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Ultrathin borophene based biosensor for early detection of alzheimer's disease and pancreatic cancer biomarkers: Acumen from DFT

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ARTICLE INFO

Keywords:
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Cancer diagnosis
Density functional theory
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ABSTRACT

Early diagnoses of Alzheimer's disease (AD) and pancreatic cancer (PC) are crucially important for the start of prognosis seeking the curing and saving of human lives. The present investigation aims to computational design materials having high selectivity towards the detection AD and PC biomarkers. Density functional theory (DFT) is explored to investigate the selective adsorption of pristine and metal-doped β12-borophene towards the volatile organic compounds (VOCs), related to AD or PC and well-known to exist in the exhaled breath of patients. Six VOCs were considered in our study; namely, **(i)** Three AD VOCs: 2,3-Dimethylheptane (2,3-DMH), Butylatehydroxytoluene (BHT), and Pivalic Acid (PVA); and **(ii)** Three PC VOCs: 2-pentanone (2p-none), 4-ethyl-1–2dimethyl benzene (4E-1,2-DMB), and n-nonanol (n-nonal). Pristine β12-borophene demonstrated selective adsorptions towards the six VOCs compared to the interfering air molecules (N_2, O_2, CO_2, H_2O) with adsorption energies at order [-0.85, -0.45] eV compared to [-0.20, -0.10], respectively. To enhance further the adsorption energies of VOCs and consequently the selectivity, the embedment of metal atoms in the small pores of β12-borophene monolayer has been explored. It is found that small-sized atoms such as alkali metal (Li) can be stably accommodated and yield large dipole moments to enhance the van der Waals interactions. For instance, using single-atom catalyst (SAC) of Li, the adsorption energies with VOCs were enhanced to become of magnitudes at order of 1.0 – 1.6 eV. While the magnetic state was maintained robust paramagnetic, the strong interactions with VOCs affected the recovery time to become huge. The SAC-Li doped β12-borophene can be proposed as candidate material for a platform of disposable nano biosensor with high sensor response to detect AD and PC biomarkers and consequently to contribute to the early diagnosis of these hazardous diseases.

PACS Numbers: 31.15.E-, 68.43.-h, 68.43.Fg, 82.33.Pt, 87.15.Aa, 87.15.Kg, 87.19.Xx, 87.19.xj

1. Introduction

The discovery of two-dimensional (2D) nanomaterials, characterized by atomic-size monolayer, has revolutionized fundamental nanoscience and nanotechnology. Specifically, the birth of a new field of 2D materials is attributed to breakthrough synthesis of Graphene by Geim and Novoselov [1]. Graphene is characterized by its remarkable mechanical strength, electronic mobility, and thermal properties [2], which have sparked widespread interest. Graphene's applications spanned broad spectrum of applications ranging from electronics [3] to energy storage [4], and to sensing [5]. In the realm of sensors, functionalized-graphene-based devices have demonstrated high sensor responses towards gas molecules ranging from small-sized toxic air molecules [6] to large-sized volatile organic compounds (VOCs) molecules [7], related to cancer diseases. Nevertheless, challenges such as the lack of bandgap and other requirements motivated researchers to explore other 2D materials beyond graphene such as silicene, germanene, borophene, transition-metal dichalcogenides (TMDs), MXenes, and MOFs [8–15].

Amongst the recently developed 2D materials, borophene has emerged and quickly gained high popularity as possessing unique properties such as cohesive structure [16], excellent mechanical strength [17], high conductivity [18], biocompatibility [19], and potential for tuneable thermal, electronic, optical, magnetic,

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Graphene-Graphullerene Heterostructure: A Novel Material for High-Performance Capacitors

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Abstract

This study introduces a novel graphene-graphullerene heterostructure as a promising material for high-performance capacitors. Compared to pristine graphene, this heterostructure exhibits a significantly larger surface area and porosity which enhance its energy storage capacity. Pristine graphullerene is a semiconductor with a bandgap of 0.92 eV and its integration with graphene effectively modifies its electronic properties, rendering it conductive as confirmed by band structure analysis. The unique combination of graphene's high conductivity and graphullerene's extended surface area and porosity presents a promising avenue for developing capacitors with exceptional performance characteristics.

