9th Semester, Center for Basic Sciences, Pt. Ravishankar Shukla University, Raipur Chhattisgarh

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

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

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Abstract

Document Sections

I. Introduction

II. Methodology

III. Results And Discussion

III. Conclusions

Authors

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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.

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

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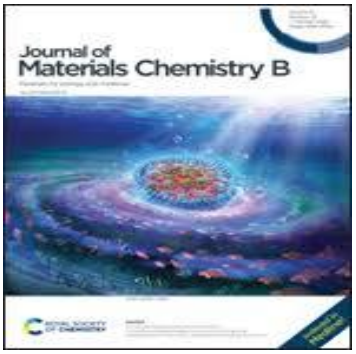

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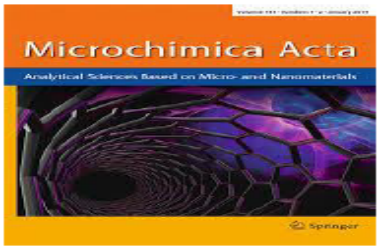

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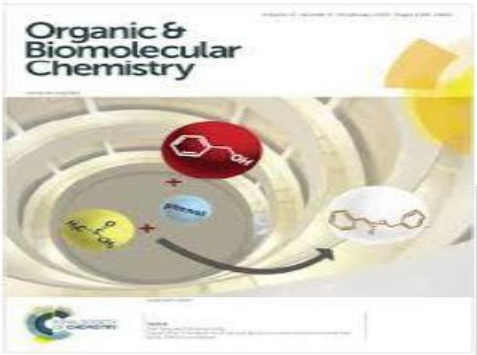

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Authors = **Kamran Ansari**, G. Pandithurai, and V. Anil Kumar

Title = Role of droplet size classes on the cloud droplet spectral dispersion as observed over the Western Ghats

Journal = Atmospheric Research

Publisher = Elsevier

Volume = 246,

Pages = 105104,

Year = 2020,

DOI = https://doi.org/10.1016/j.atmosres.2020.105104

URL = http://www.sciencedirect.com/science/article/pii/S0169809520304701

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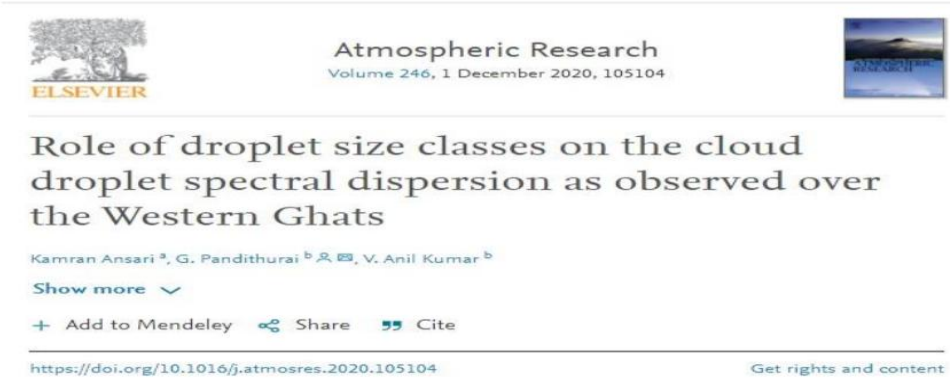

Authors = Priyanka Ghosh, Som Sharma, and **Kamran Ansari**

Title = Investigation of vertical wavenumber spectra during sudden stratospheric warming (SSW) events over the Indian region

Journal = Remote Sensing Letters

Volume = 10

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Pages = 699-708

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Publisher = Taylor & Francis

DOI = 10.1080/2150704X.2019.1601274

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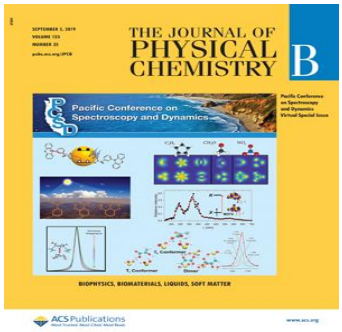

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