Exploring crystal, electronic, optical, and NLO properties of ethyl 4-(3,4-dimethoxy phenyl)-6-methyl-2-thioxo-1,2,3,4-tetrahydro pyrimidine-5-carboxylate (MTTPC)

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Abstract

Both theoretical and experimental studies are briefly discussed to shed lights on crystal shape, FT-IR, electronic, and non-linear Opto-response (NLO) characteristics of ethyl4-(3,4-dimethoxyphenyl)-6-methyl-2-thioxo-1,2,3,4-tetrahydropyrimidine-5-carboxylate (MTTHPC). Theoretical FT-IR results are in a proper concord with recorded measurements. MTTHPC has TDM (4.78 Debye) and a doublet spins that splits original FMOs into *alpha*($\uparrow$, 2.44eV) and *beta*($\downarrow$, 1.28eV) offsets, respectively. MTTHPC is a potential competitor for finest perovskite solar cells (MAPbI₃/Au-nanospheres) that possess a band offset (3.1 eV) with conversion-efficiency 24.84%. MTTHPC may be the next chapter for unique avalanche photodetectors (APD). MTTHPC 1st order hyperpolarizability is $14.15 \times 10^{-30} \text{ esu}$, surpass reference urea ($\approx 40\beta_{\text{urea}}$, $\beta_{\text{urea}} = 0.3728 \times 10^{-30} \text{ esu}$). Briefly, MTTHPC may be admitted as the next stage in forthcoming NLO technology.

Full Text

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Figures

Optimized structure for MTTHPC molecule.

Figure 2

Observed and theoretical IR charts for MTTHPC.

Figure 3

Mulliken distributions for MTTHPC charges.

Figure 4

Calculated band offsets for MTTHPC.

Figure 5

Electronic MTHPC DOS chart.

Figure 6

Figure 6 not provided with this version.

Figure 7

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