another medication with novel component of activity. Albeit one conceivable long haul answer for the issue is a superior immunization, for the time being, the significant dependence will be on chemotherapy (Tomioka H. *et al*., 2006) requiring the improvement of novel, viable and non- poisonous antitubercular agents (Berning, S.E., 2001; Reddy, V.M. *et al*., 1996 ; Barry C.E., 1997). The genome of M. tuberculosis encodes for around 4000 proteins (Cole ST *et al*., 1998). In this way, determination of a protein as a medication target is urgent for sedate disclosure for TB. Broad research, including bioinformatics based investigations has been completed to distinguish and organize tranquilize focuses for TB (Agüero F *et al*., 2008; Sundaramurthi JC *et al*., 2011).

Pantothenate (vitamin B5) is a basic forerunner for the biosynthesis of coenzyme A (CoA) and acyl bearer proteins (ACP). Since both CoA and ACPare basic in fattyacid biosynthesis that plays a key role in tenacious development and pathogenicity of MTB, pantothenate synthetase is a proper focus for creating new drugs against TB, and this comes under the classification of Ligase - an enzyme which joins two molecules (Wang S *et al*., 2003). Another potential target is hypoxanthine-guanine phosphoribosyltransferase (MtHGPRT), a key enzyme (transferase) of the purine salvage pathway (Wai Soon Eng *et al*., 2015). The Mycobacterium tuberculosis pyrR gene (Rv1379) encodes a protein that manages the expression of pyrimidine-nucleotide biosynthesis (pyr) genes in an UMP-dependent way. Since pyrimidine biosynthesis is a fundamental step in the progression of TB, the gene pyrR is an appealing antitubercular target, and this is an example of transferase (K. A. Kantardjieff *et al*., 2005). The Mycobacterium tuberculosis 30 kDa major secretory protein (antigen 85B) is the most copious protein sent out by M. tuberculosis, and in addition an intense immunoprotective antigen and a main medication target. A mycolyl transferase of 285 buildups, which is firmly identified with two other mycolyl transferases, each of molecular mass 32 kDa: antigen 85A and antigen 85C. All the three catalyze exchange of the fattyacid mycolate from one trehalose monomycolate then onto the next, bringing about trehalose dimycolate and free trehalose, in this way fabricating the bacterial cellwall, this

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