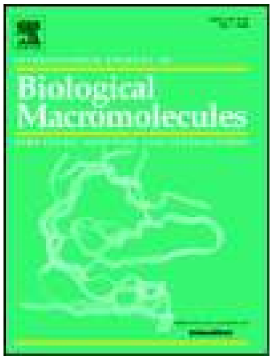

Optimization of chitosan nanoparticle synthesis and its potential application as germination elicitor of Oryza sativa L.

K. Divya, Smitha Vijayan, Sreekumar Janardanan Nair, M.S. Jisha

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Optimization of Chitosan Nanoparticle Synthesis and its Potential Application as Germination Elicitor of *Oryza sativa* L.

K. Divya[1], Smitha Vijayan[1], Sreekumar Janardanan Nair[2], M.S. Jisha[1] *

*jishams@mgu.ac.in

[1] School of Biosciences, Mahatma Gandhi University, Kottayam, Kerala, India. PIN 686 560.

[2] Principal Scientist, Central Tuber Crops Research Institute, Sreekariyam, Thiruvananthapuram

*AUTHOR FOR CORRESPONDENCE:

Dr. M.S. Jisha,

Professor, School of Biosciences, Mahatma Gandhi University, Kottayam, Kerala, India. PIN 686 560.

Email: jishams@mgu.ac.in

Mobile No. +91-9497664697

Fax: 91-481-2731002

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Bionanocomposite films based on potato, tapioca starch and chitosan reinforced with cellulose nanofiber isolated from turmeric spent

Sreeraj Gopi[a,b,c,*], Augustine Amalraj[a], Shintu Jude[a], Sabu Thomas[b], Qipeng Guo[c]

[a] R&D Centre, Aurea Biolabs (P) Ltd, Kolenchery, Cochin 682 311, Kerala, India
[b] International and Inter University Center for Nanoscience and Nanotechnology, School of Chemical Sciences, Mahatma Gandhi University, Priyadarsini Hills P.O, Kottayam 686 560, Kerala, India
[c] Institute in Frontier Materials, Deakin University, Geelong, Victoria 3220, Australia

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ABSTRACT

The aim of this research was to enhance the physicochemical properties of potato starch (PS), tapioca starch (TS) and chitosan (CS) based bionanocomposite films by incorporating with different levels of turmeric nanofiber (TNF). The TNF was prepared from turmeric spent by acid hydrolysis accompanied with high pressure homogenization. The morphology of the bionanocomposites was analyzed by SEM and it revealed their large aggregation cluster with dense structure through tightly packed TNF in the biocomposite films. The attainment of bionanocomposites due to the formation of fresh hydrogen bonds between the hydroxyl groups of PS, TS and CS with TNF authenticated by FT-IR spectroscopy. XRD results exhibited the disappearances of peaks of TNF indicating the reinforcement of TNF in the prepared bionanocomposite matrixes. The tensile strength and Young's modulus of the bionanocomposites were improved tremendously through increasing TNF concentration due to the formation of starch-TNF and chitosan-TNF network. DSC data indicated the addition of TNF significantly increased the onset temperature, peak temperature and conclusion temperature of bionanocomposites; however, the enthalpy change values considerably decreased. The antibacterial test showed the bionanocomposites exhibited excellent antibacterial performance against *Bacillus cereus, Escherichia coli, Staphylococcus aureus* and *Salmonella typhimurium* due to the addition of TNF in the biopolymer matrixes.

1. Introduction

Biopolymers are defined as biologically degradable polymers which are produced by living organisms. They contain monomeric units that are covalently bonded to form larger structures which are generally sustainable and renewable materials, as they are made from living materials. Biopolymers have a surprising number of responsibilities in our body based on various biomolecular sciences; they hold cells together to form tissues, provide intelligent chemical signals to the cells to guide their behavior, contribute to the hydration of skin and elasticity, lubricate joints and gastrointestinal tracts and protect against pathogens by assembling into the mucus gel that covers the eyes and respiratory tract. The chemical structures and compositions of biopolymers are very similar to the macromolecules of the native extracellular environment. Utilization of these materials in living systems would possibly reduce the simulation of chronic inflammation or immunological reactions and toxicity which occur frequently when a synthetic polymer device is implanted into the host [1]. The biopolymers demonstrate an elevated prospective to be utilized as a preference to synthetic polymers and plastics, as they are more eco-friendly and are simple biodegradable and renewable materials. The development of innovative technologies and the growth of biological products decrease the confidence in synthetic polymers and plastic materials [2]. Moreover, modified biopolymers can provide the mechanical, thermal and electrical properties required for particular applications. The molecular structures of biopolymers can be altered depending on the plant sources and processing treatments applied, which probably allowed targeted modification of biopolymer molecular structures to design plant based dispersions with tailored properties. Blending of biopolymers are used with the aim to extent their applications especially from natural resources for a wide range of applications like biodegradable, packing materials, automotive industries, agricultural and pharmaceutical industries [1,3].

The natural world has proffered various natural biopolymers particularly polysaccharides such as cellulose, starch and chitosan (CS) and has proven extremely feasible alternative to confect green

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* Corresponding author at: R&D Centre, Aurea Biolabs (P) Ltd, Kolenchery, Cochin 682 311, Kerala, India.
E-mail address: sreeraj.gopi@plantlipids.com (S. Gopi).

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A brief overview of molecularly imprinted polymers supported on titanium dioxide matrices

T. Sajini [a], [b], [c], M.G. Gigimol [b], B. Mathew [c], *

[a] *Research & Post Graduate Department of Chemistry, St Berchmans College, Kottayam, Kerala, India*
[b] *Research & Post Graduate Department of Chemistry, St Thomas College, Pala, Kerala, India*
[c] *School of Chemical Sciences, Mahatma Gandhi University, Kottayam, Kerala, India*

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ABSTRACT

Molecularly imprinted polymer (MIP) is a polymer competent of mimicking selective binding of target or template molecule, which is characteristic of enzyme and antibodies. MIP has a wide range of applications in various fields of science and can be used as a sensor, catalyst, drug delivery component, etc. To overcome some demerits of MIP, the process of formation of imprinting cavity was carried out by nanoimprinting materials, which enables the imprinting technique to create more effective recognition sites than those obtained by traditional approaches. Here, in this article, we described a brief account of various discoveries happened in titanium dioxide–based molecularly imprinted polymeric system that shows a wide variety of chemical applications. The intention of this article is to provide comprehensive knowledge and information to all researchers who are interested in exploiting molecular imprinting technology toward the rational design of various chemical sensors operating on different transduction principles, ranging from electrochemical to piezoelectric, being used for the detection of different template molecules as they pose considerable impact on the understanding of the origin of life and all processes that occur in living organisms.

1. Introduction

Molecular imprinting is one of the promising techniques for the fabrication of polymers with predetermined selectivity, specificity, and high affinity toward a target molecule, which involves arrangement of polymerizable functional monomers around a template molecule [1–4]. Molecularly imprinted polymers (MIPs) have the capability to specifically distinguish and separate a particular molecule from other molecules of similar structures [5]. MIPs established widespread attention and have become attractive in many fields, such as purification and separation, chemosensing/biosensing, artificial antibodies, drug delivery, and catalysis and degradation, owing to their high physical stability, structure predictability, recognition specificity, straightforward preparation, remarkable robustness, and low cost [6]. Among the various approaches, such as covalent imprinting, non-covalent imprinting, and semicovalent imprinting, used during synthesis of MIPs, non-covalent interaction can be considered the best one because of the easy removal of the template, its applicability for a variety of molecules, and being an economical and easy method [7]. A schematic representation of the molecular imprinting process is shown in Scheme 1.

In some cases, most of the bulk part of the polymer was unavailable for further rebinding of the template molecule which will lead to its low binding efficacy and low response kinetics. In conventional imprinting techniques, organic polymers [4,14–28] and metal oxides [29–39] are used as the matrices for molecular imprinting. These bulk imprinted materials are associated with some drawbacks such as complex fabrication procedure, low binding efficiency, and slow binding process as the imprinted sites are far from the surface and ready access of guest molecules to binding sites is often suppressed. So, many efforts were taken to resolve these problems [8–11]. One of the techniques is based on the small dimension with extremely high surface-to-volume ratio of nano-imprinting materials, which enable the imprinting technique to generate more effective recognition sites than those obtained by conventional approaches that only use porogens [12]. The imprinting of molecular recognition sites supported on

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* Corresponding author.
E-mail address: beenamathew@mgu.ac.in (B. Mathew).

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Investigation on the key aspects of L-arginine Para nitrobenzoate monohydrate single crystal: A non-linear optical material

Sonia, N. Vijayan, Mahak Vij, Kanika Thukral, Naghma Khan, D. Haranath, Rajnikant, M.S. Jayalakshmy

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Materials and Product Engineering

Investigation on the key aspects of L-arginine para nitrobenzoate monohydrate single crystal: A Non-Linear Optical material

Sonia[1, 2], N. Vijayan[*, 2], Mahak Vij[1, 2], Kanika Thukral[1, 2], Naghma Khan[1,2], D. Haranath[2]
Rajnikant[3], M.S. Jayalakshmy[4]

[1]Academy of Scientific and Innovative Research, CSIR- National Physical Laboratory
New Delhi –110012, India

[2]CSIR-National Physical Laboratory, Dr. K.S. Krishnan Road, New Delhi – 110 012, India

[3]Department of Physics, University of Jammu, Jammu Tawi, India

[4] International and Inter University Centre for Nanoscience and Nanotechnology, Mahatma Gandhi University, Kottayam, Kerala, India - 686 560.

Abstract: - In the contemporary days, non-linear optical materials (NLO) are getting higher attention as per the increasing demand in optical communication and data storage technology. Consequently, they explore various physical properties of the NLO material for their industrial applications. In current report, L-arginine p-nitrobenzoate monohydrate (LANB) single crystals were obtained by adopting slow cooling technique. The structural confirmation of grown single crystal was carried out using single crystal X-Ray diffractometer. Presence of strain within single crystal was deduced using Hall–Williamson relation. Various defects associated within single crystal were assessed using high resolution XRD. Additionally, its crystalline quality was again confirmed by time resolved photoluminescence spectroscopy (TRPL). Using transmission spectra, the cut off wavelength and band gap of the host material was determined to be nearly 420 nm and 2.9 eV respectively. The dielectric property has been recorded by varying the frequency ranging from 50 Hz to 100 KHz. The curve suggests that dielectric loss value is less at high frequency ensures the suitability of crystal in photonics and NLO based devices. The laser damage threshold values were also measured for single and multiple shots. Thermal parameters of the titled compound were calculated using PPE. In photoconductivity measurement, negative photoconductivity has been observed in titled compound. Microhardness studies were also performed on single crystal to explore its mechanical properties.

polymers

MDPI

Article

Robust Superhydrophobic Cellulose Nanofiber Aerogel for Multifunctional Environmental Applications

Hasan. M. [1], **Deepu A. Gopakumar** [2,3,*], **Vishnu Arumughan** [4], **Yasir Beeran Pottathara** [3,5], **Sisanth K. S.** [5], **Daniel Pasquini** [6], **Matej Bračič** [7], **Bastien Seantier** [3], **Ange Nzihou** [8], **Sabu Thomas** [5], **Samsul Rizal** [9] and **Abdul Khalil H. P. S.** [2,*]

[1] Chemical Education Department, Universitas Syiah Kuala, Jln. Tgk. Daud Beureueh Darussalam Banda Aceh, Banda Aceh 23311, Indonesia; muhammadhasan.kimia@unsyiah.ac.id
[2] School of Industrial Technology, Universiti Sains Malaysia, Penang 11800, Malaysia
[3] Univ. Bretagne Sud, UMR CNRS 6027, IRDL, F-56100 Lorient, France; ptyasirbeeran@gmail.com (Y.B.P); bastien.seantier@univ-ubs.fr (B.S)
[4] Department of Chemistry and Chemical Engineering, Chalmers University of Technology, Kemigården 4, 412 96 Göteborg, Sweden; vishnukarumughan@gmail.com
[5] International and Inter University Centre for Nanoscience and Nanotechnology, Mahatma Gandhi University, Kottayam, Kerala 686560, India; sisanth.ks@gmail.com (S.K.S.); sabuthomas@mgu.ac.in (S.T.)
[6] Chemistry Institute, Federal University of Uberlandia-UFU, Campus Santa Monica-Bloco1D-CP 593, 38400902 Uberlandia, Brazil; danielpasquini2013@gmail.com
[7] Institute of Engineering Materials and Design, University of Maribor, 2000 Maribor, Slovenia; matej.bracic@um.si
[8] Université de Toulouse, IMT Mines Albi, RAPSODEE CNRS UMR-5302, Campus Jarlard, F-81013 Albi CEDEX 09, France; ange.nzihou@mines-albi.fr
[9] Department of Mechanical Engineering, Universitas Syiah Kuala, Banda Aceh 23111, Indonesia; samsul_r@yahoo.com
* Correspondence: deepu1789@gmail.com (D.A.G.); akhalilhps@gmail.com (A.K.H.P.S.)

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Abstract: The fabrication of superadsorbent for dye adsorption is a hot research area at present. However, the development of low-cost and highly efficient superadsorbents against toxic textile dyes is still a big challenge. Here, we fabricated hydrophobic cellulose nanofiber aerogels from cellulose nanofibers through an eco-friendly silanization reaction in liquid phase, which is an extremely efficient, rapid, cheap, and environmentally friendly procedure. Moreover, the demonstrated eco-friendly silanization technique is easy to commercialize at the industrial level. Most of the works that have reported on the hydrophobic cellulose nanofiber aerogels explored their use for the elimination of oil from water. The key novelty of the present work is that the demonstrated hydrophobic cellulose nanofibers aerogels could serve as superadsorbents against toxic textile dyes such as crystal violet dye from water and insulating materials for building applications. Here, we make use of the possible hydrophobic interactions between silane-modified cellulose nanofiber aerogel and crystal violet dye for the removal of the crystal violet dye from water. With a 10 mg/L of crystal violet (CV) aqueous solution, the silane-modified cellulose nanofiber aerogel showed a high adsorption capacity value of 150 mg/g of the aerogel. The reason for this adsorption value was due to the short-range hydrophobic interaction between the silane-modified cellulose nanofiber aerogel and the hydrophobic domains in crystal violet dye molecules. Additionally, the fabricated silane-modified cellulose nanofiber hydrophobic aerogels exhibited a lower thermal conductivity value of 0.037 $W \cdot m^{-1} K^{-1}$, which was comparable to and lower than the commercial insulators such as mineral wools (0.040 $W \cdot m^{-1} K^{-1}$) and polystyrene foams (0.035 $W \cdot m^{-1} K^{-1}$). We firmly believe that the demonstrated silane-modified cellulose nanofiber aerogel could yield an eco-friendly

Document details

1 of 1
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A new 'Washington Consensus': 'Indo-Pacific' and India's emerging role (Review)

Seethi, K.M.

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School of International Relations and Politics, Mahatma Gandhi University, Kerala, India

View additional affiliations

Abstract

The United States administration is fervently promoting the "Indo-Pacific" as an alternative geopolitical construct to mobilise a large number of countries in the Asia-Pacific region to contain Chinese and Russian influence. However, India under the Narendra Modi administration has become a strategic contraption by yielding to the pressures of the Donald Trump regime for a programmed "Indo-Pacific" ploy. In the emerging scenario, New Delhi's rhetoric on "strategic autonomy" has become a political liability. © 2019 Economic and Political Weekly. All Rights Reserved.

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Plant Growth Promoting Traits of Indigenous Phosphate Solubilizing *Pseudomonas aeruginosa* Isolates from Chilli (*Capsicum*annuum L.) Rhizosphere

M. S. Linu[a], Aju K. Asok[a], Meenu Thampi[a], J. Sreekumar[b], and M. S. Jisha[a]

[a]School of Biosciences, M G University, Kottayam, Kerala, India; [b]Section of Social Sciences, Central Tuber Crops Research Institute, Trivandrum, Kerala, India

ABSTRACT

Phosphorus (P) is the second key nutrient for plants and it affects several attributes of plant growth. Identification of a potent phosphate solubilizing microorganism capable of transforming the insoluble P into soluble and plant-accessible forms is considered as the best eco-friendly option for providing inexpensive P to plants. Hence, this study was focused to assess the growth enhancement traits of the phosphate solubilizing bacteria (PSB) isolated from chili rhizosphere. Twelve PSB were isolated by enrichment culture technique and its P solubilization efficiency was checked using Vanadomolybdate phosphoric yellow color method. Among them, two potent strains PS2 and PS3, identified as *Pseudomonas aeruginosa* KR270346 and KR270347 based on biochemical and molecular characterization, were selected for further study. The *Pseudomonas aeruginosa* isolates interestingly showed the presence of various potential plant growth-promoting properties including indole acetic acid and siderophore production. The growth enhancement effect of *Pseudomonas aeruginosa* isolates on chilli showed promising results, and the growth parameters were found to be statistically significant when compared to control. The results demonstrated an eloquent impact on various aspects, namely microbial count and PSB population, phosphatase and dehydrogenase activity, available phosphorous in the soil, plant nutrient uptake, and yield parameters. Inoculation of these two isolates together with the addition of rock phosphate increased comparable amount of available P and these treatments were statistically at par throughout the growth period. The results confirmed the growth-promoting potential of the isolates to develop as biofertilizers either alone or as components of integrated nutrient management systems.

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Available phosphorus; chili; dehydrogenase activity; phosphate solubilizing microorganisms; Pseudomonas aeruginosa

Introduction

Phosphorus is the second most abundant plant nutrient available in the soil after nitrogen (Hariprasad and Niranjana 2009). Even though soil contains high level of total phosphorus, majority of them is in insoluble form as iron and aluminum phosphates in acidic soils and calcium phosphates in alkaline soils. Plants are unable to utilize precipitated form of phosphorus. Organic matter is an important reservoir of immobilized phosphate and only a small portion (~0.1%) is available to plants. In comparison to other nutrients, P concentration in soil solution is much lower and it ranges from 0.001 to 1 mg/l (Brady and Weil 2002). Hence, most cropping systems on these soils require supplemental phosphorus to maximize their yield potential.

CONTACT M. S. Jisha jishams@mgu.ac.in School of Biosciences, M G University, Kottayam, Kerala, India

Color versions of one or more of the figures in the article can be found online at www.tandfonline.com/LCSS.

Structural and photoluminescence properties of UV-excited Er^{3+} doped Ba_2CaWO_6 yellowish-green phosphors

Sreeja E, Remya Mohan P, Subash Gopi, Cyriac Joseph, N.V. Unnikrishnan, P.R. Biju

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Structural and photoluminescence properties of UV-excited Er^{3+} doped Ba_2CaWO_6 yellowish-green phosphors

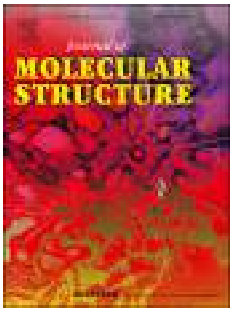
Sreeja E, Remya Mohan P, Subash Gopi, Cyriac Joseph, N.V. Unnikrishnan, P R Biju*
School of Pure and Applied Physics, Mahatma Gandhi University, Kottayam, 686560, India
**E-mail address:* prb.mgu@gmail.com

Abstract

Double perovskite Ba_2CaWO_6 phosphors doped with different concentrations of Er^{3+} have been synthesized by the conventional solid state reaction method in air at 1250 °C and are characterized by X-ray diffraction analysis (XRD), Energy Dispersive X-ray Spectrometer (EDS), Scanning electron microscope (SEM), Transmission electron microscope (TEM), Fourier transform infrared spectroscopy (FTIR) and Photoluminescence measurements. An intense green and weak red emissions are observed at 566 nm ($^4S_{3/2} \rightarrow {}^4I_{15/2}$), 680 nm ($^4F_{9/2} \rightarrow {}^4I_{15/2}$) under 314 nm, 378 nm corresponding to charge transfer band and rare earth excitations respectively. Under charge transfer excitation Ba_2CaWO_6:xEr^{3+} samples exhibit high intense emission peaks of Er^{3+} than the rare earth excitation. This is due to an efficient energy transfer from WO_6^{6-} to Er^{3+}. The maximum emission intensity was observed for 0.08 wt% concentration of Er^{3+} ions in Ba_2CaWO_6 phosphors. The critical energy transfer distance among Er^{3+} ions is calculated to be 15.18 Å and the quenching mechanism is due to dipole-dipole interaction. The energy transfer mechanism is discussed based on the energy level diagram of Er^{3+}. The radiative lifetimes were determined from the fluorescence decay analysis. The CIE color coordinates were calculated from the emission spectra. The result shows that Ba_2CaWO_6:Er^{3+} phosphor can be considered as a potential candidate for UV excited yellowish-green phosphor for display applications.

1 Introduction

UV-excited phosphors have been widely used in numerous fields of photonic applications such as phosphor based new lighting devices fluorescence tube, CFLs and display devices etc. [1]. For the generation of white light using phosphors, generally two methods have been employed. One of the commonly used methods for the production of commercial white LEDs is the combination of a blue LED chip with $Y_3Al_5O_{12}$: Ce^{3+} (YAG: Ce) phosphor and the other is the combination of red, green, blue emitting phosphors excited with UV-LED [2]. Unfortunately, these methods suffer several limitations like low color rendering index, high color temperature, low luminescent efficiency etc [3, 4]. The aforementioned problems can be resolved by using a new chemically stable trichromatic (red, green, blue) phosphor with strong absorption in the ultraviolet (UV) region. The phosphors with the different range of



Photobehaviour and *in vitro* binding strategy of natural drug, chlorogenic acid with DNA: A case of groove binding

Riju K. Thomas, Surya Sukumaran, C. Sudarsanakumar

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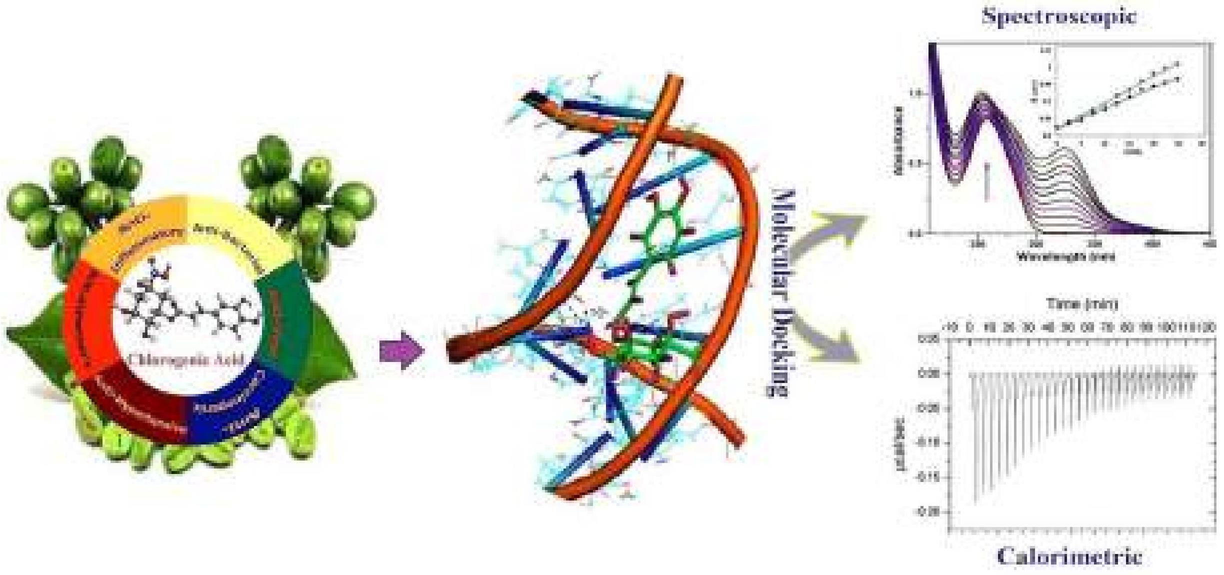

Anti-inflammatory
Anti-bacterial
Chlorogenic Acid
Molecular Docking
Spectroscopic
Absorbance
Wavelength (nm)
Time (min)
µcal/sec
Calorimetric

Photobehaviour and *In Vitro* binding strategy of natural drug, Chlorogenic acid with DNA: A case of groove binding

Riju K. Thomas[a], Surya Sukumaran[a], C. Sudarsanakumar[a*]

[a]School of Pure and Applied Physics, Mahatma Gandhi University

Kottayam, Kerala, India, 686560.

