An ab initio density functional study of the optical functions of 9-Methyl-3-Thiophen-2-Yl-Thieno [3,2e] [1,2,4] Thriazolo [4,3c] Pyrimidine-8-Carboxylic Acid Ethyl Ester crystals

Abstract

An ab initio investigation of the optical constants of 9-Methyl-3-Thiophen-2-Yl-Thieno [3,2e] [1,2,4] Thriazolo [4,3c] Pyrimidine-8-Carboxylic Acid Ethyl Ester crystal is performed within a framework of local density approximation (LDA), and the Engel-Vosko generalized gradient approximation (EV-GGA) exchange correlation potentials. It is established that there are two independent molecules (A and B) exhibiting different intra-molecular interactions: C-H···O (A) and C-H···N (B). These intra-molecular interactions favor stabilization of the crystal structure for molecules A and B. It should be emphasized that there exist remarkable π-π interactions between the pyrimidine rings of the two neighbors B molecules giving extra strengths and stabilizations to the superamolecular structure. These different intra-molecular interactions C-H···O (A) and C-H···N (B) and the π-π interaction between the pyrimidine rings of the two neighbors B molecules give principal contribution to dispersion of optical properties. With a view to seek deeper insight into the electronic structure, the optical properties were investigated. Our calculations show that theoptical constants are very anisotropic. The EVGGA calculation shows a blue spectral shift of around 0.024 eV with significant changes in the spectra compared to the LDA calculation. The observed spectral shifts are in agreement with the calculated band structure and corresponding electron density of states.