Souvenir

International Conference on Materials and Environmental Science (ICMES-2018)

December 07- 08, 2018

Jointly organized by

Shri Yashwantrao Patil Science College, Solankur

and

The New College, Kolhapur

Knowledge Partners

University Science Instrumentation Centre (USIC)
Shivaji University, Kolhapur

Department of Computer Science
Shivaji University, Kolhapur

Department of Botany
Shivaji University, Kolhapur

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MESSAGE

I am very happy to know that Shri Yashwantrao Patil Science College, Solankur and the New College, Kolhapur in collaboration with Department of USIC, Department of Botany and Department of Computer Science, Shivaji University are jointly organizing the International Conference on "Materials and Environmental Science" (ICMES-2018) on December 07-08, 2018.

I congratulate the organizers for organizing the conference on this important topic. I am sure that this conference will provide a platform for students, faculty, researchers and experts to share the knowledge and experiences of innovative techniques and there will be meaningful conversations and thought-provoking lectures from eminent resource persons. I am also confident that the deliberations during the course of conference will be very fruitful and participants will richly benefit from it.

I wish the International Conference (ICMES-2018) a grand success.

5 DEC 2018

(Devanand Shinde)
Vice-Chancellor

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Molecular structure, spectroscopic (FT-IR, FT Raman, UV, NMR and TGA/DTA) investigation and hyperpolarizability studies of (E)-1-(4-bromophenyl)-3-(2-chlorophenyl) prop-2-en-1-one

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Abstract:

A combined experimental and theoretical study on ground state molecular structure, spectroscopic and nonlinear optical properties of the chalcone derivative (E)-1-(4-bromophenyl)-3-(2-chlorophenyl) prop-2-en-1-one (2CBC) is reported. Initial geometry generated from single crystal X-ray diffraction parameters was minimized at DFT level employing B3LYP/6-311+G(d,p). The molecule has been characterized using various experimental techniques FT-IR, FT-Raman, UV-Vis, 1H NMR, Thermo gravimetric (TG) and differential thermal analysis (DTA) and the spectroscopic data have been analyzed theoretically by Density Functional Theory (DFT) method. Harmonic vibrational frequencies were calculated theoretically using the optimized ground state geometry and the spectra were interpreted by means of potential energy distribution. Time Dependent Density Functional Theory (TD-DFT) has been used to calculate energies, absorption wavelengths, and oscillator strengths of electronic singlet - singlet transitions. The calculated energy and oscillator strength complement with the experimental findings. The HOMO-LUMO energy gap explains the charge interaction taking place within the molecule. Good correlations between the experimental 1H NMR chemical shifts and calculated GIAO shielding tensors were found. The static and dynamic NLO properties such as total dipole moment (μ), mean polarizability (〈α〉), anisotropy of polarizability (Δα), total first hyperpolarizability (β) and the static second hyperpolarizability (γ) components of title molecule obtained at ω = 0.0 input frequencies at B3LYP/6-311+G(d,p) level of theory. The global chemical reactivity descriptors (GCRD) are useful tools to understand the connection between the structure, stability, and the global chemical reactivity of molecules with the help of DFT.

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Studies on Air Exposure Effect on Polythiophene Thin Films

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Abstract:

This article reports effect of air exposure on the vacuum evaporated Polythiophene thin films (includes vapor chopped and nonchopped) were studied for structural and surface morphological properties. The optical properties such as optical band gap and refractive index of the thin films were also investigated. The study of mechanical properties such as intrinsic stress and adhesion were measured using interferometric method and direct pull off method (DPO) respectively. The optical transmission loss was studied with prism coupling method. For the optical, mechanical and waveguiding properties 5 identical films for each thickness was used. The nonchopped and vapor chopped thin films were compared.

Keywords: polythiophene, thin films, optcal propertes