*Corresponding author: Prof. C. Sudarsanakumar,

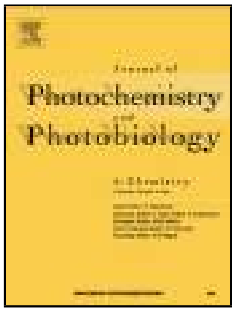
*E-mail: c.sudarsan.mgu@gmail.com

Ph: +91481-2731043, Fax: +91 481 2730423

Mob: 09447141561

Abstract

Chlorogenic acid (CHA), a non-toxic natural drug exhibits a wide range of pharmacological potential including anti-diabetic and anti-carcinogenic activities. The molecular mechanism behind the interaction of CHA with DNA has not yet been addressed, while its pharmacological activities have been reported. The sensible DNA targeting protocol by phytochemicals like CHA not only offers an insight into the designing of more efficient drugs, but also leading the way towards the establishment of therapeutic agents for the regulation of gene expressions. This study unravelled the binding mode of CHA with calf thymus DNA (ct-DNA) through a series of spectroscopic, calorimetric, dye displacement and molecular docking analysis. The binding constants obtained from the fluorescence and the UV absorption experiments were consistently in the order of 10^3 Mol^{-1} with the renowned minor groove binders. The dye displacement studies using fluorophores conjugated ct-DNA systems confirmed the minor groove binding of CHA. The energetics of interactions explored from ITC revealed a spontaneous and enthalpy driven exothermic association. The CD and



Title: Phase Transfer Reaction for the Preparation of Stable
Polymer-Quantum Dot Conjugates

Authors: Geethy P. Gopalan, Ajith Nair Anil, Ghimire
Sushant, Nidhin Joy, Ken-ichi Yuyama, Vasudevanpillai Biju,
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Pervaporation separation of an azeotropic mixture of a tetrahydrofuran–water system with nanostructured polyhedral oligomeric silsesquioxane embedded poly(vinyl alcohol)

Valiya Parambath Swapna,[1] Thomasukutty Jose,[2] Soney C. George,[2] Sabu Thomas,[3] Ranimol Stephen[1]

[1]Department of Chemistry, St. Joseph's College (Autonomous), Devagiri, Calicut, Kerala 673 008, India

[2]Centre for Nano Science and Technology, Department of Basic Sciences, Amal Jyothi College of Engineering, Kanjirapally, Kerala 686 518, India

[3]School of Chemical Sciences and International and Inter University Centre for Nanoscience and Nanotechnology, Mahatma Gandhi University, Kottayam, Kerala 686 560, India

Correspondence to: R. Stephen (ranistephen@gmail.com)

ABSTRACT: Cage - structured polyhedral oligomeric silsesquioxane (POSS) molecules were used as modifiers in the fabrication of poly (vinyl alcohol) (PVA) membrane for the separation of an azeotropic mixture of tetrahydrofuran (THF) and water system. Poly(ethylene glycol) and anionic octa(tetramethyl ammonium)-functionalized POSS were used for this study. The membranes exhibited excellent water selectivity and permeance because of their preferential interactions toward water molecules in the azeotropic THF–water mixture. In the presence of poly(ethylene glycol)–POSS and anionic octa(tetramethyl ammonium)–POSS, the PVA membrane exhibited a significant increase in selectivity. A modified Maxwell–Stefan equation was used for the computation of the theoretical flux, which was compared with the experimental values. © 2018 Wiley Periodicals, Inc. J. Appl. Polym. Sci. **2018**, *135*, 47060.

KEYWORDS: membranes; separation techniques; thermoplastics

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INTRODUCTION

Tetrahydrofuran (THF) is an extensively used highly volatile polar aprotic solvent. It is widely used in the chemical industry to manufacture pharmaceutical products, such as reagents for drug synthesis, adhesives, paints, and inks. Moreover, highly pure THF is required for the production of various polymers, including poly(tetramethylene oxide) and its copolymers.[1] THF and water can easily form azeotrope at 94.7 mol % THF. It is difficult to obtain commercially important highly pure (99.9 mol %) THF from a THF–water azeotropic mixture by conventional separation methods, such as distillation, liquid–liquid extraction, and absorption. In industry, columns filled with molecular sieves are used to remove water from THF.[2] The distillation process creates many environmental, economic, and technical challenges and carries a risk of explosion due to the reaction of THF with atmospheric oxygen.[3] The complex separation problem of the azeotrope can be solved by polymer-membrane-based pervaporation technology. It is an efficient, ecofriendly, and easily performed separation method compared to the conventional separation process. The success of the pervaporation process depends on the morphology of membrane and its properties. Membranes with good selectivity (α_{wt}) and high permeability are desirable for the better separation of solvent mixtures.[4,5] Recently, silica–polymer hybrid membranes are found to be useful in the drug release and separation of azeotropic liquid mixtures because of their unique transport properties, which are not present in the individual components.[6–8]

Poly(vinyl alcohol) (PVA) is a water-soluble, semicrystalline glassy polymer. PVA is used to manufacture membranes for separation processes, artificial biomedical devices, and drug-delivery systems because of its good film-forming nature, chemical stability, hydrophilicity, biocompatibility, and biodegradability. The polymerization degree and chain length of PVA are important parameters affecting the separation performance of its membranes. The viscosity of the PVA membrane increases with increasing polymerization degree; this is followed by a significant alteration in the fractional free volume and the separation efficiency of the membrane.[9] However, PVA membranes have the

Review

Electrospinning Tissue Engineering and Wound Dressing Scaffolds from Polymer–Titanium Dioxide Nanocomposites

Kajal Ghosal, Christian Agatemor, Zdenko Špitálsky, Sabu Thomas, Erich Kny

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Journal of Cosmology and
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Constraints on tensor to scalar ratio using WKB approximation

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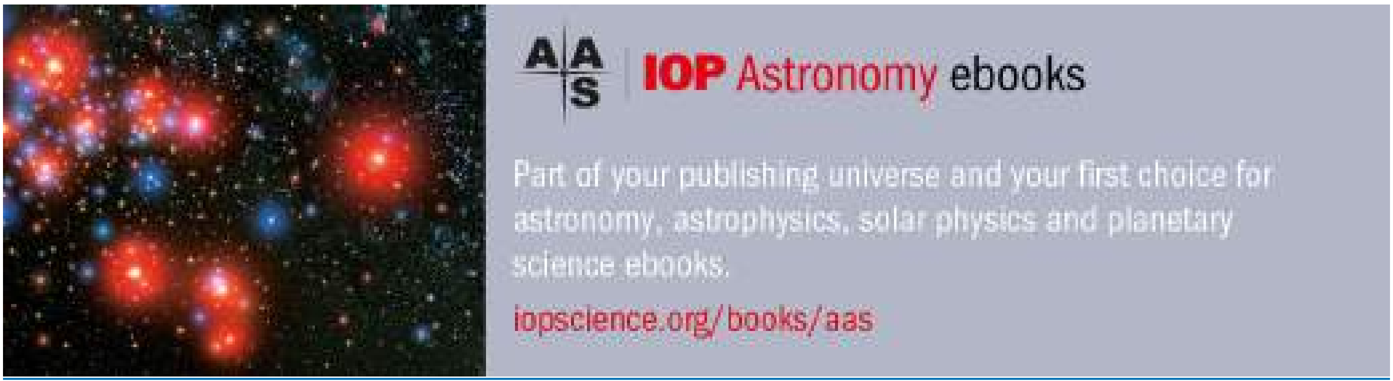

ACS Combinatorial Science

Review

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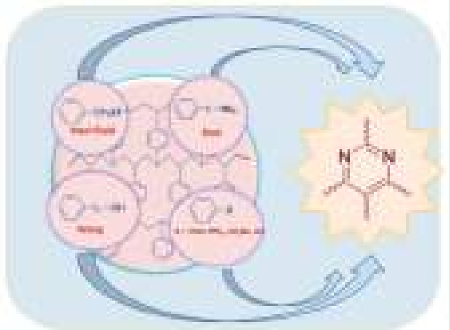
Advances in the Solid-Phase Synthesis of Pyrimidine Derivatives

E. P. Aparna and K. S. Devaky*

School of Chemical Sciences, Mahatma Gandhi University, Kottayam, Kerala 686560, India

ABSTRACT: This Review describes the existing synthetic approaches for the solid-phase synthesis (SPS) of differently substituted and fused pyrimidine derivatives. These synthetic strategies are classified on the basis of the different synthetic routes leading to the particular type of pyrimidine heterocycle formed. The Review discusses the application of a variety of polystyrene derived supports for the construction of pyrimidine rings. The effect of microwave heating on the solid-phase synthesis is also addressed in the review.



KEYWORDS: *solid-phase synthesis, pyrimidine derivatives, microwave irradiation*

INTRODUCTION

Heterocyclic compounds are molecules having cyclic structure containing at least one atom, such as sulfur, oxygen, or nitrogen, in addition to carbon as part of the ring, and they constitute the largest family of organic compounds. Nitrogen containing heterocycles especially pyrimidines form an important class of heterocyclic compounds.[1−3] Heterocycles containing pyrimidine ring has wide occurrence in nature.[4] Nucleic acid bases, such as thymine, cytosine, and uracil, and many natural products, such as vitamins (thiamine), are pyrimidine derivatives. Many pyrimidine derivatives find applications in biological and clinical field.[2,3,5] For example, drugs containing pyrimidine moieties, such as barbituric acid and Veronal, are used as hypnotics.[6] Many compounds containing fused pyrimidine systems act as pharmacophores, for example, deazapurines, a class of pyrrolo[3,2-*d*]pyrimidines, act as antagonists toward adenosine receptor subtypes[7,8] and inhibitors of enzymes.[9−12] Fused pyrimidine systems, such as 1,2,4-triazolo[1,5-*a*]pyrimidine and thiazolo[4,5-*d*]pyrimidine-5,7-dione, find extensive applications in biological fields.[13−26] Most of the polyaminopyrimidines are important therapeutic agents,[27] particularly aminopyrimidines are major components in drugs, such as Gleevec (a tyrosine kinase inhibitor) and the hypocholesterolemic agent rosuvastatin.[28,29] Recently, arylimidazopyrimidines appear to be essential in the pathology of Alzheimer's disease for detecting β-amyloid (Aβ) plaques in the brain. Many marine alkaloids have shown inherent biological activity because of the presence of dihydropyrimidinone moiety.[30] Thus, nitrogen-containing heterocycles, especially pyrimidines, have been accepted as special in pharmacophores. This Review discusses the different strategies employed in the solid-phase synthesis of substituted pyrimidines owing to their broad range of applications.

Combinatorial chemistry has emerged as an integral part of research in the synthesis of new pharmacophores by using "split and pool" protocols in association with solid-phase synthesis,[31−40] which was expanded from Merrifield's polymer-supported peptide synthesis to the field of small organic molecules. Traditionally developed methods for the synthesis of drug libraries are too slow and costly to effectively address the needs of drug discovery. In recent decades, solid-phase synthesis has been exploited to overcome this problem by synthesizing libraries of molecules that are biologically active, as well as powerful alternative method for the optimization of potential drug candidates.[41−45] One of the most important features of solid-phase organic synthesis in drug discovery is the elimination and purification of intermediates, allowing the rapid synthesis of libraries of structurally related compounds. In solid-phase organic synthesis, the product workup is easy and could be achieved by simple procedures like filtration and washings. Further, the reaction can be driven to completion by the use of excess soluble reagents without causing separation problems leading to increased product yield. Reactions that are impractical in solution phase are also carried out in solid-phase mechanism.[46,47] Application of microwave irradiation to chemical reactions has introduced a new dimension to solid-phase synthesis to aid the development of new, ecofriendly, synthetic protocols. From an environmental point of view, microwave reactions proceed via "dry media reaction" and "solvent less synthesis" mechanisms and play an important role in protecting the environment in addition to providing an increased yield of products by minimizing decomposition.[48−51] Solid-phase synthesis accelerates the production of targeted compounds by eliminating purification and isolation of intermediates, whereas microwave heating reduces the time required for completion of the reaction. Combining the two

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RESEARCH PAPER

Anticancer, antimicrobial, antioxidant, and catalytic activities of green-synthesized silver and gold nanoparticles using *Bauhinia purpurea* leaf extract

Remya Vijayan[1] · **Siby Joseph**[2] · **Beena Mathew**[1]

Received: 11 August 2018 / Accepted: 2 November 2018

Abstract

The synthesis of metal nanoparticles by green methods attained enormous attention in recent years due to its easiness, non-toxicity, and eco-friendly nature. In the present study, noble metal nanoparticles such as silver and gold were prepared using an aqueous leaf extract of a medicinal plant, *Bauhinia purpurea*. The leaf extract performed as both reducing and stabilizing agents for the development of nanoparticles. The formations of silver and gold nanoparticles were confirmed by observing the surface plasmon resonance peaks at 430 nm and 560 nm, respectively, in UV–Vis absorption spectrum. Various properties of nanoparticles were demonstrated using the characterization techniques such as FTIR, XRD, TEM, and EDX. The synthesized silver and gold nanoparticles had a momentous anticancer effect against lung carcinoma cell line A549 in a dose-dependent manner with IC_{50} values of 27.97 µg/mL and 36.39 µg/mL, respectively. The antimicrobial studies of synthesized nanoparticles were carried out by agar well diffusion method against six microbial strains. Silver and gold nanoparticles were also showed high antioxidant potentials with IC_{50} values of 42.37 µg/mL and 27.21 µg/mL, respectively; it was measured using DPPH assay. Additionally, the nanoparticles were observed to be good catalysts for the reduction of organic dyes.

Keywords Metal nanoparticles · Green synthesis · *Bauhinia purpurea* · Anticancer · Antimicrobial · Antioxidant · Catalysis

Introduction

Nanotechnology refers to the synthesis of material with various shapes, size, and chemical compositions within the size range of 1–100 nm. Nanoparticles have numerous applications in various fields such as medicine, optoelectronics, and catalysis [1, 2]. The noble metal nanoparticles such as silver and gold have a very important role in biology, medicine, and electronics because of their size-dependent properties [3]. Nanoparticles possess high surface to volume ratio, which is increasing with decreasing size of nanoparticles. Due to this high surface area, nanoparticles have high catalytic and related properties. As the surface area increases, the biological effectiveness of the nanoparticles also increases due to the increase in surface energy [2].

Different methods such as physical and chemical methods are used for the preparation of metal nanoparticles [4, 5], for examples, lithography [6], laser ablation [7], and photochemical reduction methods [8]. These methods are very costly and necessitate the use of harmful chemicals [9]. This leads to the contamination of nanoparticle surfaces and results in the adverse effect of its applications mainly in medical applications.

Biomolecules are suitable for consistent and eco-friendly synthesis of metal nanoparticles. A number of bacteria, fungi, and yeasts have been familiar with the production of noble metal nanoparticles [10–13]. But this microbial-mediated synthesis of nanoparticles is not industrially feasible because it needs high hygienic conditions and its maintenance also requires highly expensive medium [14, 15]. Hence, the use of plant materials for the production of nanoparticles obtained abundant attention in the past few decades. The biomolecules present in the plant extract can reduce the metal ions to nanosized particles and also stabilizes the nanoparticles formed [16]. In recent years, various

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✉ Beena Mathew
beenamscs@gmail.com

[1] School of Chemical Sciences, Mahatma Gandhi University, Kottayam, Kerala 686560, India

[2] Department of Chemistry, St. George's College, Aruvithura, Kottayam, Kerala 686122, India

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Assessment of soil fertility characteristics of chemical-fertilized banana fields of south India

J. G. Ray & K. S. Nidheesh

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ASIAN JOURNAL OF ORGANIC CHEMISTRY
Minireview

Copper-Catalysed Multicomponent Syntheses of Heterocycles

Reeba Mary Cherian,[a] Nissy Ann Harry,[a] Salim Saranya,[a] K. R. Rohit,[a] and
Gopinathan Anilkumar*[a, b]

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ORIGINAL PAPER

Novel cobalt-valine catalyzed O-arylation of phenols with electron deficient aryl iodides

Sankuviruthiyil M. Ujwaldev[1] · **Salim Saranya**[1] · **Nissy Ann Harry**[1] · **Gopinathan Anilkumar**[1]

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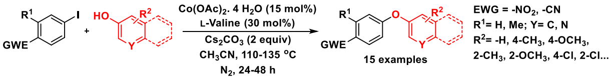
Abstract

A Novel cobalt-catalyzed O-arylation of phenols with electron deficient aryl iodides is described. The reaction employs cheap and easy-to-handle cobalt acetate tetrahydrate as the catalyst precursor and naturally occurring L-valine as the ligand without the use of any transmetallating or reducing agents. The new protocol offers a wide scope for a variety of phenols towards O-arylation with moderate to excellent yields with electron deficient aryl iodides.

Graphical abstract



Keywords Cobalt catalysis · C–O coupling · Etherification · Valine · Reducing agent

Introduction

Exploration of transition metal catalyzed methodologies for the development of carbon–heteroatom single bonds, especially carbon–oxygen bonds, has been a persistent effort in synthetic organic chemistry for the past few decades [1]. The natural abundance and biological potencies of many pharmaceutical derivatives containing ether cores easily substantiate their importance in synthetic organic chemistry [2].

After being first reported in 1904 through a stoichiometric amount of copper-mediated coupling between aryl halides with phenols [3], the advances made in the field had been very fascinating [4]. Along with the development of catalytic versions of the pioneering copper salt mediated C–O coupling protocols, use of alternate metals like palladium [5], iron [6], or nickel [7] was also interesting and sometimes more inventive. Another break through was the Chan–Lam coupling, which couples boronic acids with phenols, has also witnessed decent development [8]. In order to improve the efficiency of catalytic reactions, chemists in catalysis always showed urge in finding alternative metals or ligands in spite of the efficacy of the prevailing protocols which always led to the development of new catalysts and protocols. Cobalt-catalyzed cross-coupling chemistry is also a well-developed area having a history of more than 70 years with the initial report of homo-coupling of aromatic magnesium reagents by Kharash [9]. Although initial focus of this area was mainly on the development of carbon–carbon bonds, worthy developments also ensued in carbon–sulfur [10] and carbon–nitrogen [11] coupling reactions. However, cobalt-catalyzed carbon–oxygen coupling reactions are sparsely reported in literature and to the best of our knowledge the only report available is by Kundu et al. in 2015 [12]. The protocol was highly efficient for the coupling between phenols and aryl/styrenyl halides; but required equal amounts of copper iodide as the transmetallating agent along with cobalt catalyst making the catalytic system more complex and expensive (Scheme 1). As the catalytic activity of the cobalt in other carbon–heteroatom bond forming reactions

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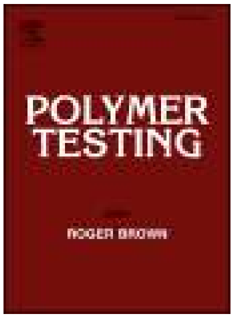
✉ Gopinathan Anilkumar
anilgi1@yahoo.com

[1] School of Chemical Sciences, Mahatma Gandhi University, P D Hills P O, Kottayam, Kerala 686560, India



Development of plasticized poly (vinyl chloride)/reduced graphene oxide nanocomposites for energy storage applications

H. Akhina, P. Mohammed Arif, M.R. Gopinathan Nair, K. Nandakumar, Sabu Thomas

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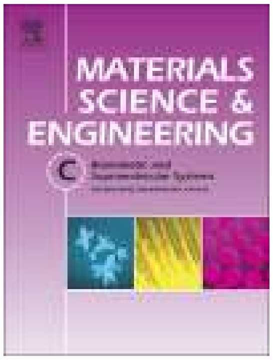

Antimicrobial properties of MFe2O4 (M = Mn, Mg)/reduced graphene oxide composites synthesized via solvothermal method

El Hadji Mamour Sakho, Jiya Jose, Sabu Thomas, Nandakumar Kalarikkal, Oluwatobi S. Oluwafemi

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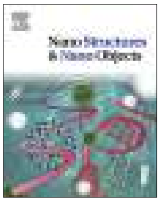
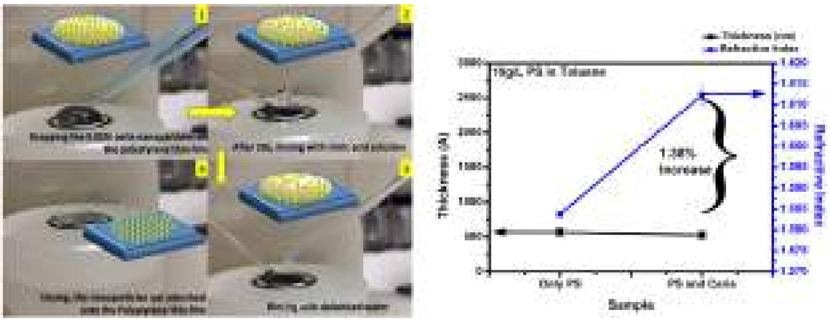


Surface engineering of polystyrene–cerium oxide nanocomposite thin films for refractive index enhancement

Jemy James [a,b], Aparna Beena Unni [c], Khadidja Taleb [d], Jean-Paul Chapel [f], Nandakumar Kalarikkal [b,e], Soney Varghese [g], Guillaume Vignaud [a,*], Yves Grohens [a]

[a] *University Bretagne Sud, UMR CNRS 6027, IRDL, F-56100 Lorient, France*
[b] *International and Inter University Centre for Nanoscience and Nanotechnology, Mahatma Gandhi University, Kottayam, Kerala, 686560, India*
[c] *NSS College of Engineering, Palakkad, Kerala, India*
[d] *Université Oran 1 Ahmed Ben Bella, Laboratoire de Synthèse Organique Appliquée (LSOA), Département de Chimie, Faculté des Sciences Exactes et Appliquées, BP 1524 EL Mnaouer, 31000 Oran, Algeria*
[e] *School of Pure and Applied Physics, Mahatma Gandhi University, Kottayam, Kerala, 686560, India*
[f] *Centre de Recherche Paul Pascal (CRPP), UPR 8641, CNRS, F-33600 Pessac, France*
[g] *School of Nano Science and Technology, National Institute of Technology, Calicut 673 601, Kerala, India*

GRAPHICAL ABSTRACT



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ABSTRACT

Polymer nanocomposites have gained much importance in the field of optoelectronics due to their unique optical properties. Refractive index engineering using nanoparticles is an effective strategy that could be applied for the fabrication of optical devices. Herein, we report three different strategies which are employed to enhance the refractive index of polymer thin films. These include incorporating cerium oxide nanoparticles onto the polystyrene matrix, secondly adding cerium oxide nanoparticles onto the cross-linkable polystyrene and thirdly by embedding functionalized cerium oxide nanoparticles onto the cross-linkable polystyrene. Refractive index of the polystyrene thin films was enhanced by dispersing neat CeO_2 nanoparticles and functionalized CeO_2 nanoparticles into the polystyrene matrix. 1.38% enhancement in the refractive index of the polymer nanocomposite thin films could be achieved using our technique. The blending of polystyrene with cerium oxide nanoparticle presents a prospective way to engineer the refractive index of polymer thin films. We firmly believe that the study will be an effective guide towards future research in the area of surface engineering of polymer thin films for refractive index enhancement.

1. Introduction

The development and advances in photonic gadgets are becoming more dependent on the availability of new functional materials, as these devices are gaining more importance in daily life

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* Correspondence to: FRE CNRS 3744, IRDL, University Bretagne Sud, F-56100, Lorient, France.
E-mail address: guillaume.vignaud@univ-ubs.fr (G. Vignaud).

