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Density functional theoretical study, spectroscopic characterization and molecular docking of the diuretic drug, spironolactone, adsorbed on AuNPs surface and in-vitro studies based on anticancer activity studies against A549 lung cancer cell line

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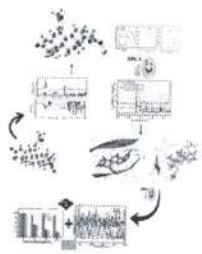
HIGHLIGHTS

- DFT calculations have been performed on the diuretic drug Spironolactone and Spironolactone adsorbed on gold nanoparticles.
- The IR, Raman, UV-Vis and SERS spectra of both the molecules were recorded to support the theoretical calculations.
- NBO, NHO, natural population analyses and HOMO–LUMO energy gap reveals the charge transfer interactions within the molecules.
- The in-silico and in-in-vitro results indicate that molecules interact with carcinoma type proteins.

GRAPHICAL ABSTRACT



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Keywords:
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ABSTRACT

In this study, the geometry, intramolecular charge transfer interactions, and harmonic vibrational frequencies of the diuretic drug, Spironolactone (SPL) and SPL adsorbed on gold nanoparticle (SPLA molecule) were investigated with the help of density functional theory method. Both molecules were found to be stabilized by intramolecular hydrogen bonds [illegible] and C_{16}-H_{47}. O_2, as well as intramolecular charge transfer interactions. These interactions were [illegible] confirmed using natural localized molecular orbitals (NLMOs) analysis. The frontier molecular orbital analysis provided a comparative picture of the reactivity, showing a low value of the energy gap, revealing electron transport in the molecule. The most reactive sites of the molecules were predicted by the molecular electrostatic potential map analysis together with the study of local and global reactivity descriptors. FT-IR and Raman spectral analysis confirmed the existence of significant hydrogen bonding, and charge delocalization in the molecules. Molecular docking performed for the biological activity

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L-Histidine with nitric acid: A comparison of crystal structures and Hirshfeld surfaces analysis

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L-histidine crystallizes [illegible] crystal structure with nitric acid, i.e. L-histidinium nitrate, L-histidinium nitrate [illegible] and L-Histidinium dinitrate. Also there is DL-histidinium dinitrate. Though the structure [illegible] nitrate monohydrate, L-Histidinium dinitrate and **DL**-histidinium nitrate [illegible] structural studies on L-histidinium nitrate is not dealt in detail. Here we have tried [illegible] the crystal structure of L-histidinium nitrate using both single crystal X-ray and [illegible]. The crystal structure consists one L-histidine molecule which has the amino and imino [illegible], but the carboxylic acid group is deprotonated. The nitrate ion is in anionic state ie [illegible]. The conformation of histidine (N1-C2-C3-C4=64.99°) is gauche (-). Also a comparison of the structure of [illegible] nitrate with other three available crystal structures retrieved using CSD have been carried [illegible] that L-histidine in L-histidinium nitrate monohydrate adopts gauche (+) conformation [illegible] three structure it is gauche (-), and L-histidinium nitrate has the lowest volume. [illegible] interaction energies analysis of all the above structures were carried out using the [illegible] nitrate monohydrate shows maximum globuarity. Interaction energy obtained [illegible] showed that L-histidinium nitrate monohydrate has maximum total energy of [illegible] of our structure L-histidinium nitrate is 0.252 indicating prolate nature unlike [illegible] complexes. The percentage of H...H contacts is maximum in L-histidinium nitrate [illegible] comparison of various contacts of histidine between the x-ray and neutron structure [illegible] maximum change is reflected in the C...H and H...H contacts with C...H having [illegible] and H...H having a lower percentage in the neutron structure indicating that the [illegible] shows the hydrogen bond interaction more accurately.

The three com[illegible] histidinium dinitrate crystallizes in a non-centrosymmetric space group and hence [illegible] optical non-linear properties, attempts were made to calculate heats of fo[illegible] polarizabilities (α) and first hyperpolarizabilities (β) using the semi empiri[illegible] using MOPAC2009 and the packing energy as implemented in MERCURY. It was [illegible] L-histidinium nitrate monohydrate was the highest amongst the three showing [illegible] for NLO material.