Keywords: DFT, Graphullerene, Electronic Band Structure.
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Introduction

Carbon's diverse bonding allows it to form a variety of structures, such as graphite, diamond, fullerenes, carbon nanotubes, and graphene [1]. These allotropes exhibit a wide range of properties; for instance, diamond is known for its hardness and thermal conductivity, while graphite displays a layered structure and electrical conductivity. Recent research has unveiled novel 2D materials like Graphullerene, a recently synthesized carbon allotrope [2-4]. Graphullerene's unique structure boasts high porosity [3-5] and a significant bandgap, making it a promising candidate for various applications. The integration of Graphullerene with graphene could yield a material with exceptional electrical and surface properties, particularly for energy storage devices such as capacitors. This study explores the Graphene-Graphullerene Heterostructuring (H-Gra/Gph) which leads to high-performance capacitor material.

Method

We conducted density functional theory (DFT) calculations using the SIESTA code [6] to investigate the electronic properties of the H-Gra/Gph. A GGA-PBE [7] functional and a DZP basis set with a confinement energy of 20 meV were applied. Geometry optimization was performed using the conjugate gradient method with a force tolerance of 0.01 eV/Å, and a 10x10x1Monkhorst-Pack k-point mesh [8] was used to sample the Brillouin zone. A 15 Å vacuum was applied along the z-axis to minimize interactions between periodic images. Norm-conserving pseudopotentials were employed for all atomic species.

Results and Discussion

The H-Gra/Gph was formed by integrating graphene sheets with graphullerene, creating a composite material with a stable, low-energy configuration. The relaxed hybrid structure of H-Gra/Gph is shown in figure 1(a). The structural optimization of H-Gra/Gph are depicted in Figure 1 (b and c).

Figure 1(b) shows the variation of total energy (E_{Total}) with respect to the lattice constant (a). The plot reveals a well-defined minimum, indicating a stable configuration for the heterostructure at an optimized lattice constant. Figure 1(c) presents the plot of total energy (E_{Total}) versus the vertical

The biofabrication of silver nanoparticles from *Artemisia maritima* Linn. and the analysis of their bioactive properties

Jagriti Rana[1] · Anand Sagar[1] · Jyoti Rana[1] · Sanjeev Kumar[2]

Received: 5 September 2024 / Revised: 11 May 2025 / Accepted: 14 May 2025

Abstract

The presented research work encompasses outcomes from different methods performed to assess the bioactive pr ties of aerial parts of *Artemisia maritima* and the biogenic synthesis of silver nanoparticles. Bioactive properties of parts were screened in terms of phytochemical components (total phenols, flavonoids, tannin contents (TPC, TFC TTC), and GCMS analysis), enzyme inhibitory potential (α-amylase), FTIR (Fourier Transform Infrared), antiox and antimicrobial activities. Biofabricated silver nanoparticles were characterized by UV-Vis spectroscopy, FTIR, FESEM, EDX, and HRTEM, their antioxidant and antimicrobial potentials were also assessed. Plant material after e tion demonstrated a higher percentage yield in methanol solvent than in acetone. Both extracts revealed the prese phenols, flavonoids, and tannins. However, between both extracts, the acetone extract revealed a higher TPC and On the other hand, methanol extract disclosed higher TFC. GCMS analysis indicated α-santonin, 1,3,6,10-cyclotetr tetraene, 3,7,11-trimethyl-14-(1-methylethyl)-, [S-(E, Z,E, E)] and tetrapentacontane as major compounds with the h percentage area in both solvents. Plant extracts also reported α-amylase inhibition potential with IC_{50} values of 5.6 mL (acetone) and 13.32 mg mL (methanol). After characterization, the obtained nanoparticles displayed the prese different functional groups (FTIR), almost spherical shapes (FESEM, HRTEM), and crystalline nature (XRD, S Nanoparticles also exhibited antioxidant and antimicrobial activities, along with plant extracts.