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Nanostructuring of 1-butyl-4-methylpyridinium chloride in ionic liquid–iron oxide nanofluids

Aswathy Joseph[1] · **Jacek Fal**[2] · **Gaweł Żyła**[2] · **Suresh Mathew**[1]

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Abstract

Understanding the behavior of ionic liquids (ILs) in ionic liquid-based nanofluids has great significance for its proper application. The phase changes and solidification observed in most ILs offer a great challenge to nanoparticles stabilization. Herein, we have synthesized and characterized a new type of IL-based iron oxide nanofluids using 1-butyl-4-methylpyridinium chloride. We have investigated the formation of dendrite-like nanostructures by 1-butyl-4-methylpyridinium chloride at the IL–nanoparticle interface. This solidification induced under high electric field was nanoparticle size dependent and may be controlled by temperature and frequency changes. Examining the rheological behavior showed that higher volume fraction of nanoparticles in this nanofluids drastically decreased the flow viscosity causing a crossover from non-Newtonian (pure IL) to Newtonian and then to shear-thinning behavior. The nanofluid stability also decreased with the increase in nanoparticle size.

Keywords Nanofluid · Ionic liquid · Ionanofluids · Viscosity

Introduction

The formation of nano- or microstructural organizations in ILs has an influential effect on their physicochemical properties and performance in various applications [1]. The root cause of these structural organizations is different kinds of inter-molecular forces acting a different extent among the ions. Different modes of interactions between an anion and a cation Π system can be observed in an IL. Some of them include (1) H-bonding between the hydrogens of the positively charged organic cation and the highly electronegative atoms of the anions, (2) X-bonding contributed by the halogen atoms present in the anions, (3) strong non-covalent anion-Π interactions, in which the anion will be located above the center of the cationic ring, (4) weak non-covalent anion-Π interactions, where the anion will be present outside the periphery of the Π-system and (5) steric interactions. The occurrence of nanostructural organization in certain ILs and IL–solvent/solute mixtures has been previously confirmed from molecular simulations and spectroscopic investigations [2]. The intermolecular forces and asymmetric nature of ions in ILs cause these nanostructural organizations leading to an ionic network or ion channels. Longer alkyl side chains (greater than or equal to C_4) can cause the segregation of polar and nonpolar domains [3, 4]. Besides, with a strong nanostructural organization tendency, many ILs are also used as a template or a surfactant for template-assisted, shape-controlled synthesis of different nanostructures [5].

However, the tendency of IL for nanostructuring can be disadvantageous also for some applications. For instance, some research groups working on imidazolium IL-based electrospray thrusters for nanopropulsion systems report the formation of radiation-induced needlelike or dendritic structures by ILs [6]. This reportedly affected the smooth

✉ Gaweł Żyła
gzyla@prz.edu.pl

Aswathy Joseph
aswathyj@gmail.com

Jacek Fal
jacekfal@prz.edu.pl

Suresh Mathew
sureshmathewmgu@gmail.com

[1] School of Chemical Sciences (SCS), Mahatma Gandhi University, Kottayam, Kerala, India

[2] Department of Physics and Medical Engineering, Rzeszow University of Technology, Rzeszow, Poland

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ChemistrySelect Communications

Catalysis

Ligand-Free Cu-Catalyzed Suzuki Coupling of Alkynyl Bromides with Boronic Acids in Ethanol Under Microwave Irradiation

Sheba Ann Babu,[a] Salim Saranya,[a] K. R. Rohit,[a] and Gopinathan Anilkumar*[a, b]

A ligand-free microwave assisted synthesis of internal alkynes using copper-catalyzed Suzuki type coupling reaction of alkynyl bromides with boronic acid derivatives has been developed. This protocol uses cheap CuI, greener solvent ethanol and K_3PO_4 base under microwave irradiation. This strategy does not need any ligand or sealed tube conditions. This methodology provides an efficient way to synthesize 1,2-diarylacetylenes in good to excellent yields.

1. Introduction

The Carbon-Carbon bond forming reactions are important tools in organic chemistry,[1] and among this, transition metal-catalyzed[2] protocols are of great significance because transition metal catalysts make nearly impossible reactions possible. Suzuki coupling is one such reaction, in which coupling between an organoboron reagent and an organic halide or pseudohalide takes place in presence of palladium catalyst, phosphine ligand and a base.[3] Suzuki coupling is one of the most efficient methods for the synthesis of diaryl acetylenes that constitutes important building blocks for ligands,[4] polymers,[5] biologically active pharmaceuticals[6] and other materials.[7]

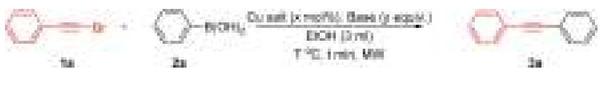
Most of the Suzuki reactions involve costly palladium and toxic air- and moisture- sensitive phosphine as the catalytic system. Therefore, a better, cost effective and greener catalytic system is required. For these reasons, latest interest has been turned towards using less costly transition metal catalysts,[8] especially copper, to replace the palladium. Copper is one such metal having low cost, high abundance, low toxicity, easy recyclability, high catalytic activity and excellent functional group tolerance. Copper chemistry is incredibly diverse because of its variable oxidation state. It can effectively coordinate to heteroatoms and to π-bonds. It should also be noted that copper activates terminal alkynes for useful reactions.

Internal alkynes are important structural units present in many natural products and are used in the synthesis of antimycotics,[9] antibiotics,[10] polymers[11] and optical or electronic materials.[12] The construction of $C_{(sp^2)}$-$C_{(sp)}$ bond can be made possible by Sonogashira type coupling using traditional Pd[13] or other transition metal[14] catalytic system. Bolm[15] and Liu[16] independently developed methodologies based on Fe(III) catalytic system for Sonoghashira reaction. Later, our own group reported the first iron-catalyzed Sonogashira coupling in water[17] and the first Zn-catalyzed Sonogashira coupling[18] between aryl iodides and terminal alkynes affording good yields of diarylacetylenes. Other catalysts based on cobalt[19] and nickel[20] have also been developed for Sonogashira type coupling reactions. We have also disclosed a copper-catalyzed Sonoghashira coupling using *trans* 1,2-diaminocyclohexane as the ligand.[21] Copper-catalyzed Suzuki type coupling of 1-bromo-2-substituted acetylenes and organoboronic acids was reported by Wang *et al.*[22] in 2011.

As part of our interest in transition metal-catalyzed coupling reactions[23] and to meet the demands of environmental factors, we have embarked on to find a new protocol for the synthesis of internal alkynes via palladium-free and ligand-free conditions by microwave irradiation. We herein report the first ligand-free microwave assisted synthesis of internal alkynes using copper-catalyzed Suzuki type coupling reactions of alkynyl bromides with aryl or alkylboronic acids/esters.

2. Results and discussion

At first the initial reaction was conducted by choosing phenylbromoacetylene **1a** and 4-phenylboronic acid **2a** as model substrates in ethanol expecting the formation of 1,2-diphenylacetylene as the product **3a** (Scheme 1).



Scheme 1. Preliminary experiment on Cu-catalyzed microwave assisted synthesis of internal alkynes. Reaction conditions: 1-bromophenylacetylene (1 equiv.), boronic acid (1.2 equiv.), Cu salt (10 mol%), base (2 equiv.), 3 mL ethanol, 130 °C, reaction time: 15 min, MW.

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[a] S. A. Babu, S. Saranya, K. R. Rohit, Prof. Dr. G. Anilkumar
School of Chemical Sciences, Mahatma Gandhi University, Priyadarsini Hills P O, Kottayam, Kerala, INDIA 686 560
E-mail: anilgi1@yahoo.com
[b] Prof. Dr. G. Anilkumar
Advanced Molecular Materials Research Centre (AMMRC), Mahatma Gandhi University, Priyadarsini Hills P O, Kottayam, Kerala, INDIA 686 560

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Biological Chemistry & Chemical Biology

In Vitro Study of the Interaction Between HSA and 4-Bromoindolylchalcone, a Potent Human MAO-B Inhibitor: Spectroscopic and Molecular Modeling Studies

Otávio Augusto Chaves,[a, b] Rani Sasidharan,[c, d] Cosme H. C. dos Santos de Oliveira,[b] Sreedharannair Leelabaiamma Manju,[d] Monu Joy,[e] Bijo Mathew,*[f] and José Carlos Netto-Ferreira*[a, g]

Based on our previous report, (2*E*)-3-(4-bromophenyl)-1-(1*H*-indol-3-yl) prop-2-en-1-one (**IC9**) showed potent and reversible hMAO–B inhibitor with $K_i = 0.010 \pm 0.005$ μM and a selectivity index of 120 - better than selegiline, the standard drug for hMAO–B. To continue the pharmacological investigation of **IC9**, the present study describes *in vitro* interaction between the titled compound and human serum albumin (HSA) under physiological condition by spectroscopic techniques (UV-Vis, circular dichroism, steady-state, synchronous, 3D and time-resolved fluorescence) combined with molecular docking and quantum chemical calculations. There is a moderate ground-state association between HSA:**IC9**, which is enthalpically and entropically driven. This association occurs mainly inside Sudlow's site I. There is a weak perturbation on the secondary structure and on the microenvironment around Trp residue as evidenced by circular dichroism and synchronous fluorescence. Molecular docking suggested that **IC9** can interact *via* hydrogen bonding, hydrophobic and electrostatic forces, whereas quantum chemical calculations suggested that the presence of a bromine atom is supporting the ability of binding between **IC9** and HSA through an electrostatic interaction.

Introduction

Monoamine oxidase (MAO) is one of the key enzymes responsible for catalyzing the oxidative deamination of biogenic amines that contribute to the oxidative stress and neurodegeneration.[1] MAO can be classified into two types based on its substrate and inhibitor specificity, namely MAO–A and MAO–B.[2] The level of MAO–B increases with age and its activity was found to be elevated in patients with Alzheimer's disease (AD), leading to enhanced dopamine metabolism related to the production of a significant amount of hydrogen peroxide, which ultimately results in neuronal damage.[3] Selective inhibition of MAO–B has been demonstrated to retard further neurodegeneration, thus providing another therapeutic approach for the treatment of AD.[4,5] Many particular types of MAO–B inhibitors have been developed to date, including chalcones, chromones, coumarins, isatins, pyrazoles, thiazolidinediones, (thiazol-2-yl) hydrazones and marketed drugs analogs.[6–9] Among these scaffolds, many chalcones showed selective, potent and reversible action as MAO–B inhibitors.[10–20]

Recently a series of indolylchalcones was synthesized in our lab and its human monoamine oxidase (hMAO) inhibitory activity was investigated. These studies showed that (2*E*)-3-(4-bromophenyl)-1-(1*H*-indol-3-yl) prop-2-en-1-one (**IC9**) (Figure 1) is a potent and reversible hMAO–B inhibitor with $K_i = 0.010 \pm 0.005$ μM and a selectivity index of 120. **IC9** was found to be a better hMAO–B inhibitor than the standard drug selegiline, for which $K_i = 0.20 \pm 0.20$ μM, with a selectivity index of 30.55.[21] This indolyl chalcone **IC9** was screened for its ability to cross the blood–brain barrier (BBB), since this is the first requirement for the design of successful central nervous system (CNS) drugs. The widely known parallel artificial membrane permeation assay of blood–brain barrier (PAMPA-BBB) revealed a value of $(15.27 \pm 1.09) \times 10^{-6}$ cms^{-1}, indicating that **IC9** could pass this barrier.[21] In the context of the strong biological profile of the title compound, there is an urgent need to understand its

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[a] *MSc. O. A. Chaves, Dr. J. C. Netto-Ferreira*
SENAI Innovation Institute for Green Chemistry. Rua Morais e Silva N° 53, Maracanã, 20271030, Rio de Janeiro-RJ, Brazil.
E-mail: jcnetto.ufrrj@gmail.com
[b] *MSc. O. A. Chaves, MSc. C. H. C. dos Santos de Oliveira*
Institute of Chemistry, Department of Organic Chemistry, Universidade Federal Rural do Rio de Janeiro, BR-465 Km 7, 23970-000 Seropédica-RJ, Brazil.
[c] *Dr. R. Sasidharan*
College of Pharmaceutical Science, Government T.D. Medical College, Alappuzha, Kerala, India.
[d] *Dr. R. Sasidharan, Dr. S. L. Manju*
Department of Chemistry, SAS, VIT University, Vellore 632014, Tamil Nadu, India.
[e] *Mr. M. Joy*
School of Pure & Applied Physics, M.G. University 686560, Kottayam, India.
[f] *Dr. B. Mathew*
Division of Drug Design and Medicinal Chemistry Research Lab, Department of Pharmaceutical Chemistry, Ahalia School of Pharmacy, Palakkad, 678557, Kerala, India.
E-mail: bijovilaventgu@gmail.com
[g] *Dr. J. C. Netto-Ferreira*
Divisão de Metrologia Química, Instituto Nacional de Metrologia, Qualidade e Tecnologia (INMETRO), 25250-020 Duque de Caxias-RJ, Brazil

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ORIGINAL ARTICLE – NANOMATERIALS

Soft, Self-Assembly Liquid Crystalline Nanocomposite for Superior Switching

Kaushik Pal[1] · Sami Sajjadifar[2] · Mohamed Abd Elkodous[3] · Yakubu Adekunle Alli[4] · Fernando Gomes[5] · Jaison Jeevanandam[6] · Sabu Thomas[7] · Alexander Sigov[8]

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Abstract

Liquid crystal (LC) has long been a feature in Materials Science and Nanotechnology, have recently been extended into the appealing domain of complex hybrid materials. The crystalline structural effects of alkoxy chain lengths and the mesogen properties of hydrogen-bonded (n-OBASA) complexes (n = 5,6,7) have been investigated in recent studies. The LC-based hybrid nanocomposite materials–obtained by the homogeneous dispersion of zinc oxide nanowires (ZnO NWs) as a dopant into hydrogen-bonded liquid-crystalline compounds—seem to be particularly promising in this article. Optimizing the geometry of surface stabilizing electro-optic, LC cell reveals the typical intermolecular hydrogen bond (H-bond) formation. Here, we explore molecular-colloidal hybrid composite matrix formed from LCs and dilute dispersions of orientation-ordered ZnO NWs, for eventual potential application in smart switchable display devices. In addition, we investigated the structural, dielectric and optical properties of the nanocomposite, and electro-optical studies which were performed by exploiting the potential during the conditions before the opening of spectrum acquisition. Our novel findings confirm that the electric field induces a charge transfer of the LC molecules to the nanomaterial, which acts as a trap for ionic charges. This effect may be utilized to achieve superior switching operation that is electro-optically tunable. Such dynamic novel switching could be harnessed in smart LCD technology and pave the way towards innovative display modulation techniques.

✉ Kaushik Pal
kaushikphysics@gmail.com;
kaushikpaul.nano@bharathuniv.ac.in

[1] Department of Nanotechnology, Bharath Institute of Higher Education and Research(BIHER), Bharath University, 173 Agharam Road, Selaiyur, Chennai, Tamil Nadu 600073, India

[2] Department of Chemistry, Payame Noor University (PNU), Ilam, P.O. Box 19395-4697, Tehran, Iran

[3] Center for Nanotechnology (CNT), School of Engineering and Applied Sciences, Nile University, Sheikh Zayed, Giza, Egypt

[4] Department of Chemistry, College of Physical Sciences, Federal University of Agriculture, Abeokuta, Ogun State, Nigeria

[5] Instituto de Macromoléculas:Professora Eloisa Mano, Centro de Technologia-Cidade Universitária, Av. Horacio Macedo, 2030, Bloco J.LaBioS Centro de Tecnologia, Rio de Jenerio, Brazil

[6] Department of Chemical Engineering, Curtin University, CDT250, 98009 Miri, Sarawak, Malaysia

[7] IIUCN, School of Chemical Sciences, Mahatma Gandhi University, Kottayam, Kerala 686560, India

[8] Department of Nanoelectronics, MIREA - Russian Technological University, Prospekt Vernadskogo, 78, Moscow, Russian Federation 119454

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Synthetic Communications

An International Journal for Rapid Communication of Synthetic Organic Chemistry

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Facile synthesis of 2-benzoxazoles *via* CuI/2,2'-bipyridine catalyzed intramolecular C–O coupling of 2-haloanilides

Thachora Venu Saranya, Pambingal Rajan Sruthi & Saithalavi Anas

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Synthetic Communications
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A convenient route to 1,3-diynes using ligand-free Cadiot–Chodkiewicz coupling reaction at room temperature under aerobic conditions

Sujatha Asha, Sasidharan Anjana, Anns Maria Thomas, Minu Elizabeth Thomas, K. R. Rohit, K. Keerthi Krishnan, Sankuviruthiyil M Ujwaldev & Gopinathan Anilkumar

To cite this article: Sujatha Asha, Sasidharan Anjana, Anns Maria Thomas, Minu Elizabeth Thomas, K. R. Rohit, K. Keerthi Krishnan, Sankuviruthiyil M Ujwaldev & Gopinathan Anilkumar (2019): A convenient route to 1,3-diynes using ligand-free Cadiot–Chodkiewicz coupling reaction at room temperature under aerobic conditions, Synthetic Communications, DOI: 10.1080/00397911.2018.1554142

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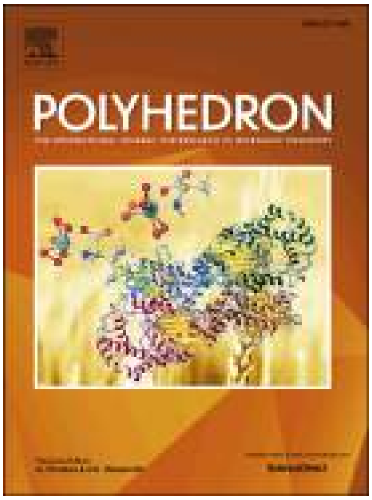
An Efficient Protocol For The Synthesis Of Thioethers Via Iron-Catalyzed Cross-Coupling Reaction And Its Mechanistic Investigation



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Nickel accumulation, localisation and the biochemical responses in *Eclipta prostrata* (L.) L

Chandana Chandrasekhar & Joseph George Ray

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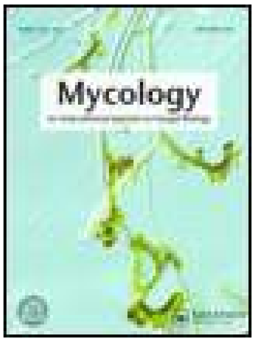

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Mycology

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Penicillium setosum, a new species from *Withania somnifera* (L.) Dunal

Tijith K. George, Jos Houbraken, Linu Mathew & M. S. Jisha

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Feature Fusion Approach for Differently Exposed Images with Weighted Guided Filter

Aparna Vijayan(✉) and V. R. Bindu

M. G. University, Kottayam, Kerala, India
aparnavijayan22@gmail.com, binduvr@mgu.ac.in

Abstract. Multi-exposure image fusion methodologies collect image information from multiple images and convey to a single image. Fusion with the aid of edge aware smoothing filters is a new trending area. The difficultes of multi-scale processing and low level fusion operations are the main problems of the existing algoritms. In this paper we propose a novel multi-exposure image fusion method which uses a feature fusion method based on an edge aware weighted guided filter. Three important image features accounting for the quality of an image viz. contrast, sharpness and exposedness are extracted from the differently exposed input images and fused together to form a single saliency map which holds all the important information. A decision map is constructed for the fused feature and an efficient edge aware filtering technique called weighted guided filter is used for optimizing the obtained decision map. A two scale decomposition of input images is done in parallel with the initial feature extraction procedure. This decomposed image representation is fused with the optimized decision map to get the final result. The proposed method encompasses the advantages of simple two scale decomposition, optimization with edge weighting and simplicity of using a single fused feature. The experimental results and objective evaluations demonstrate that the proposed method can produce more accurate results with very good visual quality.

Keywords: Multi-exposure image fusion · Two scale decomposition · Feature fusion · Weighted guided filter

1 Introduction

The increasing popularity of digital images and image editing tools has brought a wide variety of image enhancement operations within a mouse click of the creative consumer. While considering image enhancement operations, apart from existing techniques there is still room for improvement. Under different classes of enhancement approaches there are different methods for enhancing different kinds of images. Coupled with the ever growing image fusion area, research area

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International Journal of Environmental Science and Technology
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ORIGINAL PAPER

Unmodified silver nanoparticles for dual detection of dithiocarbamate fungicide and rapid degradation of water pollutants

P. N. Ragam[1] · B. Mathew[1]

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Abstract

Herein, for the first time, any phytochemical-based silver nanoparticle is reported as a dual sensor to detect toxic dithiocarbamate fungicide (Thiram) spectrophotometrically and electrochemically. Green approach was employed for the silver nanoparticle synthesis utilizing the stem extract of *Coscinium fenestratum* via a microwave-assisted route. The characterization of silver nanoparticles was carried out by methods such as UV–visible, Fourier transform-infrared, and X-ray diffraction spectroscopy, as well as transmission electron microscopy techniques. The diffraction and microscopic studies proved that the nanoparticles were essentially crystalline and almost spherically shaped with average size of 20.72 ± 4.25 nm. The nanoparticles were found very stable for more than 6 months and hence are appropriate for remediation of several issues regarding environment such as detection of fungicide as well as organic dye degradation. Thus, the nanoparticles were explored for selective recognition of Thiram and obtained a low limit of detection of 0.18 ppm, much lower than 7 ppm, the maximal residue limit as per the environmental protection agency of the USA. Moreover, the nanoparticles successfully detected Thiram from real samples from tap, canal, and river water in the state of Kerala, India. Furthermore, the nanoparticles were utilized for their excellent catalytic efficiency toward the swift degradation of three water contaminant organic dyes, namely methylene blue, methyl orange, and naphthol green B within a couple of minutes.