1. Introduction

Histidine is an essential amino acid. The side chain has [illegible] isable imidazole ring with two nitrogen's whose pKa is [illegible] the physiological pH. Based on the pH, histidine takes di[illegible] tautomeric forms. At a slightly acidic pH, the imidazole nitrogen[illegible] are protonated to form cationic imidazolium. At around [illegible] are two tautomeric forms Nε2-protonated τ tautomer [illegible]-protonated π tautomer. At mildly basic pH, there is [illegible]ne with neutral side chain [1]. Because of its tau[illegible] based on the pH values, it has been proved im[illegible]zyme catalysis [2,3], proton conduction [4,5], proton [illegible] photosynthetic complexes [7] and metalloproteins [8,9]. [illegible]ine can exist in two different polymorphs, ie monoclinic [illegible]rhombhic. Recently single crystal neutron diffraction has [illegible] to study the crystal structure of both the polymorphs [illegible] temperatures [10]. L-Histidine and Nitric acid in wa[illegible]se to three different crystals. L-histidine nitrate [11],

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Review

Recent Advances in Polymer Nanocomposites for Electromagnetic Interference Shielding: A Review

Lekshmi Omana, Anoop Chandran,* Reenu Elizabeth John, Runcy Wilson, Kalapurackal Cheriyan George, Nellipparambil Viswambharan Unnikrishnan, Steffy Sara Varghese, Gejo George, Sanu Mathew Simon, and Issac Paul*

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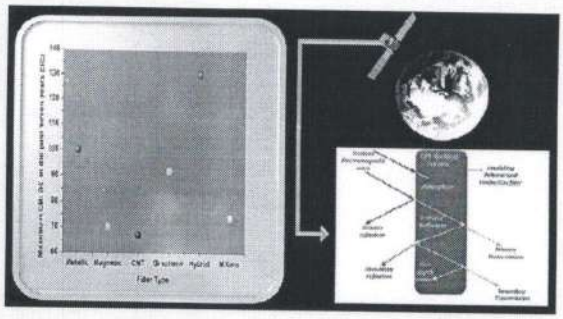
ABSTRACT: The mushrooming utilization of electronic devices in the current era produces electromagnetic interference (EMI) capable of disabling commercial and military electronic appliances on a level like never before. Due to this, the development of advanced materials for effectively shielding electromagnetic radiation has now become a pressing priority for the scientific world. This paper reviews the current research status of polymer nanocomposite-based EMI shielding materials, with a special focus on those with hybrid fillers and MXenes. A discussion on the theory of EMI shielding followed by a brief account of the most popular synthesis methods of EMI shielding polymer nanocomposites is included in this review. Emphasis is given to unravelling the connection between microstructures of the composites, their physical properties, filler type, and EMI shielding efficiency (EMI SE). Along with EMI shielding efficiency and conductivity, mechanical properties reported for EMI shielding polymer nanocomposites are also reviewed. An elaborate discussion on the gap areas in various fields where EMI shielding materials have potential applications is reported, and future directions of research are proposed to overcome the existing technological obstacles.



1. INTRODUCTION

The rapid growth of technology and proliferation of electronic devices in recent years have yielded a novel class of pollution coined as electromagnetic interference (EMI). These interferences may be mainly caused by radio frequency interference, electrostatic discharge, electromagnetic coupling, and electromagnetic conduction or induction from various sources. Besides, the introduction and development of 5G technology have also led to an increase in the presence of high-energy electromagnetic (EM) signals in the atmosphere. Mutual interference among EM radiations emitted from devices can sabotage device performance.[1] EMI has dreadful effects on electronic devices and electrical systems used in high-end applications like communication, military, medical, and remote sensing.[2−7] Since the interference of EM radiation occurs at the high-frequency radio frequency (RF) and microwave bands, they have adverse effects on the human body.[8−11] A prolonged exposure to EM radiation augments the risk of cancer, asthma, heart diseases, migraines, and even miscarriages.[12] Considering the extent of the threat EMI can cause, it is obligatory to reduce the electromagnetic radiations effectively. The practice of jamming EM radiations by means of barriers fabricated from conducting or magnetic materials is called EMI shielding.[13,14] EMI shielding of a material is understood with reference to shielding efficiency (SE) and is the ability of the material to attenuate the incident EM radiation. It can be defined mathematically as