Keywords Himalaya · GCMS · Silver-nanoparticles · Antioxidant · Disk-diffusion · MIC

Introduction

From time immemorial, plants and their products have been utilized for the therapy of numerous ailments. Over the past decades, novel drugs like taxol, quinine, digitoxin, atropine, codeine, reserpine, etc. have also been isolated from the plants (Balandrin et al. 1993). Suntar (2020) has fabulated more than eighty plants with their respective phytochemicals, which have been used in health care in the past and present. To date, a number of medicinal plants all over

Benabdallah et al. 2016; Nikolova et al. 2022). Ran (2022) have suggested that more than 150 Indian m plants have been evaluated for their antibacterial pr within the past two decades. Additionally, approx medicinal plants for nanoparticle synthesis have al in trend due to their bioavailability, cost-effectivene friendliness and application in the fields of biom biosensing, and bioimaging (Kotcherlakota et al. Rafique et al. (2017) have listed more than 80 pl cies in their review that were used for silver nanc synthesis. In the recent years, some Himalayan m

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PEARSON CORRELATION OF PHYSICO-CHEMICAL PARAMETERS AND MACRO-INVERTEBRATES IN JUKHALA VALLEY, BILASPUR DISTRICT, HIMACHAL PRADESH, INDIA

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Association of beta-arrestin gene expression with corticosteroids -long-acting beta-agonist step-up therapy in children with asthma

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Show more

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Highlights

- *LABA plays a crucial role in asthma management.*
- *Beta-arrestin-1 can be associated with symptomatic conditions in patients.*

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Base metals (Ni, Cu, Zn, Fe) oxide nanomaterials mediated photo/sono-catalytic removal of emerging pharmaceutical contaminants from wastewater

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Metal oxide nanomaterial
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Sonophotocatalytic
Pharma-based contaminants
Wastewater

ABSTRACT

Photo/sono-catalytic techniques are being extensively considered for the degradation and removal of emerging contaminants (EC), including pharma based organic pollutants. Transition metal-based nanomaterials have been studied as adsorbent/catalytic material in photo/sono-catalytic techniques for complete elimination/degradation/mineralization of pharmaceutical-based EC from wastewater streams. Various structural properties with dimensionalities of earth-abundant base metals (Ni, Fe, Cu, and Zn) oxides and their doped hybrid composites have been recently studied for removal/degradation/mineralization of EC from solution on the laboratory scale and industrial effluent of pharma sectors. The oxides of earth-abundant base metals nanomaterials have been summarized and discussed in this review along with the general mechanism of degradation/elimination with acceptable results related to wastewater stream detoxification and recyclability of catalytic material during degradation/removal of EC. The surface properties like transfer of electrons and holes, surface area, surface modification and doping with [illegible] value of these materials are primary factors for their applicability in the degradation/removal of organic pollutants from wastewater and subsequent treatment. This study would be helpful for their use and development of cutting-edge materials for waste/surface water treatment on a large scale in a sustainable and cost-effective manner.

1. Introduction

The world is under a phase of industrial growth and transformation for society but also faces environmental crises and tremendous challenges namely chemical waste, pharmaceutical, personal care products, industrial pollutants, dyes based hazardous pollutants etc. of emerging contaminants (EC) classes [1–3]. Numerous industries (paper & pulp, textile, food, dyes and pharmaceutical etc.) have been producing enormous contaminants and wastes in different spheres of the earth. This causes a number of severe problems in the hydrosphere along with the negative impacts on living organisms of the biosphere. This is also raising the strength of EC in waste/surface water due to the presence of various pollutants such as dyes, heavy metals, toxic chemicals, pharmaceuticals pollutant and pesticides [4–6]. Among the various emerging contaminates, the pharma-based biomedical waste particularly, drugs and medicines (antibiotics, antihypertensives, antidepressant, anti-convulsant, steroids and anti-inflammatory etc.), prescription/non-prescription medicines, damaged, spilled and expired

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Catalysis Today

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...avalent metals modulated Zn-based layered double hydroxides and their mixed metal oxides for catalytic depolymerization of carbonyl-coordinating plastic waste

Smita Soni, Sonika Kumari, Ajay Sharma, Shashi Kant Bhatia, Anil Kumar Sharma

[illegible]

ARTICLE INFO

Keywords: [illegible]

ABSTRACT

Plastic waste generation has become a global issue and presents a significant challenge [illegible]