Keywords Dye degradation · Electrochemical sensing · Optical sensing · Silver nanoparticles · Thiram

Introduction

Tetramethylthiuram disulfide or Thiram is one of the most renowned dithiocarbamates used worldwide in rubber processing, as fungicide and animal repellent (Hasan 2010). It is a noted allergen which induces the excess release of histamine in humans leading to headache, digestive problems, nausea, elevation of blood pressure, vomiting, and so forth (Rouabhi 2010). Moreover, Thiram is observed to inactivate glutathione reductase enzyme which can increase oxidative stress in human cells as a result of the accumulation of dangerous free radicals (Cereser et al. 2001). It is also known as a mutagen, inducing variation in chromosomes (Slimani et al. 2018; Paschin and Bakhitova 1985). From industrial wastes and agricultural fields, Thiram directly pollutes the environment and eventually affects aquatic beings, birds, and humans creating severe health impacts. Hence, monitoring Thiram in the environment is exceedingly relevant (Rouabhi 2010). Recently, several reports on the recognition of Thiram utilized surface-enhanced Raman spectroscopy (SERS), fluorescence spectroscopy, colorimetry, cyclic and square wave voltammetry, and HPLC. However, one can see that the materials used in such cases employ toxic chemicals during their synthesis and thus not safe in practical applications (Rohit and Kailasa 2014; Wang et al. 2015; Yang et al. 2014; Fei Chan et al. 2013; Yuan et al. 2011; Silva Junior et al. 2014; Filipe et al. 2014; Stathi et al. 2006). Metal nanoparticles (NPs) and their combinations have been used for detection of thiocarbamate fungicides such as Thiram and Paraquat (Yuan et al. 2011; Silva Junior et al. 2014; Filipe et al. 2014; Stathi et al. 2006). In this regard, no such reports

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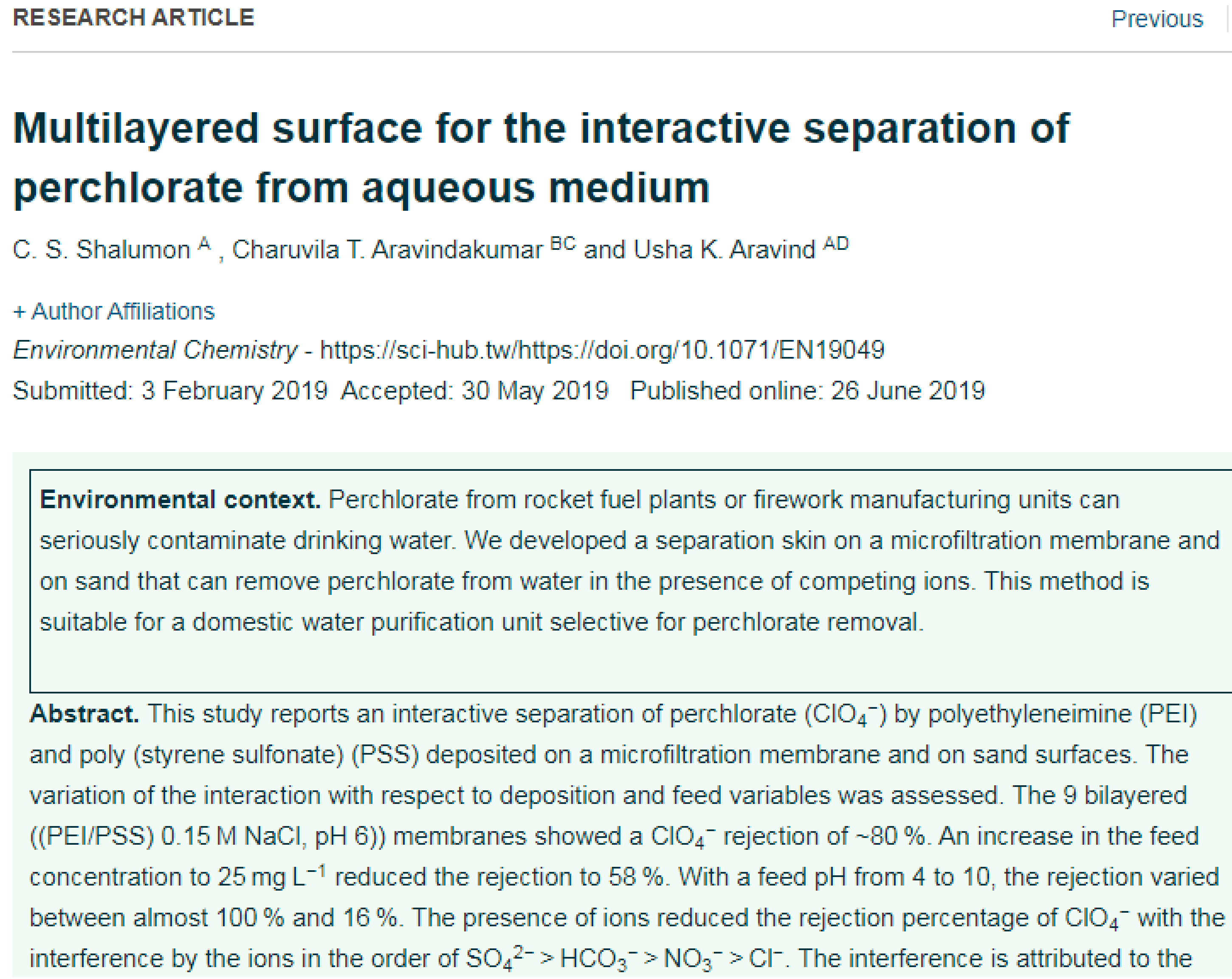
✉ B. Mathew
beenamscs@gmail.com

[1] School of Chemical Sciences, Mahatma Gandhi University, Kottayam, Kerala 686560, India



Multilayered surface for the interactive separation of perchlorate from aqueous medium

C. S. Shalumon [A] , Charuvila T. Aravindakumar [BC] and Usha K. Aravind [AD]

+ Author Affiliations

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Environmental context. Perchlorate from rocket fuel plants or firework manufacturing units can seriously contaminate drinking water. We developed a separation skin on a microfiltration membrane and on sand that can remove perchlorate from water in the presence of competing ions. This method is suitable for a domestic water purification unit selective for perchlorate removal.

Abstract. This study reports an interactive separation of perchlorate (ClO_4^-) by polyethyleneimine (PEI) and poly (styrene sulfonate) (PSS) deposited on a microfiltration membrane and on sand surfaces. The variation of the interaction with respect to deposition and feed variables was assessed. The 9 bilayered ((PEI/PSS) 0.15 M NaCl, pH 6)) membranes showed a ClO_4^- rejection of ~80 %. An increase in the feed concentration to 25 mg L^{-1} reduced the rejection to 58 %. With a feed pH from 4 to 10, the rejection varied between almost 100 % and 16 %. The presence of ions reduced the rejection percentage of ClO_4^- with the interference by the ions in the order of $SO_4^{2-} > HCO_3^- > NO_3^- > Cl^-$. The interference is attributed to the

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Multilinear Principal Component Analysis with SVM for Disease Diagnosis on Big Data

Juby Mathew & R. Vijaya kumar

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RESEARCH ARTICLE

Molecular Docking Study of Bioactive Compounds of *Withania somnifera* Extract Against Topoisomerase IV Type B

Tijith Kuzhiyil George[1] · **Anju Tomy**[1] · **Manakulam Shaikmoideen Jisha**[1]

Received: 16 August 2017 / Revised: 26 May 2019 / Accepted: 27 May 2019

Abstract The rapid emergence of multi-drug resistant bacteria and reduced susceptibility of bacteria to antibiotics adds urgency to search for new compounds having noticeable action on new and re-emerging infectious diseases. *Withania somnifera* is a remarkable source of new therapeutic agents for antimicrobial activity as well as antioxidant activity. The root powder of *Withania somnifera* was extracted sequentially with hexane, chloroform and methanol, by both hot and cold extraction method. *In vitro* antibacterial activity of extract was screened against both gram-negative and gram-positive bacteria. The chloroform extract of *Withania somnifera* root showed significant antibacterial activity against *Staphylococcus aureus* and *Salmonella typhi*. The methanol extract showed comparable antioxidant potential with ascorbic acid (standard compound). These extracts were analyzed structurally and qualitatively, to identify the phytocompounds responsible for the activity. The antimicrobial potential of major phytoconstituents was screened using docking software AutoDock 4 against a target protein topoisomerase IV type B. It was found that withasomnine was an efficient antibacterial compound which showed significant inhibition with minimum docking energy -6.22 kJ mol^{-1}, binding energy -10.07 kJ mol^{-1} and inhibition constant 4.14e−008. This was the first report on the antimicrobial docking studies on withasomnine by proving its antimicrobial activity.

Keywords Antimicrobial activity · Antioxidant activity · AutoDock 4 · Withasomnine

Introduction

The medicinal plants contain a mass array of bioactive compounds which can be utilized for the development of potent therapeutic drugs. The beneficial medicinal effects of plant materials typically result from combinations of secondary products in them. Since secondary metabolites from natural resources have been elaborated within the living systems, they are often perceived as showing more "drug-likeness and biological activities than totally synthetic molecules" making them good candidates for further drug development [1]. The drug resistance found in antimicrobial agents is variable with different geographic areas and are related to the consumption of antibiotics in the general population [2]. Reactive oxygen species are formed as a metabolic by product, but high levels can cause significant damage to cell structures [3]. These reactions are displayed during the microbial infection, UV or heat exposure, radiation and so on. *Withania somnifera* is commonly known as Ashwagandha, holds the most prominent place among the Ayurveda rasayana herbs with multiple pharmacological actions. More than 91 pharmaceutical products are produced from this plant [4]. The biologically active chemical constituents of *W.*

Significance Statement The antibacterial and antioxidant activity of *Withania somnifera* shows the sustenance of its Rasayana property. Withasomnine a pyrazole alkaloid was found as an efficient compound against an antibacterial drug target topoisomerase IV type B.

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✉ Manakulam Shaikmoideen Jisha
jishams@mgu.ac.in

[1] School of Biosciences, Mahatma Gandhi University, Kottayam, Kerala, India

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ARTICLE

Recent advances and prospects in the nickel-catalyzed C-H activation

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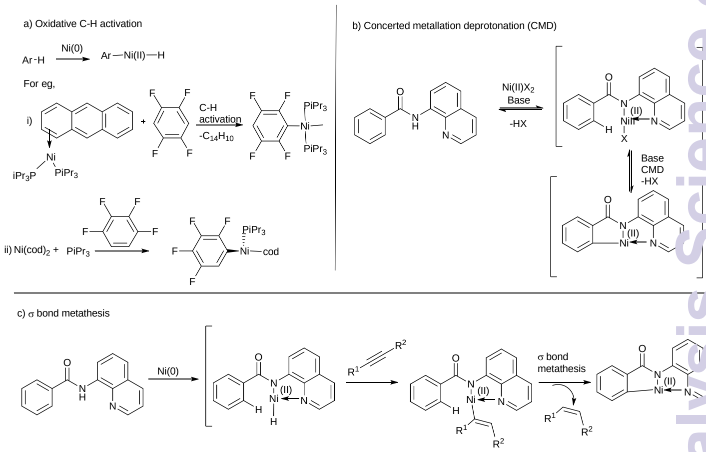
Nissy Ann Harry[a], Salim Saranya[a], Sankuviruthiyil M. Ujwaldev[a], Gopinathan Anilkumar[a,b]*

Nickel-catalyzed C-H activation has become a predominant and omnipresent research area in Organic Chemistry. Direct functionalization of inert C-H bond to create functionally enriched molecules by rapid elaboration of simple organic substrates in a single step has gained profound interest in recent times. Nickel is an abundant and inexpensive metal widely used in C-H activation by replacing toxic and expensive 4d and 5d transition metals. This review focuses on the recent advances in nickel-catalyzed C-H activation and covers literature from 2015-2018.

Introduction

C-H bonds are traditionally considered as unreactive because of their high bond dissociation energy, and very low polarity. A great amount of research has been devoted to activate C-H bonds selectively, since its derivatization could convert cheap and inert alkanes and arenes to valuable functionalized organic compounds, without using any pre-functionalized starting materials. Recently transition metal-catalyzed C-H activation have become powerful tool for the synthesis of important synthons and functionally enriched molecule. [1] The precious 4d and 5d transition metals, such as palladium, ruthenium, rhodium and iridium have shown to be effective as catalytic system and have been proven for highly important transformations through C-H activation. However, the low natural availability, relatively high price, and partly strong toxicity limited their applications.

Nickel-catalyzed reactions have a rapid advancement in the past decade.[2] Nickel as an abundant and cheap first row transition metal is of great importance to organic chemists to construct various functionalized molecules. Nickel has been proven as a valuable transition metal catalyst for the cross-coupling reactions involving secondary and tertiary alkyl halides, ethers and phenol derivatives.[3] Recently nickel-catalyzed direct C-H activation has shown a tremendous advancement. [4] This direct functionalisation of inert C-H bonds to make C-C bonds by nickel catalysts, using various organometallic compounds and organic halides as the coupling partners and enabling arylation, alkenylation, alkylation, carbonylation, dehydrogenation, amination, oxidation, silylation, and borylation has proven to be a versatile technique for one step synthesis with applications to material sciences, pharmaceutical industries and natural product chemistry. Several advancements in mechanistic studies were also occurred in this field.[5] The most commonly proposed mechanism during nickel catalyzed C-H activation step involves i) Oxidative C-H activation b) concerted metallation deprotonation process (CMD) c) σ-bond metathesis etc (**Scheme 1**). The oxidative C-H activation involves a change in oxidation state from Ni(0) to Ni(II) during C-H activation step. This type of mechanism is most commonly found in the C-H activation of perfluoro arenes[6] and pyridines.[7] The CMD maintains the oxidation state and requires a base and some directing groups.[8] The σ-bond metathesis also works with a Ni(0)-catalyst in the presence of a bidentate moiety, but without the need of a base.



Scheme 1: General mechanism for nickel-catalyzed C-H activation step

This review focuses on the recent advances in Ni-catalyzed C-H activation reactions, their importance and applications. For

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[a] School of Chemical Sciences, Mahatma Gandhi University, PD Hills, Kottayam, Kerala, INDIA 686560, E-mail: anilgi1@yahoo.com
[b] Advanced Molecular Materials Research Centre (AMMRC), Mahatma Gandhi University, PD Hills, Kottayam, Kerala, INDIA 686560

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RESEARCH ARTICLE

Native arbuscular mycorrhizal fungal isolates (*Funneliformis mosseae and Glomus microcarpum*) improve plant height and nutritional status of banana plants

Nidheesh Kammadavil Sahodaran, Abju K. Arun and Joseph George Ray*

Laboratory of Plant Science and Ecology, School of Biosciences, Mahatma Gandhi University, Kottayam, Kerala 686560, India
*Corresponding author. Email: jgray@mgu.ac.in

(Received 08 January 2018; revised 27 October 2018; accepted 23 January 2019)

Abstract

An experiment was carried out to assess the benefits of native arbuscular mycorrhizal fungi (AMF) for banana plants cv. ‘Nendran’. The AMF species applied were *Funneliformis mosseae* and *Glomus microcarpum*, which were identified in a previous survey as the most common root associates of *Musa* spp. in traditional monoculture banana fields. Spores of both the AMF species isolated from the natural banana fields were mono-cultured and used in the experiment, individually and in combination, at two inoculum spore levels (2500 or 5000 spores). We evaluated the root colonising potential of AMFs and their effects on plant height, chlorophyll content and leaf N, P and K concentrations at regular intervals up to 90 days after inoculation. All the inoculated plants showed more than 80% root colonisation. Increase in chlorophyll content in the leaves was found significant in all treatments, with the exception of the combination of 5000 spores of *F. mosseae and* 5000 spores of *G. microcarpum* each. Increases in leaf N, P and K were found in all the inoculated plants as compared to control (sterile soil without any AMF). While a significant reduction in soil available nitrogen and soil pH was observed in all treatments with inoculation, the soil available phosphorus and soil total organic carbon were increased by inoculation. Overall data revealed positive effects of AMF species in banana, especially during its early growth. As AMF species were isolated from fields differing in relation to banana variety and soil type and have positive effects in banana nutrition, an integrated soil fertility management using AMF appears promising.

Keywords: *Funneliformis mosseae*; *Glomus microcarpum*; Native AM fungi; Nendran; South Indian Banana

Introduction

Banana, one of the most consumed fruits worldwide, is a common crop in tropics, where it is cultivated in monoculture traditional farms and requires high amount of nutrients as well as chemical control of insects and diseases. However, environment contamination by overusing chemical fertilisers and pesticides is common in banana production systems all over the world (Mahecha-Vásquez *et al.*, 2017). Excessive chemical application in fields due to the intensive crop production strategies is usual in India. In order to overcome the widespread environment pollution quite common from such ‘chemicalised’ green revolution fields, an alternative farming strategy with minimum environment impact is desirable.

Arbuscular mycorrhizal fungi (AMF) are well-known root symbionts capable of increasing the effective absorbing area of plant roots. AMF are also capable of bringing about biochemical changes in nutrient-deficient soils and to enhance the availability of nutrients to associated plants (Balakrishnan and Subramanian, 2016). Beneficial effects of different species of AMF towards

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Fabrication of a Structure-Specific Molecular Imprinted Polymer–Based Electrochemical Sensor Based on CuNP-Decorated Vinyl-Functionalized Graphene for the Detection of Parathion Methyl in Vegetable and Fruit Samples

M. P. Sooraj[1,2] **· Beena Mathew**[1]

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Abstract

Molecular imprinted polymers on copper nanoparticle–decorated vinyl-functionalized graphene (CuNPs@GR-MIPs) are fabricated. The copper nanoparticles (CuNPs) are synthesized by the reduction of diaminopropane copper complexes (DAPCu) using sodium borohydride as reducing agent. The synthesized CuNPs are successfully decorated on vinyl-functionalized graphene (V-fGR) on which MIPs are fabricated. All intermediates during the synthesis of CuNPs@GR-MIP are characterized in detail by Fourier-transform infrared spectroscopy, ultraviolet-visible spectroscopy, powder X-ray diffraction analysis, transmission electron microscopy, and scanning electron microscopy techniques. The fabricated CuNPs@GR-MIPs are developed as a sensor for organophosphorus pesticide parathion methyl. The recognition cavities formed on CuNPs@GR-MIP during the synthesis are mainly responsible for the sensing property. The result of the electrochemical studies shows that CuNPs@GR-MIP material has good recognition and sensing capacity towards parathion methyl (PM). The sensitivity is found to be directly proportional to the amount of PM molecules in solution with a detection limit of 0.24×10^{-9} mol L^{-1} ($S/N = 3$). The selectivity studies of the fabricated CuNPs@GR-MIP sensor give a fine discrimination between PM and its structurally similar compounds such as 2,4-dinitrophenol, nitrobenzene, nitroaniline, p-nitrophenol, ascorbic, dopamine acid, and malathion. Most promisingly, the sensing capacity of the synthesized CuNPs@GR-MIP is successfully demonstrated in vegetables and fruits which shows us the real time applicability of the sensor in food analysis.

Keywords Parathion methyl · Cyclic voltammetry · Molecular imprinted polymer · Graphene · Copper nanoparticles

Introduction

Parathion methyl (PM), an organophosphorus compound (OPs), has been widely used in agricultural crops as herbicides and insecticide (Govindasamy et al. 2017a). However, the high toxicity and large persistence of PM resulted in the increasing pollution of natural water sources, vegetables, and fruits. The oral administration of these vegetables and fruits having high concentration of PM can inhibit acetylcholinesterase resulting in the gathering of acetylcholine at the nerve endings (Edwards and Tchounwou 2005). Excess acetylcholine at the nerve endings can cause weak neural transmissions. OPs have been categorized as extremely hazardous for the environment by the WHO (Diagne et al. 2007). However, still PM remains as a major insecticide in agricultural pest control in some undeveloped and developing countries. Therefore, monitoring of residual PM in vegetables, fruit, and water becomes a need of the time. Familiar measurement methods for PM are gas chromatography–mass spectrometry (GC–MS) (Susana and Pieter 2016; Darlan et al. 2015), high-performance liquid chromatography (HPLC) (Hu et al. 2017; Ling et al. 2018), enzyme-linked immunosorbent assay (ELISA) (Ge et al. 2017; Dau et al. 2011), and enzyme analysis (Dau et al. 2011; Kanchanmala et al. 2011; Lipeng et al. 2013). These reported techniques require expensive analytical resources, longer analysis time, and complex treatment processes of samples. Electrochemical method (Turaj et al. 2018; Mohamed et al. 2018; Minh et al. 2015) has shown great potentials over other method for the monitoring of OPs because of its simplicity, sensitivity, fast responses, selectivity, and stability.

✉ Beena Mathew
beenamscs@gmail.com

[1] School of Chemical Sciences, Mahatma Gandhi University, Kottayam, Kerala 686560, India

[2] Advanced Molecular Materials Research Center, Mahatma Gandhi University, Kottayam, Kerala 686560, India

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Research Paper

Oxidative degradation of ranitidine by UV and ultrasound: identification of transformation products using LC-Q-ToF-MS

Misha T. Elias,[A] *Jisha Chandran,*[B] *Usha K. Aravind*[A] *and*
Charuvila T. Aravindakumar[B,C,D]

[A]Advanced Centre of Environmental Studies and Sustainable Development, Mahatma Gandhi University, Kottayam, 686560, Kerala, India.
[B]Inter University Instrumentation Centre, Mahatma Gandhi University, Kottayam, 686560, Kerala, India.
[C]School of Environmental Sciences, Mahatma Gandhi University, Kottayam, 686560, Kerala, India.
[D]Corresponding author. Email: cta@mgu.ac.in

Environmental context. Ranitidine, a widely prescribed antiulcer drug commonly found in surface waters, has been identified as an emerging contaminant due to its toxicity and the enhanced toxicity displayed by its transformation products. Mechanisms for the formation of ranitidine transformation products and their degradation pathways induced by UV oxidation processes are presented. This work provides insight into treatment processes to remove these toxic chemicals from environmental water bodies.

Abstract. The transformation products (TPs) of pharmaceuticals formed during advanced oxidation processes (AOPs) are of great significance, but there are still gaps in our knowledge regarding the persistence of such compounds in the water matrices, their impact on human health and the applicability of such techniques during water treatment processes. Ranitidine (RAN), a highly prescribed gastrointestinal drug, has been widely detected in various surface waters and experiments, along with its TPs, which show enhanced toxicity. The present study analyses the TPs formed from the degradation of RAN in aqueous solution induced by three AOPs; namely UV-photolysis, UV/peroxodisulfate (PDS) and sonolysis. The degradations followed pseudo first-order kinetics, with removal efficiencies of 99.8, 100 and 98.8 % after 60 min under UV photolysis, UV/PDS, and sonolysis, respectively, with a corresponding decrease in chemical oxygen demand (COD) of 25, 100 and 75 %. Structures of the main TPs were elucidated by using LC-Q-ToF-MS in positive mode, and possible degradation pathways are proposed which mainly involved C-N and C-H bond cleavage, hydroxylation and reduction of nitro groups. Possible mechanisms for the formation of the identified TPs (elucidated by using electrospray ionisation–collisionally induced dissociation) support their structural assignments. Seven out of the 11 TPs presented here (namely **TP-1**, **TP-4**, **TP-5**, **TP-6**, **TP-7**, **TP-9** and **TP-10**) were not reported in previous studies of RAN using any other AOPs, while four (*m/z* 331, 270, 288 and 286) were found to retain the NO_2 group, which might contribute to the formation of halonitromethanes (HNMs) during chlorination of drinking water. Interestingly, we identified an additional sonolysis product, **TP-3**, whose formation can only be rationalised by invoking ozone.

Additional keywords: advanced oxidation processes, ESI-CID, halonitromethanes, pharmaceutical pollution, photodegradation.

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Introduction

Whereas the pharmaceutical industry has revolutionised the health sector by providing solutions for many human and veterinary diseases, the consistent use of pharmaceuticals such as antibiotics, bronchodilators and antihistamines has been a subject of serious environmental concern (Llor and Bjerrum 2014; Prosser and Sibley 2015; Kümmerer 2003). The environment is generally exposed to these pharmaceuticals through the excretion process or by the direct disposal of outdated or unused pharmaceuticals. In either case, they enter water bodies and wastewater treatment plants due to their low volatility and highly polar nature. They have been detected and quantified in surface waters and wastewaters, either in their native form or as their metabolites/transformed products in nanogram to microgram per litre concentrations (Rosal et al. 2010; Rahman et al. 2009). Most of these compounds and their metabolites are highly persistent and are capable of imparting potential toxic effects on the environment (Schulze et al. 2010; Trovó et al. 2009). These chemicals are generally classified as contaminants of emerging concern (CECs), as their health impacts are still

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CHAPTER 7

High Performance Flooring Materials from Recycled Rubber

Raghvendra Mishra, M. K. Aswathi and Sabu Thomas

Recycling is one of the best ways to make a positive impact on the world. In addition, recycling requires much less energy, minimizes the need for raw materials and reduces waste materials, therefore helping to preserve natural resources along with sustainable development. From the point of view of sustainable development, recycling is eco-friendly and economic. Due to rapid growth in the automobile industry the volume of scrap tyres in the world has increased. The increasing amount of scrap tyres causes many environmental problems due to the disposal methods used for worn-tyres, such as burning or piling up in landfills. Burning of the waste tyres releases toxic fumes which pollute the air and can contaminate soil and water. Utilizing the recycled rubber derived from scrap vehicle tyres in flooring materials represents an effective technique for using huge volumes of waste materials safely. Recently, the use of recycled rubber as a flooring material has been promoted due to the importance of water resistant floorings in kitchens, bathrooms, and laundry rooms, and also for eco-friendly floorings in playground surfacing or rubber crumb for athletic fields and in other applications. This chapter discusses the different processing techniques and the importance of using recycled rubber as a flooring material.