$$SE_T(dB) = 10\log_{10}\left(\frac{P_T}{P_I}\right) = 20\log_{10}\left(\frac{E_T}{E_I}\right) = 20\log_{10}\left(\frac{H_T}{H_I}\right) \quad (1)$$

where P_I (E_I or H_I) and P_T (E_T or H_T) are the power (electric or magnetic field intensity) of incident and transmitted electromagnetic waves, respectively.[15−17] The unit of SE is prescribed as decibel (dB). EMI can be classified in two ways: one is based on its mode of propagation, and the other is based on its characteristic frequency. The mode of propagation is further classified into two: radiated and conducted interference. Radiated interference is attributed to the EM radiations emitted from any device, whereas conducted interference is the

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Changing Realities, Splattered Truths: Institutionalizing Indigeneity and its Resistance in Alexis Wright's *The Swan Book*

SUSAN ALEXANDER

Abstract

Dovetailing themes of displacement, myth, reality, a sense of belonging, attempts at assimilation and above all climate change, *The Swan Book* by Alexis Wright looks into the various aspects of aboriginal life against a background of climate change making it a novel for the future. Oblivia, the protagonist becomes a silent onlooker, a captive of her own brain, indicative of the entire aboriginal community who had to relocate and create homelands to encroach on. The process echoes with the attempts of the community to lose themselves in nature while they are forced to believe what others believed in which stands as a barometer for assimilation. The article is an attempt to trace the looming disaster of climate change, loss of culture and identity and its resistance and dispossession faced by a community.

Keywords: Aboriginal, Apocalypse, Assimilation, Displacement, Indigenous, Institutionalising.

"People on the road called her the Mother of catastrophe of flood, fire, drought and blizzard. These were the four seasons which she threw around the world whenever she liked. In every neck of the woods people walked in the imagination of the doomsayers and talked the language of extinction" (Wright 5). The flipping of weather and the creation of climate refugees among man-"the rich people flying off in armadas of planes like migratory birds" (15) and the poor people walking herd like from one place to another crossing lands and oceans, animals and birds moving from one

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Effect of Charge Transfer and Non-Covalent Interactions of the Synthesized NLO Compound p-Nitrophenol Sodium-Bisulfate Using DFT Method

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ABSTRACT

In the present work a new semiorganic single crystal p-nitrophenol sodium-bisulfate (PNSB) was synthesized and fully characterized by means of single crystal XRD, powder XRD, FT-IR, FT-Raman and UV-visible spectroscopic techniques. The optimized geometrical parameters were obtained at the DFT/B3LYP level of theory and correlate them with similar structures. Normal coordinate analysis, force constants, and potential energy distributions have been used to support the complete vibrational assignments for all vibrational modes. The computed IR and Raman frequencies correlate well with the experiments, as indicated by the correlation factor. The optimized molecular structure reveals the presence of C-H…O hydrogen bonding interaction. The stability of the molecule arising from hyper conjugative interaction and charge delocalization has been analyzed using natural bonding orbital analysis. NBO analysis proved the presence of intermolecular O-H…Na22 hydrogen bonds caused by the interaction of the lone pair of oxygen with the anti-bonding orbital. HOMO, LUMO and ESP analyses were done using DFT, whereas, the absorption band in the UV–vis spectrum was predicted and compared with the experimental data. ESP is used to identify the nucleophilic region, which is located around the sodium atom, and the electrophilic region, which is primarily located at the oxygen atoms of the PNSB molecule. The frontier orbital gap denotes the charge transfer interaction within the compound required for optical activity. Electron Localization Function, Localized Orbital Locator and Reduced Density Gradient analysis were discussed. In order to study the nonlinear optical activity of PNSB, the dipole moment, polarizability and fihyperpolarizabilities were computed. It is found that the calculated first order hyperpolarizability of PNSB is 51.75 times greater than that of urea.

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Electrostatic interactions; hydrogen bonding; hyperpolarizability; nonlinear optical crystal

Introduction

In the past few decades, there has been a growing interest in crystal growth process, particularly the increasing demand for materials for technological applications.[1,2] Nonlinear optical (NLO) materials have a nonlinear response to the electric field related with the light of a laser beam,

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