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Effect of Ni and Dy co-doping on the structural, electrical, and dielectric properties of Strontium Y-type hexaferrite

2024-25

Monika Chandel[1] · Rohit Jasrotia[2,3] · Jahangeer Ahmed[4] · Saad M. Alshehri[4] · Kirti Singha[5] · Virender Pratap Singh[6]

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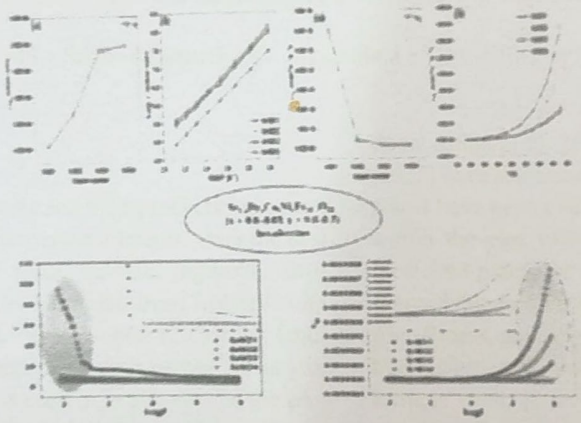
Abstract

Strontium Y-type hexaferrites, often referred to as Sr-Co_2Y hexaferrites, are widely considered for the microwave applications. The current study describes the synthesis of Ni and Dy-doped Sr Y-type hexagonal ferrites i.e. $Sr_{2-x}Dy_xCo_2Ni_yFe_{12-y}O_{22}$ ($x = 0$–0.03 and $y = 0$–0.3) by utilising the sol-gel (SG) process. The hexaferrite powders were sintered for 4 h at 1150 °C to eliminate impurities and moisture. The room temperature (RT) DC resistivity (ρ) of the S hexaferrites increases as the temperature and the Ni^{2+}/Dy^{3+} content increase. This shows the semiconducting nature o Sr-Co_2Y hexaferrites. The Ni^{2+} and Dy^{3+} doping reduces the drift mobility (μ_d) but increases the activation energy (E_a The observed E_a for the Sr hexaferrite materials showed the same trend as that of ρ. The dielectric analysis was performe within the frequency range of 82 Hz–10 MHz. Both the real permittivity (ε') and the loss tangent ($\tan\delta$) drop as th applied frequency rises. The dielectric properties also decrease after Ni and Dy substitution. The increase in ρ togeth with the small dielectric loss makes these hexaferrite materials more effective for devices and applications requiring hig resistive and high-frequency materials.

Graphical Abstract



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Self Attested

The biofabrication of silver nanoparticles from *Artemisia maritima* Linn. and the analysis of their bioactive properties

Jagriti Rana[1] · Anand Sagar[1] · Jyoti Rana[1] · Sanjeev Kumar[2]

2022-25

Received: 5 September 2024 / Revised: 11 May 2025 / Accepted: 14 May 2025

Abstract
The presented research work encompasses outcomes from different methods performed to assess the bioactive pr ties of aerial parts of *Artemisia maritima* and the biogenic synthesis of silver nanoparticles. Bioactive properties of parts were screened in terms of phytochemical components (total phenols, flavonoids, tannin contents (TPC, TFC TTC), and GCMS analysis), enzyme inhibitory potential (α-amylase), FTIR (Fourier Transform Infrared), antiox and antimicrobial activities. Biofabricated silver nanoparticles were characterized by UV-Vis spectroscopy, FTIR, FESEM, EDX, and HRTEM, their antioxidant and antimicrobial potentials were also assessed. Plant material after e tion demonstrated a higher percentage yield in methanol solvent than in acetone. Both extracts revealed the prese phenols, flavonoids, and tannins. However, between both extracts, the acetone extract revealed a higher TPC and On the other hand, methanol extract disclosed higher TFC. GCMS analysis indicated α-santonin, 1,3,6,10-cyclotetr tetraene, 3,7,11-trimethyl-14-(1-methylethyl)-, [S-(E, Z,E, E)] and tetrapentacontane as major compounds with the h percentage area in both solvents. Plant extracts also reported α-amylase inhibition potential with IC_{50} values of 5.6 mL (acetone) and 13.32 mg/mL (methanol). After characterization, the obtained nanoparticles displayed the prese different functional groups (FTIR), almost spherical shapes (FESEM, HRTEM), and crystalline nature (XRD, S Nanoparticles also exhibited antioxidant and antimicrobial activities, along with plant extracts.