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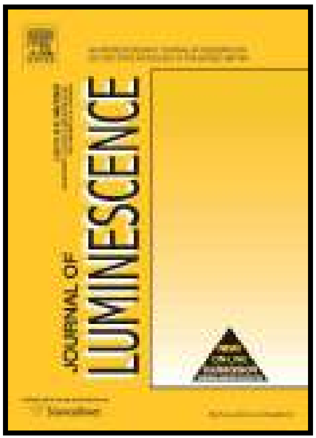

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Revealing the interaction strategy of Diosmin functionalized gold Nanoparticles with ctDNA: Multi-Spectroscopic, Calorimetric and Thermodynamic approach

Riju K. Thomas, Surya Sukumaran, S. Prasanth, C. Sudarsanakumar

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Revealing the interaction strategy of Diosmin functionalized gold Nanoparticles with ctDNA: Multi-Spectroscopic, Calorimetric and Thermodynamic approach

Riju K. Thomas, Surya Sukumaran, S. Prasanth, C. Sudarsanakumar[*]

School of Pure and Applied Physics, Mahatma Gandhi University Kottayam, Kerala, India, 686560.

[*]Corresponding author. Prof. C. Sudarsanakumar, School of Pure and Applied physics. Tel.: +91481-2731043; fax: +91 481 2730423; Mob: 09447141561. c.sudarsan.mgu@gmail.com

Abstract

The interactions of natural drug functionalized metal nanoparticles with DNA plays a pivotal role in developing effective therapeutic agents having a wide range of potential biomedical applications. The focus of this study was to decipher the binding mechanism of diosmin capped gold nanoparticles (DM-AuNPs) with calf thymus DNA (ctDNA) through a combination series of spectroscopic and calorimetric studies. The gold nanoparticles were successfully synthesized by the facile one-pot synthesis using DSM as a capping and reducing agent. The DM-AuNPs were characterized using UV-Visible spectroscopy, XRD, FTIR, DLS and HRTEM analysis confirming the formation of stable AuNPs with an average size of 30±3 nm. A series of experiments such as UV-Vis absorbance, fluorescence dye displacement studies, temperature melting and viscosity analysis unravelled the binding mode of DM-AuNPs by establishing a typical groove binding mode upon its complexation with ctDNA. The CD and FTIR measurements provided clear-cut evidences regarding the

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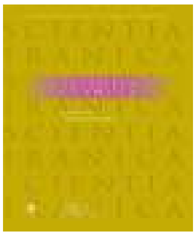

Microwave aided and plant reduced gold nanoparticles as talented dye degradation catalysts

S. Francis[a], **E.P. Koshy**[a], **and B. Mathew**[b,*]

a. *Department of Chemistry, St. Joseph's College, Moolamattom, Idukki, 685591, Kerala, India.*
b. *School of Chemical Sciences, Mahatma Gandhi University, Kottayam, 686560, Kerala, India.*

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KEYWORDS
Microwave;
Elephantopus scaber;
Gold nanoparticles;
Dye degradation.

Abstract. Green alternatives prevail over hazardous and expensive pathways of nanoparticle synthesis. This study reports eco-friendly manufacturing of gold nanoparticles by microwave assistance. The water-soluble organic constituents of the tropical herb *Elephantopus scaber* function as the three-electron donor and the aggregation preventer. XRD spectra certified *fcc* crystal lattice, and the TEM images supported mixed spherical and triangular geometries of the nanoparticles with an average particle size of 18.97 ± 5.86 nm. Ecological relevance of the gold nanoparticles lies in their ability to degrade methylene blue and methyl orange. The catalytic capacity of the gold nanoparticles is exploited for the reduction of 4-nitrophenol. Large-scale production of gold nanoparticles in an easy manner using renewable sources improves the 'green' significance of the present synthesis.

1. Introduction

The beauty of miniature science is put on display by nanotechnology. Biogenic synthesis of metal nanoparticles is the eco-friendly modification of nanoscience. Nanobiotechnology is an umbrella term that encompasses the synthesis, characterization, and exploitation of its biomedical applications [1]. Secondary process on the surface of nanoparticles makes them promising material as low-cost nanocatalysts, value-added products, a commodity for environmental pollution controlling systems, antibacterial coatings, etc. [2]. Plant reduced gold nanoparticles generally have spherical, triangular, and cubical shapes; flavonoid, polyphenol, ascorbic acid, citric acid, and alkaloid contents present in the plant extracts make them captivate reducing and capping agents [3]. Unique physical and chemical characteristics of gold nanoparticles make them suitable for biological and chemical sensing applications [4].

The medicinal plant *Elephantopus scaber* belongs to the family of sunflower. Healing power of *Elephantopus scaber* for fevers, diarrohea, ulcers, bronchitis, stomach disorders, and various viral and bacterial infections is well known [5]. The microwave fabrication of stable gold nanoparticles using phytoreducer *Elephantopus scaber (E. scaber)* is reported here for the first time. The effects of different microwave irradiation times and the amounts of leaf extract on the formation of nanoparticles were studied. UV-visible, FTIR, powder XRD, and TEM-EDAX characterizations were performed on the nanoparticles. The catalytic power of the newly synthesized gold nanoparticles was explored in the degradation of dyes

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*. *Corresponding author. Tel./Fax: +91-481-2731036*
E-mail address: srsijofrancis@gmail.com (S. Francis); epkosh@gmail.com (E.P. Koshy); beenamscs@gmail.com (B. Mathew)

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In situ S-doped ultrathin gC_3N_4 nanosheets coupled with mixed-dimensional (3D/1D) nanostructures of silver vanadates for enhanced photocatalytic degradation of organic pollutants†

Subi Joseph,[a] Sinoj Abraham,[b] Ragam N. Priyanka,[a] Thomas Abraham,[a] Arya Suresh[a] and Beena Mathew *[a]

A novel plasmonic Z-scheme sulphur doped $gC_3N_4/Ag_3VO_4/\beta\text{-}AgVO_3/Ag$ (SGA-*x*) hybrid quaternary photocatalyst was successfully fabricated *via* the ultrasonic assisted Kirkendall effect and diffusion processes followed by low temperature phase conversion. The obtained samples were characterized by X-ray diffraction, scanning electron microscopy, transmission electron microscopy, UV-vis diffuse-reflectance spectroscopy (UV-vis DRS) and X-ray photoelectron spectroscopy. The photocatalytic activities of the obtained photocatalysts were measured by degradation of methylene blue (MB), methyl orange (MO) and 2,4-dichlorophenoxy acetic acid (2,4-D) under visible-light irradiation. Among the composites with various levels of $\beta\text{-}AgVO_3$, SGA-7 exhibited the highest degradation efficiency with 95.45% MB degradation for 30 min, which was about 1.47 times higher than that of $S\text{-}gC_3N_4/Ag_3VO_4$ (SGA). The inter-particle electronic coupling in hollow nanoflower leads to self-narrowing of the band gap of Ag_3VO_4. Moreover, electrochemical impedance spectroscopy (EIS) and photoluminescence (PL) spectral analysis indicate that the introduction of a minute amount of $\beta\text{-}AgVO_3$ by low temperature phase conversion of Ag_3VO_4 could efficiently promote the separation efficiency of photogenerated charge carriers. This enhanced photocatalytic activity is attributed to the synergistic effects of heterostructured semiconductor photocatalysis, increased surface area, improved utilization of solar light due to a hollow structure, decreased photocorrosion and the surface plasmon resonance (SPR) of Ag nanoparticles (NPs). Besides, trapping experiments implied that holes and $^{\bullet}O^{2-}$ were the predominant active species during the degradation process. A possible combination of conventional and Z scheme mechanisms of enhanced photocatalytic activity of SGA-7 is proposed.

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Introduction

Semiconductor photocatalytic processes have shown great potential as a low-cost, environmentally favourable, and sustainable treatment technology, to align with the "zero" waste scheme, capable of surmounting two global problems of the whole world *i.e.* "Energy and Water". Traditional photocatalysts such as TiO_2, ZnO, and SnO_2 are active exclusively in the ultraviolet region due to their wide band gap (~3.0 to 3.4 eV) and are capable of utilizing only 5–7% of the solar spectrum. Visible-light-responsive photocatalysts attract great attention because they can harvest and potentially utilize more sunlight than conventional photocatalysts. The engineering of both the morphology and chemical composition by designing a heterojunction is of significant importance in enhancing the photocatalytic activity.

In the carbon nitride family, 2D metal-free graphitic carbon nitride ($g\text{-}C_3N_4$) has received much attention due to its interesting electronic properties, potential catalytic activities, high inplane nitrogen content and ecofriendly features, which has been investigated in the field of photocatalysis, CO_2 reduction and other energy conversion processes.[1–3] Although $g\text{-}C_3N_4$ is visible light active, its photocatalytic activity is low due to the high recombination rate of photogenerated electron–hole pairs. The band gap of $g\text{-}C_3N_4$ is about 2.7 eV, which can absorb visible light up to 450 nm. The efficiency can be proliferated by decreasing the band gap by doping with non-metals.[4–6] Since the electronegativity of sulphur is lower than that of the substituted carbon or nitrogen atom, the dopant anion has a radius comparable to that of the

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[a] *School of Chemical Sciences, Mahatma Gandhi University, Kottayam-686560, Kerala, India. E-mail: beenamscs@gmail.com*

[b] *Mechanical Engineering Department, University of Alberta, Edmonton, Alberta, Canada T6G 2V4. E-mail: sinoj@ualberta.ca*

† Electronic supplementary information (ESI) available: XRD patterns showing the formation of $\beta\text{-}AgVO_3$, HPLC chromatograms for the degradation of MB, MO and 2,4-D, comparison of the photocatalytic activity of SGA-7 with previous literature, TOC, and the scavenger effect. See DOI: 10.1039/c9nj01353a

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In situ S-doped ultrathin gC_3N_4 nanosheets coupled with mixed-dimensional (3D/1D) nanostructures of silver vanadates for enhanced photocatalytic degradation of organic pollutants†

Subi Joseph,[a] Sinoj Abraham,[b] Ragam N. Priyanka,[a] Thomas Abraham,[a] Arya Suresh[a] and Beena Mathew*[a]

A novel plasmonic Z-scheme sulphur doped $gC_3N_4/Ag_3VO_4/\beta\text{-}AgVO_3/Ag$ (SGA-*x*) hybrid quaternary photocatalyst was successfully fabricated *via* the ultrasonic assisted Kirkendall effect and diffusion processes followed by low temperature phase conversion. The obtained samples were characterized by X-ray diffraction, scanning electron microscopy, transmission electron microscopy, UV-vis diffuse-reflectance spectroscopy (UV-vis DRS) and X-ray photoelectron spectroscopy. The photocatalytic activities of the obtained photocatalysts were measured by degradation of methylene blue (MB), methyl orange (MO) and 2,4-dichlorophenoxy acetic acid (2,4-D) under visible-light irradiation. Among the composites with various levels of $\beta\text{-}AgVO_3$, SGA-7 exhibited the highest degradation efficiency with 95.45% MB degradation for 30 min, which was about 1.47 times higher than that of $S\text{-}gC_3N_4/Ag_3VO_4$ (SGA). The inter-particle electronic coupling in hollow nanoflower leads to self-narrowing of the band gap of Ag_3VO_4. Moreover, electrochemical impedance spectroscopy (EIS) and photoluminescence (PL) spectral analysis indicate that the introduction of a minute amount of $\beta\text{-}AgVO_3$ by low temperature phase conversion of Ag_3VO_4 could efficiently promote the separation efficiency of photogenerated charge carriers. This enhanced photocatalytic activity is attributed to the synergistic effects of heterostructured semiconductor photocatalysis, increased surface area, improved utilization of solar light due to a hollow structure, decreased photocorrosion and the surface plasmon resonance (SPR) of Ag nanoparticles (NPs). Besides, trapping experiments implied that holes and $^{\bullet}O^{2-}$ were the predominant active species during the degradation process. A possible combination of conventional and Z scheme mechanisms of enhanced photocatalytic activity of SGA-7 is proposed.

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Structure and dynamics of gold nanoparticles decorated with chitosan–gentamicin conjugates: ReaxFF molecular dynamics simulations to disclose drug delivery†

Susanna Monti, *[a] Jiya Jose,[b] Athira Sahajan,[b] Nandakumar Kalarikkal [b] and Sabu Thomas *[b]

With the aim of designing an efficient procedure for producing biocompatible drug delivery systems based on nanoparticle carriers for *in situ* controlled antibiotic release, we have defined a novel computational approach resorting to a reactive force field capable of realistically describing hybrid systems. The modeling procedure was focused on well-known components, namely gold nanoparticles, citrate, chitosan and gentamicin, and the experiments tuned on purpose. On the one hand, gold nanoparticles were synthesized, fuctionalized with chitosan, loaded with gentamicin and characterized by means of transmission electron microscopy (TEM), scanning electron microscopy (SEM), dynamic light scattering (DLS), UV-visible (UV-vis) spectroscopy, and Fourier transform infrared spectroscopy (FTIR). On the other hand, an effective model of a functionalized gold nanoparticle was created and its structure and dynamics were explored by classical reactive molecular dynamics simulations in solution based on the ReaxFF atomistic description. The structure, dynamics and drug release were reproduced realistically disclosing the motion of all the molecular components, their adsorption on the metal support, desorption, intermolecular interactions and self-assembly. The system size was very close to the experimental conditions and all the calculations could efficiently identify the most probable binding modes, the locations of the adsorbed molecules, the characteristic arrangements of the chains and the effects due to the surrounding environment. The role played by the substrate and water molecules in the releasing process was described in detail. In line with the literature it was found that the antibiotic activity was preserved and the drug release from the carrier could be tuned by changing the chitosan/getamicin weight ratio and the deposition pattern of the adsorbed layers.

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Introduction

Chitosans are a family of copolymers of *N*-acetylglucosamine and glucosamine obtained by the deacetylation of chitin. Due to their biocompatibility, biodegradability and solubility, these molecules can be easily manufactured in different forms, such as films, microspheres, nanospheres, sponges, *etc.*, and combined with other compounds for a wide variety of applications related to the biocatalysis, biomedicine and pharmaceutical sectors. Indeed, as reported in several papers, the antimicrobial activity of chitosan-based materials seems due to two main mechanisms: the interference with bacterial metabolism through electrostatic interactions between the chitosan positively charged sites and the negatively charged microbial cell membranes;[1–5] and the blockage of RNA transcription by complexation of chitosan with DNA molecules.[6] These two types of action are connected to the molecular weight and to the structural characteristics of the polymer chains.[7] Chitosan with greater molecular weight has shown weaker antibacterial activity,[8] whereas a higher degree of deacetylation determined a stronger action.[9,10] These findings suggest that the use of proper chitosan-based materials enriched with natural or synthetic antibiotics can be very effective for drug delivery and treatment of specific infections. According to the literature the delivery action can be further improved by combining these compounds with metal-based nano-vehicles. Indeed, these hybrid biocomposites demonstrated to be a convenient alternative for: (1) improving the penetrative capabilities of existing antimicrobials; (2) overcoming thick bacterial biofilm barriers; and

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[a] *CNR-ICCOM, Institute of Chemistry of Organometallic Compounds, via G. Moruzzi 1, I-56124 Pisa, Italy. E-mail: sapeptides@gmail.com*

[b] *International and Inter University Centre for Nanoscience and Nanotechnology, Mahatma Gandhi University, Kottayam-686 560, Kerala, India*

† Electronic supplementary information (ESI) available: Figures of the model AuNPs, RDF plots, antimicrobial activity: Petri dish at 24 h after application of AuNP solutions (1–2), gentamicin (3) and a CG–AuNP mixture, MD simulated GENT release. See DOI: 10.1039/c9cp02357g

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A nanocomposite of N-doped carbon dots with gold nanoparticles for visible light active photosensitisers†

Takashi Nozaki,[a] Tomomi Kakuda,[a] Yasir Beeran Pottathara[b] and Hideya Kawasaki*[a]

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This study aims to report the synthesis of nitrogen-doped carbon dots (N-CDs) derived from biomass, tannic acid and polyethyleneimine, which is a N-doping agent. The N-doping of CDs is found to enhance singlet oxygen ($^1O_2$) generation under visible light irradiation. Additionally, the N-CDs work as both a reducing agent and stabiliser, and hence the N-CDs can directly reduce chloroauric acid to form gold nanoparticles (Au NPs) without adding other reducers and stabilisers. The as-prepared N-CD–Au NP nanocomposite possesses 2.3 times higher photosensitising ability for producing $^1O_2$ than N-CDs. To the best of our knowledge, this is the first report on the enhancement of the photosensitising ability of N-CDs by Au NPs. We suggest that the plasmon coupling of Au NPs with the N-CDs causes the energy transfer from the N-CDs to the ground state oxygen ($^3O_2$), thus resulting in an increased $^1O_2$ generation.

Introduction

Carbon dots (CDs) are small carbon-based spherical nanoparticles, which are typically less than 10 nm in size can be modified with surface passivation and heteroatom doping.[1] The light absorbing ability of CDs has attracted a significant amount of attention in photoluminescence for bioimaging and fluorescence sensing applications owing to their advantages, such as tunable fluorescence emission, long-term stability and low toxicity.[2–7]

More recently, CDs have been recognised as a new generation of carbon nanomaterials for photocatalysis.[8–12] Among them, the photosensitising property of CDs is attractive for the generation of singlet oxygen ($^1O_2$) for photodynamic therapy used in the treatment of cancer and the inactivation of bacteria.[13–17] The energy transfer from photo-excited CDs to triplet oxygen ($^3O_2$) in the ground state is a key factor for producing highly reactive $^1O_2$. Ge *et al.* reported that C-dots exhibit dual photodynamics with $^1O_2$ and photothermal effects under 635 nm laser irradiation.[14] Zhang *et al.* demonstrated phosphorescent C-dots for highly efficient $^1O_2$ generation and their photo-oxidative nanozyme behaviour.[17] Several studies have been conducted based on the strategies to improve the $^1O_2$ generation efficiency of organic photosensitisers.[18,19] However, it is still challenging to find such strategies for CDs.

Herein, nitrogen-doped C-dots (N-CDs) were synthesised using tannic acid and polyethyleneimine. The N-CDs can work as photosensitisers to yield $^1O_2$ under visible light, and the N-doping of CDs is found to enhance the $^1O_2$ generation. In addition, we found that the N-CDs can directly reduce chloroauric acid to form gold nanoparticles (Au NPs) without the need for other reducers and stabilisers. Interestingly, the resultant nanocomposite of N-CDs with Au NPs (N-CD–Au NP nanocomposite) possesses a stronger photosensitising capability to produce $^1O_2$ under visible light in comparison with N-CDs alone. To the best of our knowledge, this is the first report on the enhancement of the photosensitising ability of N-CDs by Au NPs in the nanocomposite. The mechanism occurring on the gold (*i.e.* the metal-surface that leads to the photosensitising enhancement) is discussed.

Experimental

Materials

Tannic acid (TA), polyethyleneimine (MW.600) (PEI), *N*,*N*-dimethylformamide (DMF) (99.5%), hydrogen tetrachloroaurate (III) tetrahydrate ($HAuCl_4·4H_2O$, 99.9%), L-tyrosine (99.0%), trisodium citrate dihydrate, 0.1 mol L^{-1} silver nitrate solution, quinine sulphate dihydrate (98%) and methanol (99.7%, HPLC grade) were purchased from Wako Chemical, Japan.

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[a] *Department of Chemistry and Materials Engineering, Faculty of Chemistry, Materials and Bioengineering, Kansai University, Suita-shi, Osaka 564-8680, Japan. E-mail: hkawa@kansai-u.ac.jp*

[b] *International and Inter University Centre for Nanoscience and Nanotechnology, Mahatma Gandhi University, 686560 Kottayam, Kerala, India*

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Preface to the SI-NFAB

Neural functions of the aging brain: Daily living, developmental and geriatric disabilities

ARTICLE INFO

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ABSTRACT

Neuronal, microglial, astrocytic and oligodendrocytic functions of the brain are significantly affected during normal aging, and more so if inflicted with neurological diseases. Aging is a consistent risk factor for many neurodegenerative diseases that are sporadic in nature, whereas developmental neurological disabilities stem from errors in brain development. The neuronal functions are affected in both developmental disabilities and geriatric diseases. This special issue, is based on the two-days meeting at Thiruvanathapuram, India on 'Neural Functions of Aging Brain', which had several original presentations, as well as full reviews by neurobiologists and clinicians from India. Out of these, thirteen peer reviewed contributions are published in the present Special Issue of this Journal. This 'Foreword' is also a brief overview on the current scenario of neurobiology research on developmental disabilities and ageing in India based on the manuscripts included in the special issue, *vis-s-vis* the global scenario. Apparently, there is a void in geriatric and developmental neuroscience research in India since huge data mining and translation, concerted efforts on clinical neuroscience research, and consistent efforts on pure basic research resulting in 'first in the field' novelty are largely missing. Overall, Indian neuroscience excels in making meaningful relevance of contemporary discoveries in neuroscience and contributing towards advances in their applications.

1. Introduction

This special issue on "Neural Functions of the Aging Brain' (NFAB) of *J. Chem. Neuroanat.* contains peer reviewed manuscripts from the selected presentations made at a national symposium on the same subject, which was held during 27-28 September 2016, prior to the 'World Day of the Aged' on the 1st of October. The meeting was jointly organised by the Inter University Centre for Biomedical Research and Super Speciality Hospital (IUCBR & SSH), Kottayam and Rajiv Gandhi Centre for Biotechnology (RGCB), Thiruvananthapuram, Kerala, India.

As per the census of India in 2011, the aging (above 60 years old) population in Kerala is about 13% of the total population, where the country average is 8.6% ("ECONOMIC REVIEW 2017 | State Planning Board, Thiruvananthapuram, Kerala, India," 2017). The study quotes the report of Centre for Disability Studies, Thiruvananthapuram as 2.3% population growth rate among old-age people, and it is predicted that the proportion of the elderly will be about 20% by 2025. Currently, the global population of elderly, i.e., over 60 years of age is about 12%, which is expected to reach over 20% by 2050 (Wasay et al., 2016). World's older population who reside in developed or developing countries currently, is predicted to rise to 80% or more residing in *lesser* developed countries by 2050 (Wasay et al., 2016).

At a time when no dedicated institute for research on aging exists in India, the following institutions have major laboratories on aging research: Institute of Life Sciences, Bhubaneswar, Orissa; Centre for Geriatric Research in Banaras Hindu University, Varanasi; Centre for Research on Ageing, Sri Venkateswara University, Tirupati; School of Life Sciences, Central University of Hyderabad, Hyderabad; All India Institute of Medical Sciences, New Delhi, National Institute of Mental Health & Neurosciences, Bengaluru. In addition to these, several small groups across the nation have also contributed significantly to neurogerontology in India. The newly instituted Inter University Centre for Biomedical Research and Super Speciality Hospital (IUCBR & SSH), Kottayam, Kerala specifically have in-depth interests in ageing research, and committed to initiate a Centre for Aging Research to focus research on genetic, cellular and molecular basis of developmental disabilities and geriatric neurodegenerative diseases, so as to improve the quality of lives of individuals affected with normal or abnormal aging.

This special issue contains thirteen articles, which address basic, applied and translational biomedical research on developmental and geriatric disabilities, and the present-day predicament of the aging population in India. These articles deal with dietary patterns, stress-induced glucocorticoids, bioenergetics of the neurons, protein phosphorylation, intracellular calcium regulation and calcium mediated signalling in relation to normal ageing and age-related diseases. Fig. 1 depicts molecular, cellular, tissue-specific and behavioural changes in the CNS as human brain ages. Healthcare advises as provided by international agencies/associations such as Centre for Disease Control and Prevention and World Federation of Neurology are incorporated into the image of Fig. 1.

