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materialstoday: PROCEEDINGS
Volume 44, Part 2, 2021, Pages 3032-3039

The effect of molecular twisting on electronic and transport properties of Chitosan: Ab initio approach

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Available online 12 March 2021.

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https://doi.org/10.1016/j.matpr.2021.02.439

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Impact Factor- 1.24
Year-2021
Volume-44
URL- https://doi.org/10.1016/j.matpr.2021.02.439

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Structural, Electronic and Optical properties of (P3HT)n in context of Organic Solar Cells: DFT Based Approach

Publisher: IEEE

Cite This PDF

Rahul Baghel ; Mohan L Verma ; Hemant Kumar ; Swati Verma All Authors

32 Full Text Views

ISBN:978-1-7281-5791-7
Year-2021
URL- 10.1109/ICAECT49130.2021.9392484

Abstract

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I. Introduction

II. Methodology

III. Results And Discussion

III. Conclusions

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Abstract:
With increase in energy demand, major contribution is expected to be imparted from solar energy. Also it is renewable and provides a clean source of electricity. Organic photovoltaic (OPV) offer as a promising candidate of solar energy production having attractive features like environment friendly, cheap and light-weight. This also motivated the researchers to explore new materials to design more efficient organic solar cells through enhancement in structural and electronic properties. Poly(3-hexylthiophene) (P3HT) is widely employed in field of organic electronics research, and is a representative member of material family of soluble organic semiconducting polymers.P3HT is used as a standard polymer for research in organic solar cells. In the proposed work, theoretical study is conducted to explore the structural, electronic and optical properties of P3HT polymer. The effect of the increasing the monomer units as side chain on the structural, electronic and optical properties of (P3HT)n polymer is also investigated based on DFT study.

Published in: 2021 International Conference on Advances in Electrical, Computing, Communication and Sustainable Technologies (ICAECT)

Date of Conference: 19-20 Feb. 2021

Date Added to IEEE *Xplore*: 06 April 2021

ISBN Information:
Electronic ISBN:978-1-7281-5791-7
Print on Demand(PoD) ISBN:978-1-7281-5792-4

INSPEC Accession Number: 20840468

DOI: 10.1109/ICAECT49130.2021.9392484

Publisher: IEEE

Conference Location: Bhilai, India

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IOP Conference Series: Materials Science and Engineering

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Ab-initio Modeling of Functionalized 2D-Stanene nanostructure in context of FET based Toxic Gas Sensor

Swati Verma[1], Arun Kumar[2], Hemant Kumar[3], Rahul Baghel[4], Latika Pinjarkar[5] and Mohan L Verma[6]

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IOP Conference Series: Materials Science and Engineering, Volume 1166, International Conference on Materials Science and Manufacturing Technology (ICMSMT 2021) 8th-9th April 2021, Coimbatore, India

Citation Swati Verma *et al* 2021 *IOP Conf. Ser.: Mater. Sci. Eng.* **1166** 012052

Article PDF

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DOI

https://doi.org/10.1088/1757-899X/1166/1/012052

Impact Factor- 0.51
Year-2021
Volume-1166
URL- https://doi.org/10.1088/1757-899X/1166/1/012052

ELSEVIER

Physica E: Low-dimensional Systems and Nanostructures

Volume 135, January 2022, 114962

Ab-initio modelling for gas sensor device: based on Y-doped SnS_2 monolayer

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Received 12 June 2021, Revised 24 August 2021, Accepted 1 September 2021, Available online 24 September 2021.

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https://doi.org/10.1016/j.physe.2021.114962

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Impact Factor- 3.382
Year-2022
Volume-135
URL- https://doi.org/10.1016/j.physe.2021.114962

Original Paper | Published: 25 January 2022

Effects of non-essential protein on D-glucose to control diabetes: DFT approach

Impact Factor- 1.810
Year-2022
Volume-28

Shreya Tiwary, Hemant Kumar, Deepti Pateria & Mohan L. Verma

Journal of Molecular Modeling **28**, Article number: 42 (2022) | Cite this article

Metrics

URL- https://doi.org/10.1007/s00894-021-05013-7

Abstract

Diabetes is a disease found in every 1 out of 4 people in the world. The glucose molecule is one of the sources of energy in the body and the lack of the digestion of glucose causes diabetes type 1 and type 2. Arginine and cysteine are nonessential amino acids that contain sulfur and help maintain the metabolisms of humans. We explored the glucose-arginine (Glc-arg) and glucose-cysteine (Glc-cys) molecules by finding their structural properties, electronic properties, chemical reactivity, mechanical strength, and transport properties because these non-essential amino acid molecules inhibit glucose-stimulated insulin secretion. Density functional theory (DFT) has been implemented to study all the properties of Glc-arg and Glc-cys using SIESTA software. Glucose-arginine (Glc-arg) inhibits a large percentage of glucose secretion and shows high chemical reactivity.

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