Keywords Himalaya · GCMS · Silver-nanoparticles · Antioxidant · Disk-diffusion · MIC

Introduction

From time immemorial, plants and their products have been utilized for the therapy of numerous ailments. Over the past decades, novel drugs like taxol, quinine, digitoxin, atropine, codeine, reserpine, etc. have also been isolated from the plants (Balandrin et al. 1993). Suntar (2020) has fabulated more than eighty plants with their respective phytochemicals, which have been used in health care in the past and present. To date, a number of medicinal plants all over the world have been assessed for their phytocompounds and bioactive properties (Vladimir-Knezevic et al. 2014; Benabdallah et al. 2016; Nikolova et al. 2022). Ran (2022) have suggested that more than 150 Indian me plants have been evaluated for their antibacterial pr within the past two decades. Additionally, approa medicinal plants for nanoparticle synthesis have al in trend due to their bioavailability, cost-effectivene friendliness and application in the fields of biom biosensing, and bioimaging (Kotcherlakota et al. Rafique et al. (2017) have listed more than 80 pl cies in their review that were used for silver nan synthesis. In the recent years, some Himalayan m plants *Bergenia ligulate*, *Trillium govanianum* (V al. 2024), *Ocimum kilimandscharicum* (Singh et a and *Phlomis bracteosa* (Rana et al. 2024) have al utilized for the silver nanoparticle synthesis. The mechanism of nanoparticle antibacterial activity ha be determined. However, literature suggests some p pathways, including silver nanoparticle interacti membrane and intercellular contents, as well as th tion of reactive oxygen species (ROS) and Ag^+ ion

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ORIGINAL PAPER

Comparative study of electrical and dielectric properties of Ho/Y ions modified Ba-Co-Sr Z-type nanohexaferrites

Kirti Singha[1] · Rohit Jasrotia[2,3] · Jahangeer Ahmed[4] · Saad M. Alshehri[4] · Abhishek Kandwal[5] · Monika Chandel[6] · Pankaj Sharma[7]

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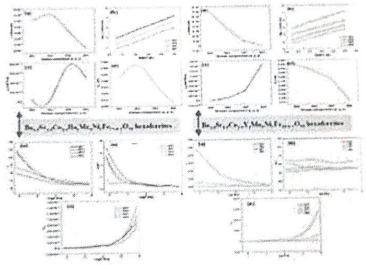
Abstract

Two different compositions of Ho^{3+} and Y^{3+} doped Ba-Sr Z-type hexaferrite having composition, $Ba_{1.5}Sr_{1.5}Co_{2-z}Ho_xMn_xNi_yFe_{24-x-y}O_{41}$ and $Ba_{1.5}Sr_{1.5}Co_{2-z}Y_xMn_xNi_yFe_{24-x-y}O_{41}$ (x = y = 0.0, 0.25, 0.50, 0.75, z = 0.0, 0.05, 0.10, 0.15) were fabricated through a sol-gel auto-combustion mechanism. Analysis of dielectric and electrical properties of both compositions was undertaken. The dc electrical resistivity of Ba-Sr hexaferrites decreased from 7.09 to 2.41 ($\times 10^7$) Ω-cm as a function of Ho-Mn-Ni doping. A similar trend is followed by Y-Mn-Ni substituted samples with lesser values for each electrical parameter. Both the compositions' activation energy was studied using the dc electrical resistivity data. The ambient temperature dielectric characteristics of the prepared hexaferrites were investigated at varying frequencies between 64 Hz to 734 KHz. With increasing frequency, it was found that both the values of loss tangent (tanδ) and the real part of permittivity (ε') decreased. The ac conductivity (σ_{ac}) remained relatively constant at the lower frequencies but increased at the higher frequencies, especially when the Ho^{3+} and Y^{3+} ions are incorporated. With these excellent electric and dielectric characteristics, the prepared compositions are highly applicable for high-frequency and antenn miniaturization usages.

Graphical Abstract



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