2. Burden of neurological disabilities in India

Globally, disabilities associated with aging are compounded by incidences of communicable diseases including viral diseases (highly prevalent in certain regions of the country, significantly in the southern Indian Sate, Kerala) at any stage of their life, continue to affect brain faculties and mental capabilities when aged (Kyu et al., 2018). Astute examples are increasing incidents of autism spectrum disorders (Arora et al., 2018) and attention deficit-hyperactivity disorders in children,

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Influence of POSS Fillers on the Transport Properties of Natural Rubber Nanocomposites

S. Lakshmipriya,[1] **S. Anil Kumar**,[2] **K. Nandakumar**,[1] **Sabu Thomas**[1*]
[1]*International and Inter University Centre for Nanoscience and Nanotechnology, Mahatma Gandhi University, Kottayam, India*

[2]*N S S Hindu College, Changanacherry, India*

Three types of polyhedral oligomeric silsesquioxane (POSS)—octaphenyl (OP), POSS@TESPT (TT), and MWCNT@POSS (VC)—were incorporated into natural rubber (NR) to fabricate nanocomposites. The transport properties of POSS–NR nanocomposites were studied through solvent diffusion techniques. Diffusion studies were done with toluene (aromatic solvent) and the influence of nanofiller structure, concentration and compatibility with the NR matrix on various diffusion parameters were analyzed. The fillers that have good interaction with the polymer matrix showed the lowest solvent uptake. The network structure analysis revealed that the polymer chains deformed affinely. The effect of fillers on the chain flexibility was also discussed based on mechanical property studies. POLYM. COMPOS., 2018. © 2018 Society of Plastics Engineers

INTRODUCTION

The knowledge of transport properties of polymers is important as it throws light into their suitability in applications like structural engineering materials where they often come in contact with hazardous solvents, vapors and temperatures. Barrier properties like diffusion studies of polymer matrices help in designing food packaging materials, solvent reservoirs, biomedical devices, and so on. The concentration difference between two phases is the driving force behind these processes [1]. Transport properties of solvents through polymer matrices are influenced by various factors like nature of the polymer and penetrant, crosslink density of the matrix [2], temperature, geometry, and chemical nature of fillers [3], interaction of fillers with the polymer [4] and so on [5].

Diffusion is a kinetic parameter that depends upon polymer free volume, segmental mobility, and nature of penetrant molecule. Many studies have been done on the transport properties of rubber-based nanocomposites [6]. Diffusion studies throws light into the nature of filler–polymer interactions based on the rate of solvent absorption. Unnikrishnan and Thomas [7]studied the diffusion of solvents through carbon black (CB)-filled natural rubber (NR) composites and found that the solvent uptake and diffusion coefficient decreased with decrease in the size of CB particles due to reduction in polymer chain mobility. Choudhary et al. [8] found that good dispersion and effective polymer–filler interactions could reduce the solvent swelling properties of vulcanized hydrogenated nitrile rubber nanocomposites. Kumar and Thomas [9]found that the solvent uptake by sisal fiber/SBR composites decreased as the penetrant size increased. According to Chaudhari et al. [2], the swelling extent of nanocomposites in various solvents depends on the polymer–solvent interaction and the structure /size of the solvent molecule.

Polyhedral oligomeric silsesquioxanes (POSSs) are a class of organic–inorganic hybrid materials having the general formula $R_n(SiO_{3/2})_n$ (R represents organic group). The thermal and mechanical properties of these materials are intermediate between silica and organic polymers. The presence of organic groups at the surface makes it compatible with various polymers and hence used as both nanofillers and as inorganic building blocks. Recently, POSS based systems have been extensively applied in the fabrication of amphiphilic surfactants [10], synthesis of non-spherical Janus particles [11], as micro initiators for growing polymer chains [12], scaffolds for liquid crystalline supermolecules [13], and so on. POSS based hybrid systems are also in demand for use in specific technological applications and are popular due to their tunable surface groups and diverse properties [14]. POSS nanoparticles also form hybrids with other nanoparticles like carbon nanotubes [15], graphene oxide [16], silica [17], nanoclay [18] and so on which greatly reduces the problem of nanoparticle agglomeration. Although various works has been done with POSS-elastomer systems, their nanocomposites with NR are an unexplored area. Our study focusses on the solvent transport properties of POSS–NR nanocomposites. Gen et al. [19] studied the diffusion and pervaporation characteristics of

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Correspondence to: S. Thomas; e-mail: sabuthomas@mgu.ac.in

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Synthesis and electrochemical characterization of electroactive IoNanofluids with high dielectric constants from hydrated ferrous sulphate†

Aswathy Joseph,*[a] Marylin Mary Xavier,[b] Jacek Fal,[c] Gaweł Żyła,[c] Soorya Sasi,[b] P. Radhakrishnan Nair,[b] A. S. Padmanabhan[a] and Suresh Mathew*[ab]

An iron oxide based-electroactive IoNanofluid with a high dielectric constant, high stability and low viscosity was synthesized from ferrous sulphate heptahydrate *via* a facile microwave assisted one-step route in 1-butyl-4-methylpyridinium chloride. The IoNanofluid exhibited CE coupled faradaic redox reactions involving reversible chemical reaction and reversible electron transfer steps. A transition from diffusion controlled to surface controlled capacitive processes was observed at varying scan rates. The efficiency of the charge–discharge process was greater than 94% even after 100 cycles.

Ferrous sulphate heptahydrate ($FeSO_4{\cdot}7H_2O$) or melanterite is a major industrial by-product of titanium dioxide and steel surface treatment plants that causes serious environmental issues. Many efforts are being focused on utilizing this excess by-product for purposes like iron recovery, wastewater treatment, production of sodium or potassium ferrates, *etc.*, in an attempt to cover its production volume by these industries.[1–3] Recyclable industrial by-products like these often under-utilized in large quantities are an ingenious source of starting materials for nanofluid production. When combined with ionic liquids (ILs), they can offer distinctive and intriguing redox chemistry also. Herein, we investigate the fascinating redox reactions of electroactive IoNanofluids (complex dispersions of nanofluids in ILs) for the first time. The IoNanofluid electrochemistry can be promising if brought to the cognizance of the scientific community. This is mainly due to the wide electrochemical potential window offered by ILs, unlike conventional nanofluid dispersion mediums. In such systems, the IL anion–cation interaction energy, weak inter-ionic forces and nanoparticle–IL surface–interface interactions also have a decisive role in determining the nanofluids' colloidal stability and electrochemical properties. Here, we present a new aspect of IoNanofluid redox chemistry that involves both coupled reversible chemical reaction (C_r) and reversible electron transfer reaction (E_r).

Electroactive nanofluids consist of electrochemically active nanoparticles that can undergo electrochemical redox reactions during the charge–discharge process.[4] Iron oxide based-IoNanofluids also exhibit a complicated electroactive nature. The redox processes of iron/iron oxide magnetic nanoparticles (MNPs) and ionic liquids are commonly investigated in many electrochemical systems.[5–8] Similarly, nanomaterials of carbonaceous materials, hybrid polyoxometalates, metals, metal alloys, metal oxides, intermetallic or mixed metal oxides, metal phosphates, partially fluorinated metal oxides and phosphates, *etc.*, freely dispersed in electrolytes of Li salts or anchored onto ionic liquid cations like alkyl-ammonium, phosphonium, imidazolium, and pyrrolidinium ions have also been explored as electroactive nanofluids.[9–18] The practicality of such systems for implementation in redox flow batteries is also being explored tremendously nowadays.[19–23] Characteristics such as very low viscosity, high solid loading, excellent thermal and colloidal stability, superior heat transfer capabilities, maximum discharge capacity, *etc.*, are considered as desirable qualities for an electroactive nanofluid.[19,24] Besides, the energy capacity of rechargeable systems working with electroactive nanofluids depends on the mass of electroactive nanomaterials in them.[25]

In this study, we used $FeSO_4{\cdot}7H_2O$ along with 1-butyl-4-methylpyridinium chloride and ammonia solution to prepare the IoNanofluid. For this, about 1 wt% of $FeSO_4{\cdot}7H_2O$ was dissolved in 1-butyl-4-methylpyridinium chloride (IL) at 100 °C and added few microlitres of 30 wt% ammonia solution until a pH greater than 10 was achieved. At higher pH, $FeSO_4{\cdot}7H_2O$ easily forms solid iron(II) hydroxide colloidal particles. This mixture was then microwave irradiated at 100 °C for 15 minutes in an Anton Paar Monowave 300 microwave reactor (reaction profile shown in Fig. S1 of the ESI†). The resultant IoNanofluid had exceptionally high colloidal stability greater than one year without the use of any stabilizers or surfactants. A compact IL

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[a] School of Chemical Sciences (SCS), Mahatma Gandhi University, Kottayam, Kerala 686 560, India. E-mail: aswathyj@gmail.com, sureshmathewmgu@gmail.com
[b] Advanced Molecular Materials Research Centre (AMMRC), Mahatma Gandhi University, Kottayam 686560, Kerala, India
[c] Department of Physics and Medical Engineering, Rzeszów University of Technology, Rzeszów, Poland

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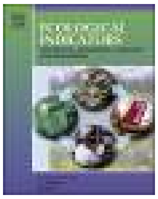

Original Articles

Polyphasic approach revealed complex bacterial community structure and function in deep sea sediment of ultra-slow spreading Southwest Indian Ridge

Rupesh Kumar Sinha[a,*], K.P. Krishnan[a,*], Femi Anna Thomas[a], M.B. Binish[b], Mahesh Mohan[b], P. John Kurian[a]

[a] National Centre for Antarctic and Ocean Research, Headland Sada, Vasco da Gama 403804, Goa, India
[b] School of Environmental Sciences, Mahatma Gandhi University, Kottayam 686560, Kerala, India

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ABSTRACT

The Southwest Indian Ridge (SWIR) is one of the least explored mid-ocean ridges and contains a high frequency of hydrothermal vents. We examined the bacterial community structure and metabolic potential of surface sediments collected from a sea mount at 2681 m depth and a ridge-flank at 3776 m in SWIR. High throughput 16S rRNA amplicon sequencing combined with Community Level Physiological Profiling (CLPP) revealed that hydrothermal sediments hosted a diverse microbial community with significant difference in structure and function between seamount and ridge-flank. The ridge-flank community was primarily comprised of facultative chemoautotrophic members of *Burkholderiales* (43.0%) while copiotrophic members of *Alteromonadales* (56.9%) and *Oceanospirillales* (14.6%) were dominant in seamount sample. These results coincided with CLPP of microbial community with higher utilization of carbohydrates such as D-cellobiose, β-methyl-D-glucoside, glucose 1-phosophate and pyruvic acid methyl ester observed in seamount. Culture-dependent approach using array of nutrient media enabled the isolation of heterotrophic genera that exhibited ability to degrade refractory organic matter such as phenanthrene, anthracene, pyrene, fluorene and fluoranthene. These results indicate that bacterial community present in the deep-sea hydrothermal sediment can act as bioreactor for mineralization of refractory organic matter. Thus our study emphasize on the significance of polyphasic approach in comprehensive and rapid assessment of physiological and taxonomic characteristics of the deep seabed bacterial community and further suggested that the bacterial community can act as ecological indicators of the metabolic sources prevalent in the ridge environment.

1. Introduction

At mid-oceanic ridges, chemical and isotopic exchange reactions between the heated seawater and oceanic basement have a profound influence on seawater chemistry (Kastner, 1999; Edmond et al., 1979) and thus effect the mineralogy, geochemistry and physical properties of the oceanic basement. Precipitation of minerals occurs when the hot acid, sulfide and metal-rich fluids mix with cold oxidizing alkaline seawater. The entire ocean volume circulates through oceanic basement at spreading centers in 5–7 million years (Kastner, 1999). Thus, hydrothermal vents play important role in fertilization of oceans with biologically significant minerals such as iron and manganese. Microbial diversity of marine sediments has been studied extensively in the past decades and available knowledge provides a coherent framework for understanding the composition of microbial communities and their *in situ* function. However, our understanding of benthic microbes is strongly skewed towards studies from shallow depths and continental margins. Data sets from open ocean sites and deep sea sediments are scarce, particularly from the mid oceanic ridge systems (Walter et al., 2018; Gold, 1992). Seabed of mid oceanic ridges are characterized with a variety of chemical substances such as manganese, iron, sulphur compounds, methane, hydrogen gas and polycyclic aromatic hydrocarbons (PAH) which form dynamic habitats with distinct chemical gradients that influence the microbial structure (Jannasch and Mottl, 1985; Baker et al., 2013; Yuan et al., 2015). Composition of benthic microbial community in mid oceanic ridges varies with carbon and oxygen content, hydrothermal influence and sediment depth. Oxic surficial sediments harbor relatively diverse bacterial communities with

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* Corresponding authors.
E-mail addresses: kineto.magnetic@gmail.com (R.K. Sinha), kpkrishnan@gmail.com (K.P. Krishnan).

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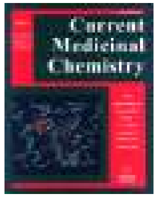

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Review Article

The Medicinal Chemistry of Therapeutic Peptides: Recent Developments in Synthesis and Design Optimizations

Author(s): Anutthaman Parthasarathy, Sasikala K. Anandamma, Karunakaran A. Kalesh*.

Affiliation: School of Chemical Sciences, Mahatma Gandhi University, Priyadarshini Hills, Kottayam, Kerala – 686560, India

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Abstract:

Peptide therapeutics has made tremendous progress in the past decade. Many of the inherent weaknesses of peptides which hampered their development as therapeutics are now more or less effectively tackled with recent scientific and technological advancements in integrated drug discovery settings. These include recent developments in synthetic organic chemistry, high-throughput recombinant production strategies, highresolution analytical methods, high-throughput screening options, ingenious drug delivery strategies and novel formulation preparations. Here, we will briefly describe the key methodologies and strategies used in the therapeutic peptide development processes with selected examples of the most recent developments in the field. The aim of this review is to highlight the viable options a medicinal chemist may consider in order to improve a specific pharmacological property of interest in a peptide lead entity and thereby rationally assess the therapeutic potential this class of molecules possesses while they are traditionally (and incorrectly) considered 'undruggable'.

Keywords: Therapeutic peptides, solid-phase peptide synthesis, high-throughput screening, stapled peptides, unnatural amino acids, liposome encapsulation, cyclic peptides/peptoids, cell-penetrating peptides.

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Development of Electrochemical Nanosensor for the Detection of Malaria Parasite in Clinical Samples

Olaoluwa R. Obisesan[1,2], *Abolanle S. Adekunle*[1*], *John A. O. Oyekunle*[1], *Thomas Sabu*[2], *Thabo T. I. Nkambule*[3] *and Bhekie B. Mamba*[3]

[1] *Department of Chemistry, Obafemi Awolowo University, Ile-Ife, Nigeria,* [2] *International and Inter University Center for Nanoscience and Nanotechnology, Mahatma Gandhi University, Kottayam, India,* [3] *Nanotechnology and Water Sustainability Research Unit, College of Science, Engineering and Technology, Univeristy of South Africa, Johannesburg, South Africa*

In this study, electrochemical nanosensors were developed from the synthesized metal oxide (MO) nanoparticles by supporting it on a gold electrode (Au). The activity of the developed nanosensor toward the detection of malaria biomarker (β-hematin) was determined and the optimum conditions at which the maximum detection and quantification occurred were established. β-Hematin current response at the sensors was higher when compared with the bare Au electrode and followed the order Au-CuO (C) > Au-CuO (M) > Au-Fe_2O3 (M) > Au-Fe_2O3 (C) > Au-Al_2O3 (M) > Au-Al_2O3 (C) > bare Au. The developed sensors were stable with a relatively low current drop (10.61–17.35 %) in the analyte. Au-CuO sensor had the best performance toward the biomarker and quantitatively detected *P. berghei* in infected mice's serum samples at 3.60–4.8 mM and *P. falciparum* in human blood serum samples at 0.65–1.35 mM concentration.

Keywords: β-hematin, metal oxide nanoparticles, sensor, cyclic voltammetry, square wave voltammetry, malaria, clinical samples, biomarker

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Northeastern University, United States
Jiahua Zhu,
University of Akron, United States

***Correspondence:**
Abolanle S. Adekunle
sadekpreto@gmail.com

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INTRODUCTION

Medical diagnosis and biological monitoring of diseases in the clinical laboratory are important because they're useful in detecting various diseases or onset of several diseases. The use of markers (biomarkers) has been the main cornerstone in the identification and quantification of target metabolites in biological fluids (blood, urine, and saliva) (Gil and Pla, 2001; Angerer et al., 2006). Detection of most diseases using sophisticated techniques mainly involves expensive and time-consuming processes. Development of sensitive, selective, accurate, rapid as well as affordable techniques for clinical diagnosis has been a major focus of researchers recently. Electrochemical sensors using nanoparticles have emerged as one of the suitable technologies for the detection of analytes of interest in clinical chemistry due to their high sensitivity and selectivity, rapid response time, and low cost (Wang, 1994).

Malaria is an intricate, infectious, hematologic disease instigated by a protozoan parasite named *Plasmodium falciparum* (Priyamvada et al., 2014). The parasite spends part of its life in humans and part in Anopheles mosquitoes. Malaria is transmitted to humans through infected Anopheles mosquitos. Although there are more than 50 species of *Plasmodium*, only four species, *P. falciparum, P. vivax, P. malariae,* and *P. ovale,* are known to cause malaria in humans (Priyamvada et al., 2014). The malaria parasite depends on iron for growth because many enzymes of the parasite metabolic pathways depend on iron (Weinberg and Moon, 2009). Malaria clinical symptoms occur during the intra-erythrocytic stage. At this stage, *P. falciparum* degrades more than 80% of

JOURNAL OF Applied Polymer SCIENCE

Exploring the filler-polymer interaction and solvent transport behavior of nanocomposites derived from reduced graphene oxide and polychloroprene rubber

M. G. Maya,[1,2] Jiji Abraham,[3] Soney C. George ,[1] Sabu Thomas[2]
[1]Centre for Nanoscience and Technology, Department of Basic Sciences, Amal Jyothi College of Engineering, Kanjirappally, Kottayam 686518, Kerala, India
[2]International and Inter University Centre for Nanoscience and Nanotechnology, Mahatma Gandhi University, Kottayam 686550, Kerala, India
[3]Department of Chemistry, Vimala College (Autonomous), Thrissur 68009, Kerala, India
Correspondence to: S. C. George (E-mail: soneygeo@gmail.com)

ABSTRACT: Aliphatic solvent resistance of polychloroprene rubber (CR) reinforced reduced graphene oxide (RGO) nanocomposites were explored in the temperature range of 30–50 °C using hexane, heptane, and octane. Microstructure-assisted solvent resistant property is evident from transmission electron microscopy images of fabricated composites. Different transport parameters such as diffusion, permeation, and sorption constants were moderate while increasing RGO content. Diffusion mechanism was explained based on the permeating molecule and is found to be close to Fickian mechanism except for heptane. Evaluation of kinetic and thermodynamic parameters shows the ability of nanoreinforcement to alter thermodynamic characteristics and rate constant values. The extent of reinforcement was also evaluated by Kraus equation. From swelling studies, molecular mass between crosslinks was evaluated using Flory–Rehner equation and compared these values with theoretical predictions such as phantom and affine models to analyze the deformation and mobility of the network during swelling. Temperature plays a significant role in the transport of organic solvent through CR/RGO nanocomposites. © 2019 Wiley Periodicals, Inc. J. Appl. Polym. Sci. **2019**, *136*, 48168.

KEYWORDS: chloroprene rubber; crosslink density; network structure; reduced graphene oxide; solvent transport; swelling coefficient; thermodynamic parameters

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INTRODUCTION

In recent years, researchers in industry and academic circles have focused their interest on polymeric nanocomposites, which stand for a radical alternative to conventional filled polymers or polymer blends. As we know that, in nanocomposites, at least one dimension is in the nanometer range. This distinctive enables the nanoreinforcement to enhance the overall material performance. Nanomaterials are more effective in reinforcements than their conventional counterparts because a smaller amount of nanomaterials causes a significant improvement of the polymer matrix properties. The field of nanoscience has blossomed over the last two decades by the discovery of graphene[1] and graphene-based polymer nanocomposites. A better enhancement in modulus, failure properties such as tensile and tear strength, barrier properties, thermal properties, and so forth was obtained by the incorporation of graphene-based filler in elastomeric matrices.

Sorption and diffusion of small molecules through the polymer is a matter of the broad range of application in many industrially important phenomena. Solvent diffusion studies are vital in elastomeric composites because this method predicts the life span of the product used in the liquid atmosphere; as well, it is used to characterize the chemical structure, crosslink density, and interfacial characteristics of rubber composites. There is a rapidly increasing demand for polymer specified permeability such as selective membrane for packaging application, foaming, and plasticization. Transport properties such as diffusivity relate how rapidly molecules move through the polymer matrix.

These things are very important in many applications of polymer for films and membranes. Various factors such as nature of the polymer, nature of the solvent, crosslinking system and temperature, and so forth, were influenced the diffusion phenomenon. According to the free volume concept, chain mobility provides a

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Epoxy/methyl methacrylate acrylonitrile butadiene styrene (MABS) copolymer blends: reaction-induced viscoelastic phase separation, morphology development and mechanical properties

Jomon Joy,[a] Krzysztof Winkler,[b] Kuruvilla Joseph,[c] S. Anas[ad] and Sabu Thomas *[ae]

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This article examines for the first time the effect of the addition of methyl methacrylate acrylonitrile butadiene styrene (MABS) copolymer on the phase separation, morphology and mechanical properties of epoxy systems. Blends of epoxy resin/MABS containing 5, 10, 15 and 20 phr MABS were prepared using a solution mixing technique. The homogenous blends obtained by this technique undergo a polymerization reaction-induced phase separation process by the introduction of the curing agent 4,4′-diaminodiphenyl sulfone (DDS). The optical microscopy analyses revealed that at low concentration of the MABS, the phase separation was by a nucleation and growth process. However, at higher concentration of MABS, the phase separation was by a spinodal process as evidenced by the formation of a co-continuous phase morphology followed by coarsening at later stages leading to phase separated domains. The morphology of the completely cross linked samples was probed by SEM, TEM and AFM analyses. A phase-in-phase morphology was noticed in all the compositions as a result of a viscoelastic phase separation process due to strong dynamic asymmetry arising from the molecular weight and T_g differences between the component polymers (high molecular weight MABS and liquid epoxy). In other words, the phase separated MABS and epoxy phases were not pure phases, both had sub-inclusions of the other phase leading to an interpenetrating polymer network (IPN) type of structure. The dynamic mechanical spectroscopy data also indicated a phase-in-phase morphology as evidenced by the shift in the T_g of the phases. It was also observed that the mechanical properties of the blends were enhanced effectively by the addition of MABS. The tensile strength and impact strength of epoxy increased by 25% and 72%, respectively, upon loading of MABS. This article also provides a correlation between the morphology and mechanical properties of the blended systems.

1. Introduction

Among the various thermosetting resin-based blends used in engineering applications,[1] epoxy resins (ERs) are extensively used as matrixes for high-performance composites in the aerospace and automotive industry, due to their excellent properties like high tensile strength and modulus, ease of processing, excellent thermal and chemical resistance and low shrinkage on curing.[2] These resins are also utilised widely in protective coatings and structural applications including fiber-reinforced composites, electrical laminates, casting, encapsulation, tooling and adhesives.[3–5] Epoxy resins generally require a high level of cross linking for many applications, which results in a brittle behavior. Various studies have been carried out on the toughening of epoxy polymers.[6] The most familiar method to improve the toughness of epoxy matrixes is to incorporate low molecular weight liquid rubbers into epoxy resins. Reactive functionalized butadiene-*co*-acrylonitrile rubbers such as carboxyl terminated (CTBN), amine terminated (ATBN) and epoxy terminated (ETBN) butadiene acrylonitrile were widely used as modifiers for epoxy resins.[7–9] The rubber-toughened epoxy often exhibits outstanding fracture characteristics and increased impact properties. However the presence of the rubbery phase decreases the modulus, glass transition temperature (T_g) and thermal stability of the material with a further

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[a] *School of Chemical Sciences, Mahatma Gandhi University, Kottayam, Kerala, India. E-mail: sabuthomas@mgu.ac.in*
[b] *Institute of Chemistry, University of Bialystok, Bialystok, Poland*
[c] *Department of Chemistry, Indian Institute of Space Science and Technology, Thiruvananthapuram, Kerala, India*
[d] *Advanced Molecular Materials Research Centre, Mahatma Gandhi University, Kottayam, Kerala, India*
[e] *International and Inter University Centre for Nanoscience and Nanotechnology, Mahatma Gandhi University, Kottayam, India*

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CORRECTION

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Correction: Cascade energy transfer and tunable emission from nanosheet hybrids: locating acceptor molecules through chiral doping

Goudappagouda,[ab] Vivek Chandrakant Wakchaure,[ab]
Kayaramkodath Chandran Ranjeesh,[ab] Chalona Antony Ralph Abhai[c] and
Sukumaran Santhosh Babu*[ab]

Correction for 'Cascade energy transfer and tunable emission from nanosheet hybrids: locating acceptor molecules through chiral doping' by Goudappagouda *et al.*, *Chem. Commun.*, 2017, **53**, 7072–7075.

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The Royal Society of Chemistry apologises for these errors and any consequent inconvenience to authors and readers.

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[a] *Organic Chemistry Division, National Chemical Laboratory (CSIR-NCL), Pune-411008, India. E-mail: sb.sukumaran@ncl.res.in; Web: http://academic.ncl.res.in/sb.sukumaran/home*

[b] *Academy of Scientific and Innovative Research (AcSIR), New Delhi-110020, India*

[c] *School of Chemical Sciences, Mahatma Gandhi University, Kottayam-686560, India*

Editors
Inamuddin
Department of Applied Chemistry
Aligarh Muslim University
Aligarh, India

Sabu Thomas
School of Chemical Sciences
Mahatma Gandhi University
Kottayam, Kerala, India

Raghvendra Kumar Mishra
Mahatma Gandhi University
Kottayam, Kerala, India

Abdullah M. Asiri
Chemistry Department, Faculty of Science
King Abdulaziz University
Jeddah, Saudi Arabia

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Effect of $CoFe_2O_4$ weight fraction on multiferroic and magnetoelectric properties of $(1-x)Ba_{0.85}Ca_{0.15}Zr_{0.1}Ti_{0.9}O_3 - xCoFe_2O_4$ particulate composites

Ajith S. Kumar[1] · **C. S. Chitra Lekha**[1] · **S. Vivek**[1] · **K. Nandakumar**[2] · **M. R. Anantharaman**[3] · **Swapna S. Nair**[1]

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Abstract

Different compositions of the composite lead-free multiferroic magnetoelectric systems are fabricated by employing piezoelectric $Ba_{0.85}Ca_{0.15}Zr_{0.1}Ti_{0.9}O_3$ (BCZT) and magnetostrictive $CoFe_2O_4$ (CFO) by varying the CFO weight fraction. The magnetic, dielectric, ferroelectric and magnetoelectric (ME) properties of the system are analyzed and found to be varying with the ferrite concentration. Even though the composite systems exhibit high magnetocapacitance (MC) properties (~35%), the possible stray contributions from magnetoresistance and magnetostriction make it unreliable for the quantitative determination of ME coupling coefficient (MECC). Therefore, a dynamic method is chosen for the measurement of magnetoelectric coupling. All the compositions have shown fairly good ME coupling. It is found that the ME coupling increases with ferrite fraction and the highest ME coupling of 14.8 mV/(cm Oe) is observed for 0.6BCZT–0.4CFO composite. It is also observed that the ME voltage increases linearly with the ac modulating field with a voltage generation of 1.25 V/cm (for $x=0.4$) for a small ac modulating field of 100 Oe. This high sensitivity and linear response of ME coupling to the ac magnetic fields offer the possibility of employing these particulate composites for a wide range of applications from magnetic field sensors to energy harvesters.

1 Introduction

Research on novel functional materials like magnetoelectric multiferroics attracts significant interest, due to its profound physics behind them as well as the large application potentials specifically in the field of energy harvesters [1–3], magnetoelectric sensors [4, 5] and storage devices [6, 7]. This special class of material exhibits both ferroelectric and magnetic properties in a single material or in an artificially engineered composite [8]. Beyond the concurrent existence of several order parameters in a single component, the switching of magnetic or electric polarization by the other's conjugate field can involve in the development of low-power consuming multifunctional memory devices, which can have the best properties of FeRAMs and MRAMs [9]. In single phase multiferroics, such as bismuth ferrite (BFO) [10, 11], the ME coupling is often due to the local interaction between the ordered ferroelectric and magnetic sublattices. They, however, exhibit weak coupling properties at room temperature [12], making them unusable for any practical applications. To obtain better ME coupling, an alternative strategy is to fabricate artificial heterostructures consisting of ferroelectric and magnetic phases [8, 13, 14]. In this kind of heterostructures, individual phases can be separately optimized for achieving high ME coupling at room temperature.

Magnetoelectric particulate composites belong to the class of engineered artificial systems, where the coupling is achieved via strain-mediated mechanical interaction at the piezoelectric/magnetostrictive interfaces. Since ME coupling is a product property, the piezoelectric constant and magnetostrictive properties of the individual ferroelectric and magnetic phases should be very high in order to obtain high coupling. Along with the high ferroic properties, the

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✉ Swapna S. Nair
swapna.s.nair@gmail.com

[1] Dept. of Physics, Central University of Kerala, Kasaragod 671316, India

[2] Dept. of Physics, Mahatma Gandhi University, Kottayam 686560, India

[3] Dept. of Physics, Cochin University of Science and Technology, Kochi 682022, India

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TECHNICAL ARTICLE

Highly Ordered Good Crystalline ZnO-Doped WO_3 Thin Films Suitable for Optoelectronic Applications

V.S. KAVITHA,[1] R. JOLLY BOSE,[1] R. SREEJA SREEDHARAN,[1]
C. SUDARSANAKUMAR,[2] RADHAKRISHNA PRABHU,[3]
and V.P. MAHADEVAN PILLAI[1,4]

1.—Department of Optoelectronics, University of Kerala, Kariavattom, Thiruvananthapuram, Kerala 695581, India. 2.—School of Pure and Applied Physics, Mahatma Gandhi University, Priyadarsini Hills, Kottayam, Kerala 686560, India. 3.—School of Engineering, Robert Gordon University, Aberdeen, UK. 4.—e-mail: vpmpillai9@gmail.com

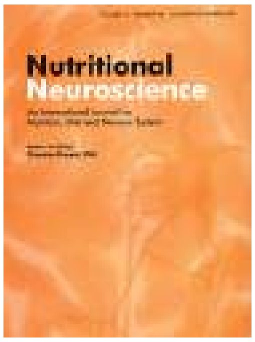
Highly ordered ZnO-doped WO_3 thin films with good crystalline quality are prepared using radio frequency magnetron sputtering technique, and its morphological and structural properties are studied using various characterization tools such as field emission scanning electron microscopy, energy-dispersive x-ray spectroscopy, x-ray diffraction technique, micro-Raman spectroscopy, and x-ray photoelectron spectroscopy. Morphological analysis shows a smooth surface for pure film, whereas the ZnO-doped films presents a dense distribution of grains of larger sizes with well-defined grain boundary. X-ray diffraction studies reveal the enhancement of crystalline quality of the films with increase in ZnO doping concentration up to 5 wt.%, beyond which the crystalline quality gets deteriorated. A phase modification from a single monoclinic WO_3 phase to mixed monoclinic WO_3 and $W_{18}O_{49}$ phases is observed for films with higher ZnO doping concentrations.

INTRODUCTION

Tungsten trioxide (WO_3) is an important semiconductor oxide material showing a broad spectrum of novel properties.[1] It shows structural and stoichiometric transitions upon change in conditions that fascinated scientists to explore their future technological applications in different fields.[2,3] Since structural and morphological properties of nanomaterials show a vital role in device performance, the designing of nanomaterials is a crucial problem when technological applications are concerned.[4] From an application point of view, it is utmost desirable to synthesize highly crystallized nanomaterial thin films by controlling their structural and morphological properties. WO_3 thin films are better known for their important physiochemical properties, which make them a suitable candidate in catalysis, gas sensors, electro-chromic devices, etc.[5–7] The structural and morphological properties of WO_3 thin films (at sub-micrometric scale) have profound effects on its physiochemical properties, which strongly depends on its preparation methods and conditions.[8] WO_3 thin films have been prepared by many groups through different techniques like chemical vapor deposition,[9] RF magnetron sputtering,[10] solvothermal process,[11] electrodeposition,[12] sol–gel processs,[13] hydrothermal techniques,[14] atomic layer deposition,[15] pulsed laser deposition technique,[16,17] etc. Among this radio frequency (RF) magnetron sputtering technique is relatively simple, and one can grow homogeneous, high-quality thin films of larger area suitable for device applications. Here we report the fabrication of ZnO-doped WO_3 thin films of superior crystalline quality using RF magnetron sputtering technique and its morphological and structural studies using different techniques such as field emission scanning electron microscopy (FESEM), energy-dispersive x-ray spectroscopy (EDX), x-ray diffraction (XRD), micro-Raman spectroscopy, and x-ray photoelectron spectroscopy (XPS).

EXPERIMENT

ZnO-doped tungsten oxide thin films were prepared using the RF magnetron sputtering technique from sputtering targets made of WO_3 powder



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Autistic traits and components of the folate metabolic system: an explorative analysis in the eastern Indian ASD subjects

Sharmistha Saha, Tanusree Saha, Swagata Sinha, Usha Rajamma & Kanchan Mukhopadhyay

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Scope of surface-modified molecular and nanomaterials in gel/liquid forms for developing mechanically flexible DSSCs/QDSSCs

Soorya Sasi,[a] Sunish K. Sugunan,[a,b] P. Radhakrishnan Nair,[a] K. R. V. Subramanian[c] and Suresh Mathew *[a,d]

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The advanced lifestyle of the human race involves heavy usage of various gadgets which require copious supplies of energy for uninterrupted functioning. Due to the ongoing depletion of fossil fuels and the accelerating demand for other energy resources, renewable energy sources, especially solar cells, are being extensively explored as viable alternatives. Flexible solar cells have recently emerged as an advanced member of the photovoltaic family; the flexibility and pliability of these photovoltaic materials are advantageous from a practical point of view. Conventional flexible solar cell materials, when dispersed in solvents, are usually volatile and create severe stability issues when incorporated in devices. Recently, non-volatile, less viscous functional molecular liquids/gels have been proposed as potential materials for use in foldable device applications. This perspective article discusses the scope of surface-modified non-volatile molecular and nanomaterials in liquid/gel forms in the manufacturing and deployment of flexible photovoltaics.

1. Introduction

The modern era of technology has created unprecedented transformations in the lifestyle of the human race and has led to the introduction of many electronic, electrical, mechanical and photovoltaic devices. Excessive usage of these devices has increased rates of energy consumption to new peaks, and the excessive consumption of traditional energy sources is leading

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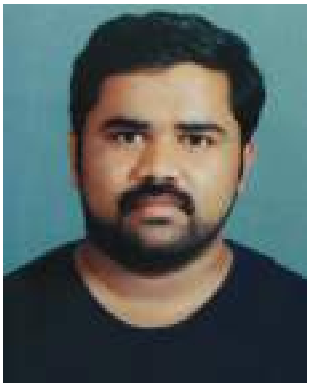
[a] *Advanced Molecular Materials Research Centre, Mahatma Gandhi University, Kottayam, Kerala, India. E-mail: sureshmathewmgu@gmail.com*
[b] *Department of Chemistry, CMS College (Autonomous) – affiliated to Mahatma Gandhi University, Kottayam, Kerala, India*
[c] *Department of Mechanical Engineering, GITAM University, Nagadenahalli, Dodballapur Taluk, Bengaluru 562103, India*
[d] *School of Chemical Sciences, Mahatma Gandhi University, Priyadarshini Hills, Kottayam, Kerala, India*

Soorya Sasi

Miss Soorya Sasi is a Research Scholar working towards her Ph.D. in the area of functional molecular liquids and composites for energy applications at the Advanced Molecular Materials Research Centre (AMMRC), Mahatma Gandhi University (MGU), Kottayam, Kerala, India. She received her M.Tech. in nanotechnology from Amrita Vishwa Vidya Peetham, India and worked as a Senior Research Fellow at the Amrita Center for Nanosciences and Molecular Medicine, Kochi, Kerala, India. Her areas of interest are flexible nanomaterial composites, dye/quantum dot-sensitized solar cells, supercapacitors and flow capacitors.



Sunish K. Sugunan

Dr Sunish K. Sugunan received his Ph.D. in Chemistry from the University of Saskatchewan, Canada and completed a subsequent two-year Post-doctoral term at Durham University, UK. Later, he worked as a research officer at Advanced Molecular Materials Research Centre (AMMRC), Mahatma Gandhi University (MGU), Kottayam, Kerala, India. Currently, he is working as an Assistant Professor at CMS College – Kottayam, Kerala, India. His areas of research are experimental and theoretical studies of materials for solar cells, flexible nanomaterials and composites, OLEDs, photosynthetic complexes and photocatalysis.

ORIGINAL PAPER

Nonlinear Optical Materials

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Synthesis, Crystal Growth, and Optical Characterization of a Novel Nonlinear Optical Organic Material: *N*,*N*-Diarylbenzamide

Radhakrishnan Lakshmi, Peethambaram Prabukanthan, Gurusamy Harichandran, and C. Sudarsana Kumar*

Nonlinear optical organic materials of *N*,*N*-diphenylbenzamide (NNDPB) and 4-fluoro-*N*,*N*-diphenylbenzamide (FNNDPB) are synthesized from benzoylation of *N*,*N*-diphenylamine using the substituted benzoyl chlorides. The single crystals of NNDPB and FNNDPB are grown by a slow evaporation technique. Single-crystal X-ray diffraction shows that both the crystals belong to orthorhombic crystallographic system with space group *Pbca*. Fourier transform infrared spectrum shows the chemical bonding and various functional groups, the carbonyl peak appeared at 1647 and 1651 cm^{-1} in NNDPB and FNNDPB compounds, respectively. ^1H and ^{13}C nuclear magnetic resonance analysis examines the placement of aromatic protons and carbons are identified to the synthesized materials. UV–vis near IR spectra analysis showed 100% transmission in the visible region for both NNDPB and FNNDPB crystals. As-grown crystal dielectric constant and dielectric loss are inversely proportional to the frequency at all the temperatures. The thermal properties of NNDPB and FNNDPB crystals are studied from thermogravimetric analysis/differential thermal analysis analysis, it is thermally stable up to 483 and 503 K. Crystal growth mechanism and defects are observed from etching studies. The relative second harmonic generation efficiency is measured by Kurtz–Perry powder technique and is found to be 1.55 and 1.7 times as that of potassium dihydrogen phosphate.

1. Introduction

Organic crystals are of great importance for the nonlinear optical (NLO) technologies in line with the trend to replace the classical electronics with organic materials. The organic materials have been of specific interest in the synthesis of materials having NLO properties and they offer an opportunity to use theoretical modeling coupled with synthetic flexibility to design and produce novel materials.[1] The organic NLO crystals are preferred to inorganic one due to their potentially high nonlinearities and rapid responses in electro-optic devices. The microscopic origin of nonlinearity in the organic molecular NLO materials is due to the presence of delocalized π-electron systems connecting donor and acceptor groups, which enhance the necessary asymmetric polarizability.[2]

The NLO property of organic crystal is governed by the NLO characteristics of the constituent individual molecular chromophores with donor– π–acceptor conjugation. Due to the presence of delocalized π-electron systems connecting the donor and acceptor groups, the materials generally exhibit high second harmonic generation (SHG) efficiencies.[3–5] A high NLO efficiency inorganic crystal arises from the large number of delocalized π electrons present in the material.[6,7] NLO materials are continuing to receive great attention due to their wide applications in laser technology, optical data storage.[8]

N-Phenyl benzamides are important biologically active compounds with NLO properties. Some of the amide-based compounds, near infrared spectroscopic studies of the hydrogen bonding between thioacetamide and *N*,*N*-disubstituted benzamide derivatives in CCl4 are reported by Choi et al.[9] The synthesis and crystal structure of 2-nitro-*N*-(4-nitrophenyl)benzamide is reported by Saeed et al.[10] In this work, we have chosen synthesis of organic compounds *N*,*N*-diphenylbenzamide (NNDPB) and 4-fluoro-*N*,*N*-diphenylbenzamide (FNNDPB) by the benzoylation of diphenylamine with benzoylchloride and 4-fluoro benzoylchloride, respectively.

Organic crystals are mostly grown by slow evaporation method.[11,12] The method is mostly used for the growth of organic single crystal and it can provide a convenient and inexpensive solution. The grown crystals of diarylbenzamides were used for structural and stability characterizations of single crystal, and powder X-ray diffraction (XRD), Fourier transform

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R. Lakshmi, Dr. P. Prabukanthan
Materials Chemistry Lab
Department of Chemistry
Muthurangam Government Arts College
Vellore 632002, India
E-mail: pprabukanthan76@hotmail.com

Dr. G. Harichandran
Department of Polymer Science
University of Madras
Guindy Campus, Chennai 600025, India

Dr. C. Sudarsana Kumar
School of Pure and Applied Physics
Mahatma Gandhi University
Kottayam 686560, India

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Tuning of nonlinear absorption in highly luminescent CdSe based quantum dots with core–shell and core/multi-shell architectures

Sneha Bhagyaraj,[abcd] Sreekanth Perumbilavil,[e] R. Udayabashkar,[f] R. V. Mangalaraja,[f] Sabu Thomas,[cg] Nandakumar Kalarikkal *[ch] and Oluwatobi Samuel Oluwafemi *[ab]

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We present our effort on an efficient way of tuning the nonlinear absorption mechanisms in ultra-small CdSe based quantum dots by implementing core–shell and core/multi-shell architectures. Depending on the size, architecture and composition of the QDs, these materials exhibited resonant and near-resonant nonlinear optical absorption properties such as saturable (SA) and reverse saturable (RSA) absorption for 5 ns pulses of 532 nm. These QDs exhibited a non-monotonic dependence of the effective two-photon absorption coefficient (β) under nanosecond excitation with a maximum value for a thinner shell. We obtained a nonlinear absorption enhancement of an order of magnitude by adopting the core–shell architecture compared to their individual counterparts. Interestingly, CdSe QDs exhibit SA and/or RSA depending on their size and show a switching over from SA to RSA as the input intensity increases. We explained the enhanced nonlinear absorption in core–shell QDs compared to their individual counterparts in view of enhanced local fields associated with the core–shell structure. Thus, the present nanostructured materials are excellent candidates as saturable absorbers and optical limiters.

Introduction

Nanostructured nonlinear optical materials have been gaining interest as optical limiters for protection applications in laser related research laboratories and industries and as saturable absorbers. Optical limiters are materials that can attenuate highly intense laser radiation by limiting the output intensity/fluence to a safe range, so that delicate instruments and human eyes can be protected from laser-induced damage.[1,2] Many materials such as graphene derivatives,[3–8] ultra-small nanoclusters,[9–11] semiconductor nanoparticles,[12–15] glasses,[16–19] magnetic nanoparticles,[20–24] liquid crystals,[25] organic materials,[26–29] quantum dots[30] and many others[31,32] have been explored for optical limiting applications. Semiconductor quantum dots (QDs), which possess some unique quantum confinement properties that enable fine tuning of their optical characteristics, have been widely explored for various optoelectronic applications.[33] In semiconductor core–shell quantum dots (CSQDs), there exist some dielectric confinement effects which place them in a favourable position to be used as third order nonlinear optical materials. They can be tuned to work off resonance as well as on resonance with a fast time response.[34] Compared to core semiconductors, several core–shell/multi-shell QDs show enhanced optical nonlinearity, which is assigned to the local field of the surrounding dielectric medium.[35]

Among the various II–VI semiconductors, CdSe QDs are efficient and their optical tuning range spans the visible region of the spectrum, which in turn has attracted a great deal of interest in terms of scientific research. Extensive research on the linear and nonlinear optical properties of colloidal CdSe QDs with various capping agents and preparation methods has been reported.[36,37] Studies have demonstrated that the surface passivation of the core can improve the stability and optical properties by formation of a core–shell structure, thereby

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[a] *Department of Applied Chemistry, University of Johannesburg, P.O. Box 17011, Doornfontein, 2028 Johannesburg, South Africa. E-mail: oluwafemi.oluwatobi@gmail.com*
[b] *Centre for Nanomaterials Science Research, University of Johannesburg, Johannesburg, South Africa*
[c] *International and Interuniversity Centre for Nanoscience and Nanotechnology, Mahatma Gandhi University, Kottayam, Kerala – 686560, India. E-mail: nkkalarikkal@mgu.ac.in*
[d] *Center for Advanced Materials, Qatar University, P.O. Box 2713, Doha, Qatar*
[e] *Laboratory of Photonics, Tampere University, P.O. Box 692, FI-33104 Tampere, Finland*
[f] *Advanced Ceramics and Nanotechnology Laboratory, Department of Materials Engineering, Faculty of Engineering, University of Concepcion, Concepcion, Chile*
[g] *School of Chemical Sciences, Mahatma Gandhi University, Kottayam, Kerala-686560, India*
[h] *School of Pure and Applied Physics, Mahatma Gandhi University, Kottayam, Kerala-686560, India*

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Effects of termite foraging activity on topsoil physical properties and water infiltration in Vertisol

Sougueh Cheik[a,b,*], Nicolas Bottinelli[b,c], Benoit Soudan[a], Ajay Harit[d], Ekta Chaudhary[e], Raman Sukumar[e], Pascal Jouquet[a,b]

[a] Indo-French Cell for Water Science (IFCWS), Civil Engineering Department, Indian Institute of Science, 560012 Bangalore, Karnataka, India
[b] Institute of Ecology and Environmental Sciences (UMR 242 iEES-Paris), Sorbonne Universités, Centre IRD, Bondy, France
[c] Soils and Fertilizers Research Institute (SFRI), Dong Ngac, Tu Liem, Ha Noi, Viet Nam
[d] School of Environmental Sciences, Mahatma Gandhi University, Kottayam, Kerala, India
[e] Centre for Ecological Sciences, Indian Institute of Science, Bangalore, Karnataka, India

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ABSTRACT

In the tropics, termites are key litter decomposers and soil bioturbators. Termite foraging activity involves the production of sheetings and galleries that influence the physical, chemical and hydraulic properties of soils. The functional impacts of these biogenic structures and biopores have been acknowledged for a long time in soils dominated by 1:1 minerals. Less is known, however, on their functional impacts in soils dominated by 2:1 minerals, such as vertisol which represent 22% of the land surface in India. Therefore, an experiment was carried out in a vertisol in southern India where elephant (*Elephas maximus*) dung pats (ED) and *Lantana camara* twigs (LT) were applied on the ground and protected (+) or not (−) from termite activity. Termite activity was only measured below ED−, showing a clear preference for organic matter derived from elephant dung. Soil sheetings had similar properties to the surrounding topsoil, with the exception of their C content that was reduced. This result raised the question of the origin of the soil used by termites for covering ED. ED− was also associated with the presence of effective macropores up to 5 cm depth and a significant increase in water hydraulic conductivity (12-fold). However, the utilization of the coefficient of linear extensibility showed that these galleries were unstable and most likely short-lived. In conclusion, this study confirmed that the structure of soils dominated by 2:1 minerals is mainly controlled by physical processes (i.e., the shrinking and swelling of soils). This study also stresses the need to better understand the dynamic of termite galleries in soil and to quantify the origin and fate of organic matter in soil sheetings.

1. Introduction

Fungus-growing termites are amongst the most important litter decomposers and soil bioturbators in arid and semi-arid environments (Bignell and Eggleton, 2000; Bottinelli et al., 2015). As "intended engineers" (*sensu* Jouquet et al., 2006), they build important and complex nest structures (i.e., mounds or termitaria) that protect colonies from predators and maintain a stable environment for the colony and their symbiotic fungus to grow (Lüscher, 1961). The functional impact of these mounds has been largely recognized (see Holt and Lepage, 2000; Jouquet et al., 2016; Khan et al., 2018 for reviews), especially in Africa where they constitute biodiversity and nutrient hot spots that increase the robustness of ecosystems (Bonachela et al., 2015).

Termites also influence ecosystem functioning through the production of subterranean galleries and sheetings to protect themselves from light, desiccation and predators while they forage (MacKay et al., 1985; Harit et al., 2017a,b; Fernandes et al., 2018). From studies carried out in sandy soils or in soils dominated by 1:1 minerals (e.g., sandy loams and Acrisol), it is usually considered that galleries constitute preferential flow paths and then increase water infiltration, reduce crust formation, water runoff and soil erosion in arid and sub-arid ecosystems (e.g., Eldridge and Pickard, 1994; Mando et al., 1996, 1999; Mando, 1997; Sarr et al., 2005; Mettrop et al., 2013; Léonard and Rajot, 2001; Léonard et al., 2004; Colloff et al., 2010: Kaiser et al., 2017). Although less known, a recent review suggests that soil sheetings are always enriched in clay in comparison with the surrounding soil but that their

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* Corresponding author at: Indo-French Cell for Water Science (IFCWS), Civil Engineering Department, Indian Institute of Science, 560012 Bangalore, Karnataka, India.

E-mail address: sougueh.cheik@ird.fr (S. Cheik).

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insects

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Article

Linking Termite Feeding Preferences and Soil Physical Functioning in Southern-Indian Woodlands

Sougueh Cheik [1,2,*], Rashmi Ramesh Shanbhag [3], Ajay Harit [4], Nicolas Bottinelli [2,5], Raman Sukumar [6] and Pascal Jouquet [1,2]

[1] Indo-French Cell for Water Science (IFCWS), Civil Engineering Department, Indian Institute of Science, Bangalore 560012, India; pascal.jouquet@ird.fr
[2] Institute of Ecology and Environmental Sciences (UMR 242 iEES-Paris), Sorbonne Universités, Centre IRD, 93143 Bondy, France; nicolas.bottinelli@ird.fr
[3] Indian Plywood Industries Research and Training Institute, Bangalore 560022, India; rashmishanbhags@gmail.com
[4] School of Environmental Sciences, Mahatma Gandhi University, Kottayam 686560, India; om.harit@gmail.com
[5] Soils and Fertilizers Research Institute (SFRI), Dong Ngac, Tu Liem, Ha Noi, Vietnam
[6] Centre for Ecological Sciences, Indian Institute of Science, Bangalore 560012, India; rsuku@iisc.ac.in
* Correspondence: sougueh.cheik@ird.fr; Tel.: +84-16-6284-0970

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Abstract: Termites are undoubtedly amongst the most important soil macroinvertebrate decomposers in semi-arid environments in India. However, in this specific type of environment, the influence of termite foraging activity on soil functioning remains unexplored. Therefore, this study examines the link between the quality of litter and the functional impact of termite feeding preferences on soil properties and soil hydraulic conductivity in a deciduous forest in southern India. Different organic resources (elephant dung: "ED", elephant grass: "EG", acacia leaves: "AL" and layers of cardboard: "CB") were applied on repacked soil cores. ED appeared to be the most attractive resource to *Odontotermes obesus*, leading to a larger amount of soil sheeting (i.e., the soil used by termites for covering the litter they consume), more numerous and larger holes in the ground and a lower soil bulk density. As a consequence, ED increased the soil hydraulic conductivity (4-fold) compared with the control soil. Thus, this study highlights that the more *O. obesus* prefers a substrate, the more this species impacts soil dynamics and water infiltration in the soil. This study also shows that ED can be used as an efficient substrate for accelerating the infiltration of water in southern-Indian soils, mainly through the production of galleries that are open on the soil surface, offering new perspectives on termite management in this environment.

Keywords: *Odontotermes obesus*; sheeting; termite foraging activity; litter quality; organic resource consumption; soil water dynamic

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1. Introduction

Soil biodiversity regulates a large number of ecological functions, such as the degradation of litter, the cycling of nutrients or the regulation of water dynamics in the soil [1,2]. Amongst soil organisms, termites are increasingly recognized as playing a role in the provisioning of key ecosystem services [3,4]. Termites are ubiquitously amongst the most abundant and active litter decomposers in tropical environments [5] and are also considered significant soil bioturbators or ecosystem engineers because of the biostructures they produce [6,7]. Indeed, a large body of literature describes the specific soil biological, chemical and physical properties of termite mound nests [8–17] and the link between

Carbon Nanotube Reinforced Poly(Trimethylene Terephthalate) Nanocomposites: Viscoelastic Properties and Chain Confinement

Madathinal Kunjappan Aswathi,[1] Moothetty Padmanabhan,[2] Lovely Mathew,[1,3] Prosenjit Saha,[4]
Roberto Terzano,[5] Nandakumar Kalarikkal,[1,6] Tatiana Volova,[7] Sabu Thomas [1,8]
[1] *International and Interuniversity Centre for Nanoscience and Nanotechnology, Mahatma Gandhi University, Kottayam, Kerala, India*
[2] *Department of Chemistry, Amrita Vishwa Vidyapeetham, Amritapuri, Kerala, India*
[3] *Department of Science and Humanities, Viswajyothi College of Engineering and Technology, Muvattupuzha, Kerala, India*
[4] *M.N. Dastur School of Materials Science and Engineering, Indian Institute of Engineering Science and Technology (IIEST)-Shibpur, Howrah, India*
[5] *Department of Soil, Plant and Food Sciences, University of Bari "Aldo Moro", Bari, Italy*
[6] *School of Pure and Applied Physics, Mahatma Gandhi University, Kottayam, Kerala, India*
[7] *Department of Biotechnology, Siberian Federal University, Krasnoyarsk, Russia*
[8] *School of Chemical Sciences, Mahatma Gandhi University, Kottayam, Kerala, India*

Through a very facile route, a new class of nanocomposites involving poly(trimethylene terephthalate; PTT) and multiwalled carbon nanotubes (MWCNTs) was developed which was found to be high performance engineering material showing high modulus. Morphological, mechanical, viscoelastic, and thermal properties of the PTT nanocomposites with varying compositions of MWCNT were systematically studied and the results were analyzed. The dynamic mechanical and tensile properties of all the nanocomposites were seen to be enhanced with the addition of MWCNT and the sample containing 2 wt% MWCNT showing a storage modulus as much as 9.4×10^8 GPa. The results were correlated with the morphological features obtained from scanning electron microscopy and transmission electron microscopy. Coefficient of effectiveness, degree of entanglement density, and reinforcement efficiency factor were estimated from the storage modulus values and, in addition, the degree of chain confinement also could be quantified. Furthermore, theoretical modelling was also done on the elastic properties of the composites. The crystallization temperature, glass transition temperature, and percentage crystallinity were estimated for all the nanocomposites and it was found that the sample with 3 wt% MWCNT content exhibited the highest glass transition temperature of 68.2°C. POLYM. ENG. SCI., 9999:1–11, 2018. © 2018 Society of Plastics Engineers

INTRODUCTION

Polymeric materials reinforced by nanofillers are of special interest in nanotechnology owing to their versatile properties and innumerable applications. The incorporation of nanofillers into the polymers can tune and modify several physical characteristics of the nanocomposites including the strength and modulus of the polymer matrix and can also enhance the thermal and thermo-oxidative degradation of the polymers [1–3]. The thermal behavior of nanocomposites can be correlated to the glass transition temperature, T_g. Among the nanocomposites, the carbon nanotube (CNTs)-based nanocomposites are known to exhibit good electrical, mechanical, and thermal properties [4,5]. The electrical conductivity shown by the multiwalled carbon nanotubes (MWCNT) is comparable to that of copper (500–10,000 S/cm) and, in addition, the tensile strength ($\sim$20 GPa) and modulus (in the order of 1 TPa) are still higher [6]. Highly favorable conductivity of MWCNT (100–1,000 W/mK), very high aspect ratio, and good physical properties of CNT are some of the factors which have made the material a very promising and attractive candidate for composite preparations [7]. The conductivity of CNT-based polymer nanocomposite is seen to be dependent on several factors including the concentration of fillers, their aspect ratio, and degree of dispersion. Paszkiewicz et al. [8] investigated the effect of hybrid fillers like single-walled carbon nanotubes (SWCNT) and graphene nanoplatelets (GNP) on PTT-block-poly (tetramethylene oxide) (PTT-PTMO) and reported that the synergic effect of SWCNT and GNP enhances the thermal conductivity of PTT-PTMO significantly. Kumar et al. [9] reported that at a total loading of 0.5 wt% the hybridizing effect of GNP with commercially functionalized MWCNT in polyetherimide (PEI) matrix improve the electrical and thermal conductivity, as well as the dynamic properties considerably. Logakis et al. [10] investigated the thermal, electrical, mechanical, and dielectric properties of poly (methyl methacrylate) (PMMA)/CNT nanocomposites and reported that the electrical percolation threshold was found to be at 0.5 vol%.

PTT which is an aromatic semicrystalline polyester was first synthesized by Whinfield and Dicksen in 1941 (British patent 578 079). Because of the presence of three methylene groups PTT shows good elastic recovery greater than that of other polyesters like poly (butylene terephthalate) (PBT) and poly (ethylene terephthalate) (PET) and it is comparable to that of nylon. PTT also shows good color fastness, uniform dye uptake, stain resistance, and so forth [11]. The properties of PTT are in between that of PBT and PET and hence it can be considered as a promising material for the applications such as fibers, films, and engineering thermoplastics [12]. However, PTT has some limitations

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Correspondence to: S. Thomas; e-mail: sabuchathukulam@yahoo.co.uk

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[2] *Department of Chemistry, Amrita Vishwa Vidyapeetham, Amritapuri, Kerala, India*
[3] *Department of Science and Humanities, Viswajyothi College of Engineering and Technology, Muvattupuzha, Kerala, India*
[4] *M.N. Dastur School of Materials Science and Engineering, Indian Institute of Engineering Science and Technology (IIEST)-Shibpur, Howrah, India*
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[6] *School of Pure and Applied Physics, Mahatma Gandhi University, Kottayam, Kerala, India*
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INTRODUCTION

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RESEARCH ARTICLE

WILEY polymers advanced technologies

Injectable poloxamer/graphene oxide hydrogels with well-controlled mechanical and rheological properties

Elaheh Rohani Rad[1] | Henri Vahabi[2,3] | Krzysztof Formela[4] | Mohammad Reza Saeb[2,3] | Sabu Thomas[5]

[1] Faculty of Health and Medical Sciences, The University of Adelaide, Adelaide, South Australia, Australia

[2] CentraleSupélec, LMOPS, Université de Lorraine, Metz, France

[3] Laboratoire Matériaux Optiques, Photoniques et Systèmes, CentraleSupélec, Université Paris-Saclay, Metz, France

[4] Department of Polymer Technology, Gdańsk University of Technology, Gdansk, Poland

[5] School of Chemical Sciences, MG University, Kottayam, Kerala, India

Correspondence
M.R. Saeb, Dr.,Laboratoire Matériaux Optiques, Photoniques et Systèmes, CentraleSupélec, Université Paris-Saclay, 57070, Metz, France.
Email: mrsaeb2008@gmail.com

S. Thomas, Department of Polymer Technology, Faculty of Chemistry, G. Narutowicza Str. 11/12, Gdańsk University of Technology, 80-233 Gdansk, Poland.
Email: sabuthomas@mgu.ac.in

Although significant progress has been made in the design and application of injectable hydrogels for biomedical applications, concurrent control of rheological and mechanical properties of injectable hydrogels has remained as an open challenge to the researchers. In this work, we introduce and put into practice a photo-curable poloxamer (also known as Pluronic)/graphene oxide (Plu/GO) injectable hydrogel with well-controlled rheological and mechanical properties. Acrylate group was anchored to hydrogel structure to endow photo-crosslinking ability through decelerating degradation rate of poloxamer hydrogels after injection. It was found that the modified Plu remains stable in biological media for a long-term period without significant weight loss. Rheological properties of hydrogels were also carried out as essential prerequisite for an ideal injectability via frequency sweep, flow curve, recovery, and yield stress before and after modification, signifying shear-thinning behavior of Plu/GO hydrogels with high recoverability. The viscosity of shear-thinning-like hydrogels dropped at higher shear stress, which facilitated injection process. Moreover, mechanical behavior of Plu was optimized by manipulating the content of Plu, degree of modification with reactive precursor, curing, and particularly incorporation of GO without deteriorating effects on rheological behavior of Plu.

KEYWORDS

injectable hydrogel, mechanical properties, photo-crosslinking, Pluronic, rheological properties

1 | INTRODUCTION

Hydrogels reveal remarkable features such as high swelling ratio, sol-gel transition, similarity to native tissue and provide acceptable permeability when subjected to oxygen and water,[1-5] making them potential candidate for biomedical applications.[6-10] For tissue engineering uses, hydrogels should additionally provide a set of appropriate characteristics, where invasive surgical operation underlines the need for implanted hydrogels in lesion site to regenerate damaged tissue.[10-14] Bearing such requirements in mind, the use of injectable hydrogels with ability to form stable network is a prerequisite to avoid invasive therapeutics.[13,15,16] Injectable hydrogels serve as carrier for cells or drugs to the target tissue, and even a scaffold in damaged site to regenerate tissue.[17-19] Although considerable progress was made in manufacturing injectable hydrogels, designing injectable hydrogel with tunable rheological and mechanical properties has remained a challenging matter.[20-22] Highly thixotropic hydrogels offer a great opportunity in the development of injectable hydrogels as shield cells against high shear stress during injection. Moreover, thermal gelation of injectable hydrogels such as N-isopropylacrylamide[23] and methylcellulose[24,25] at body temperature preserves a faithful cage for cells or drugs once they are injected by the hydrogel.

Polxamer, also known as Pluronic, is a synthetic terpolymer composed of poly (propylene oxide) (PPO) block in the middle and poly (ethylene oxide) (PEO) blocks at two opposite sides.[26,27] PEO and PPO blocks play the role of hydrophilic and hydrophobic segments,

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UV-Induced reduction of graphene oxide in cellulose nanofibril composites

Y. B. Pottathara,[abc] S. Thomas,*[b] N. Kalarikkal,[b] T. Griesser,[d] Y. Grohens,[a] V. Bobnar,[e] M. Finšgar,[f] V. Kokol*[c] and R. Kargl*[cg]

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We report on an effective dry method to reduce graphene oxide (GO) in films of cellulose nanofibrils (CNF) by UV irradiation in the presence of nitrogen gas. The reduction of GO and the removal of carbonyl and carboxyl moieties were confirmed by infrared and UV-vis spectroscopy, potentiometric charge titration and X-ray photoelectron spectroscopy (XPS). The crystallinity of native and reduced composites was elucidated by X-ray diffraction measurements. The resulting reduced graphene oxide–CNF nanocomposite films remain flexible and show improved dielectric properties. After 5 hours of UV irradiation a 3 wt% graphene oxide loaded film increased its dielectric constant from 68.9 to 88.9, which shows significant enhancement compared to previous reports. The AC conductivity of reduced GO films reaches values of 9.37×10^{-4} S m^{-1}. The electrochemical performance of the samples was tested by cyclic voltammetry and electrochemical impedance spectroscopy. UV treated samples showed a higher capacitive nature than untreated samples. The UV induced reduction of GO in the presence of CNF is seen as a promising alternative to solvent based methods.

1. Introduction

The modern electronics industry requires high dielectric constant materials for the development of energy storage devices, flexible electronics, embedded capacitors, actuators, and sensors.[1–9] Due to their light weight, flexibility, low cost, and ease of processing, polymer based composites have advantages over established inorganic materials, ceramics, and metals.[3] Biopolymers like cellulose have been proposed and investigated in the past as a base material for flexible electronics due to their low cost, light weight, and biodegradability.[10] Among them, cellulose nanofibrils (CNF) have a high aspect ratio[11] with a high elastic modulus (*ca.* 138 GPa)[12] and low thermal expansion (0.1 ppm K^{-1})[13] compared to other polymers.

Graphene-based materials such as graphene nanoplatelets (GNPs), graphene nanosheets (GNSs) and graphene oxide (GO) have a high specific surface area and a planar structure and can be obtained by simple manufacturing methods.[14–16] With the two-dimensional sheet-like structure with covalently attached carbon atoms having various functional groups on the edges and basal planes, GO shows enhanced dispersion in polymeric matrices.[17] GO incorporated cellulose composites are widely reported having high mechanical and improved thermal properties.[18–22] However, for the fabrication of electronic devices, the low conductivity of GO limits its applicability and several researchers have paid attention to reducing GO in numerous ways to obtain improved electrical properties, including the use of cellulose based composites.[2,23–28]

Some reports are available for the *in situ* chemical reduction of GO in cellulose based composites[2,22–26] mainly using poisonous hydrazine as a reducing agent. Thermally reduced graphene oxide was also reported,[21,27] but here the addition of reduced GO into the cellulose matrices required the usage of organic solvents for better dispersion. Reported biological methods used a mannitol culture medium as the reducing agent together with bacterial cellulose[29] and strong alkaline solutions for the spinning of composite fibers.[30] These authors focused on the biomedical and thermo-mechanical applications rather than electronic device fabrication. Reduction of GO, coated on a quartz crystal, in the presence of hydrazine vapor in a closed chamber at 80 °C without any damage to the films for transparent conductors was reported recently[31] and cellulose nanocrystal/GO hybrid films

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[a] *IRDL-FRE, CNRS 3744, Universite de Bretagne Sud, 56100 Lorient, France*

[b] *International and Inter University Centre for Nanoscience and Nanotechnology, Mahatma Gandhi University, 686560 Kottayam, Kerala, India. E-mail: sabuchathukulam@yahoo.co.uk*

[c] *University of Maribor, Faculty of Mechanical Engineering, Smetanova ulica 17, SI-2000 Maribor, Slovenia. E-mail: vanja.kokol@um.si, rupert.kargl@um.si*

[d] *Chair of Chemistry of Polymeric Materials, University of Leoben, Otto-Glöckel-Straße 2, A-8700 Leoben, Austria*

[e] *Jozef Stefan Institute, Condensed Matter Physics Department, Jamova 39, SI-1000 Ljubljana, Slovenia*

[f] *University of Maribor, Faculty of Chemistry and Chemical Engineering, Smetanova Ulica 17, SI-2000 Maribor, Slovenia*

[g] *Graz University of Technology, Institute of Paper, Pulp and Fibre Technology, Inffeldgasse 23, A – 8010 Graz, Austria*

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[c] *University of Maribor, Faculty of Mechanical Engineering, Smetanova ulica 17, SI-2000 Maribor, Slovenia. E-mail: vanja.kokol@um.si, rupert.kargl@um.si*
[d] *Chair of Chemistry of Polymeric Materials, University of Leoben, Otto-Glöckel-Straße 2, A-8700 Leoben, Austria*
[e] *Jozef Stefan Institute, Condensed Matter Physics Department, Jamova 39, SI-1000 Ljubljana, Slovenia*
[f] *University of Maribor, Faculty of Chemistry and Chemical Engineering, Smetanova Ulica 17, SI-2000 Maribor, Slovenia*
[g] *Graz University of Technology, Institute of Paper, Pulp and Fibre Technology, Inffeldgasse 23, A – 8010 Graz, Austria*

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Magnetic Performance and Defect Characterization Studies of Core-Shell Architectured $MgFe_2O_4$@$BaTiO_3$ Multiferroic Nanostructures

Ann Rose Abraham[a], B. Raneesh[b], Saju Joseph[c], Mohammed Arif P[c], P.M.G. Nambissan[d], Dipankar Das[e], Didier Rouxel[f], Oluwatobi Samuel Oluwafemi[g, h], Sabu Thomas[c] and Nandakumar Kalarikkal*[a,c]

[a]*School of Pure and Applied Physics, Mahatma Gandhi University, Kottayam, Kerala-686560, India*.
[b]*Department of Physics, Catholicate College, Pathanamthitta, Kerala-689 645, India*
[c]*International& Inter University Centre for Nanoscience and Nanotechnology, Mahatma Gandhi University*, Kerala-686560, *India*
[d]*Applied Nuclear Physics Division, Saha Institute of Nuclear Physics, Kolkata 700064, India.*
[e]*UGC DAE Consortium for Scientific Research, Kolkata Centre, Sector III, LB-8*
Bidhan Nagar, Kolkata 700 098, India
[f]*Universite de Lorraine, Institut Jean Lamour, Vandouvre-les-Nancy, F-54506, France*
[g]*Department of Chemistry, University of Johannesburg, Doornfontein Campus, P.O Box 17011, Doornfontein, 2028, South Africa*
[h]*Centre for Nanomaterials Science Research, University of Johannesburg, Johannesburg, South Africa.*
* Corresponding author: nkkalarikkal@mgu.ac.in

Abstract

Multiferroics that permit manipulation of magnetization vector exclusively by electric fields have spawned extensive interest for memory and logic device applications. In line with this understanding, we herein report about the encapsulation of non-ferroelectric magnesium ferrite ($MgFe_2O_4$) nanoparticles in a ferroelectric shell of $BaTiO_3$ to produce a system with engineered dielectric, magnetic, magneto-electric and ferroelectric properties. The interface effect on the strain transfer was observed to strongly influence the magneto-electric coupling and the electric

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From Science to Evidence – How Biodiversity Indicators Can Be Used for Effective Marine Conservation Policy and Management

Abigail McQuatters-Gollop[1]*, Ian Mitchell[2], Cristina Vina-Herbon[3], Jacob Bedford[1], Prue F. E. Addison[4], Christopher P. Lynam[5], P. N. Geetha[6], Estee Ann Vermeulan[7], Kaylee Smit[7], Daniel T. I. Bayley[8], Elisabeth Morris-Webb[9], Holly J. Niner[10] and Saskia A. Otto[11]

[1] Centre for Marine and Conservation Policy, University of Plymouth, Plymouth, United Kingdom, [2] Joint Nature Conservation Committee, Aberdeen, United Kingdom, [3] Joint Nature Conservation Committee, Peterborough, United Kingdom, [4] Interdisciplinary Centre for Conservation Science, Department of Zoology, University of Oxford, Oxford, United Kingdom, [5] Centre for Environment, Fisheries and Aquaculture Science, Lowestoft Laboratory, Lowestoft, United Kingdom, [6] PG and Research Department of Zoology, Mahatma Gandhi University, Kottayam, India, [7] Institute for Coastal and Marine Research, Ocean Sciences Campus, Nelson Mandela University, Port Elizabeth, South Africa, [8] Centre for Biodiversity and Environment Research, University College London, London, United Kingdom, [9] School of Ocean Sciences, Bangor University, Menai Bridge, United Kingdom, [10] Faculty of Engineering, University College London, Adelaide, SA, Australia, [11] Institute of Marine Ecosystem and Fishery Science, Center for Earth System Research and Sustainability, University of Hamburg, Hamburg, Germany

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Spain

***Correspondence:**
Abigail McQuatters-Gollop
abigail.mcquatters-gollop@plymouth.ac.uk

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Indicators are effective tools for summarizing and communicating key aspects of ecosystem state and have a long record of use in marine pollution and fisheries management. The application of biodiversity indicators to assess the status of species, habitats, and functional diversity in marine conservation and policy, however, is still developing and multiple indicator roles and features are emerging. For example, some operational biodiversity indicators trigger management action when a threshold is reached, while others play an interpretive, or surveillance, role in informing management. Links between biodiversity indicators and the pressures affecting them are frequently unclear as links can be obscured by environmental change, data limitations, food web dynamics, or the cumulative effects of multiple pressures. In practice, the application of biodiversity indicators to meet marine conservation policy and management demands is developing rapidly in the management realm, with a lag before academic publication detailing indicator development. Making best use of biodiversity indicators depends on sharing and synthesizing cutting-edge knowledge and experience. Using lessons learned from the application of biodiversity indicators in policy and management from around the globe, we define the concept of 'biodiversity indicators,' explore barriers to their use and potential solutions, and outline strategies for their effective communication to decision-makers.

Keywords: ecosystem approach, assessment, monitoring, baselines, thresholds, policy communication, cumulative effects