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Geometrical and crystal structures, optical absorption and device characterization of *N*-(5-{[antipyrinyl-hydrazono]-cyanomethyl}-[1,3,4]thiadiazol-2-yl)-benzamide

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ABSTRACT

The molecular structure of the *N*-(5-{[antipyrinyl-hydrazono]-cyanomethyl}-[1,3,4]thiadiazol-2-yl)-benzamide (ACTB) is optimized theoretically in which the energies of highest occupied molecular orbital and lowest unoccupied molecular orbital are calculated. ACTB crystalizes in triclinic structure with a space group, *P*2. ACTB thin films were prepared by using thermal evaporation technique onto quartz and n-Si single crystal substrates. The optical properties of the films are investigated in terms of the spectrophotometric measurements of the transmittance and reflectance. The current–voltage (*I*–*V*) characteristics of the fabricated In/ACTB/n-Si/Au diode are studied in temperature range 298–398 K. The device showed rectification behavior. At low forward voltage, the thermionic theory is applied for determining the ideality factor and barrier height as a function of temperature. The series resistance of the device is found to decrease with increasing temperature. At relatively high forward voltage, the space charge limited current dominated by exponential distribution of traps is found to be the operating mechanism in which the trapping parameters and charge carriers mobility are estimated.

1. Introduction

Due to the increasing importance of organic materials in science, technology, industry and medical applications, they have been received considerable attention by researchers in different fields. They have recently been widely investigated due to simple and cost-effective processes in synthesis and application versatility owing to their flexibility and light weight. They have an interest occurrence in connection with the development of the organic optoelectronic devices, such as organic light-emitting diodes [1], solar cells [2], photodetectors [3], field-effect transistors [4] and Schottky junctions [5].

The organic/inorganic hybrid heterojunctions have attracted great attention due to the potential to become high stable devices. The inorganic semiconductors in such devices are studied in the form of thin films or single crystals. The latter has recently been focused on due to easy processing techniques. A large number of studies concerning organic/inorganic heterojunctions have been fabricated and investigated in order to benefit from advantages of both organic and inorganic materials in a single device [6–10]. The main importance of these studies originates from that the presence of organic films in such diodes may influence the basic diode parameters and electrical conduction mechanisms [10].

N-(5-{[antipyrinyl-hydrazono]-cyanomethyl}-[1,3,4]thiadiazol-2-yl)-benzamide (ACTB) compound has recently been prepared as a novel material and investigated by the authors

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[11]. ACTB showed semiconductor behavior and thermal stability up to 241 °C. This compound contains 1,3,4-thiadiazole moiety which acts as a strong electron acceptor unit and was used in molecular design of organic sensitizers [12]. This moiety is usually employed to modulate the HOMO or LUMO energy levels in optoelectronic and photophysical devices [13]. Organic materials included thiadiazole moiety are used as active materials in manufacturing devices including chemosensors [14]. Bithiophene azo dyes functionalized with thiadiazole acceptor group exhibited second order nonlinear optical properties [15]. The triazole–thiadiazole compounds possess good conjugated plane, rigid structure and various coordination sites, are theoretically suitably used as the organic ligand of the rare earth luminescent complexes [16]. Thiadiazole ring systems are extensively studied due to their properties with respect to versatile biological activities including antibacterial, antifungal, anticancer, antitubercular, and analgesic activities [17,18], and have been widely investigated for applications as bioactive compounds, lubricant additives, corrosion inhibitors, polymercross-linkers, cathode components of battery schemes and other potential applications [19–21].

The aim of this work is to study the geometrical and crystal structures of ACTB compound. The optical properties of ACTB films and the electrical properties of In/ACTB/n-Si/Au heterojunction are also investigated.

2. Experimental

The powder of ACTB was prepared by the authors elsewhere [11]. The molecular structures of the investigated compounds were optimized by HF method with 3-21G basis set. The molecules were built with the Perkin-Elmer ChemBio Draw and optimized using Perkin-Elmer ChemBio 3D software [22]. Geometry optimization option was employed to obtain the most stable structure in which transport gap is determined.

Thin films of ACTB and metal electrodes were deposited, at room temperature, onto quartz and n-Si substrates by using thermal evaporation technique. High vacuum evaporation coating unit (Edwards 306A) was used for depositing films. The vacuum of working chamber was pumped down to base pressure of 10^{-5} Pa before evaporation processes. The hot point probe showed that the ACTB films have p-type conductivity.

An inorganic semiconductors substrate, n-type Si single crystal, doped with phosphor and (100) orientation, was used for junction manufacture. The n-Si wafer was chemically cleaned by boiling in $NH_3+H_2O_2+6H_2O$ for 10 min followed by 10 min in $HCl+H_2O_2+6H_2O$ at 60 °C and finally was rinsed thoroughly in deionized water for three minutes. The native oxide on the front surface of the substrates was removed in HF/H_2O (1:10) solution and finally was rinsed thoroughly in deionized water. Right away after cleaning operation, high purity gold metal was coated the back surface of the n-Si wafer. The wafer-coated gold film was annealed at 450 °C for 10 min in argon atmosphere. Then, thin layer of

Table 1
The bond lengths for ACTB compound.

Bond lengths (Å)			
C(1)–C(2)	1.365	C(11)–S(10)	1.458
C(1)–O(8)	1.209	N(24)–N(23)	1.363
C(1)–N(9)	1.365	N(23)–C(21)	1.275
C(16)–N(17)	1.164	C(21)–C(20)	1.364
C(15)–C(16)	1.383	C(20)–C(26)	1.343
N(18)–N(19)	1.259	N(24)–C(26)	1.276
C(21)–O(22)	1.214	C(2)–C(3)	1.348
N(24)–C(25)	1.485	C(3)–C(4)	1.343
C(26)–C(27)	1.509	C(4)–C(5)	1.341
N(23)–C(28)	1.279	C(5)-C(6)	1.341
N(19)–C(20)	1.275	C(6)–C(7)	1.343
C(15)–N(18)	1.293	C(2)–C(7)	1.347
C(14)–C(15)	1.361	C(28)–C(29)	1.349
N(9)–C(11)	1.348	C(29)–C(30)	1.343
C(11)–N(12)	1.265	C(30)–C(31)	1.34
N(12)–N(13)	1.252	C(31)–C(32)	1.34
N(13)–C(14)	1.27	C(32)–C(33)	1.342
C(14)–S(10)	1.481	C(28)–C(33)	1.349

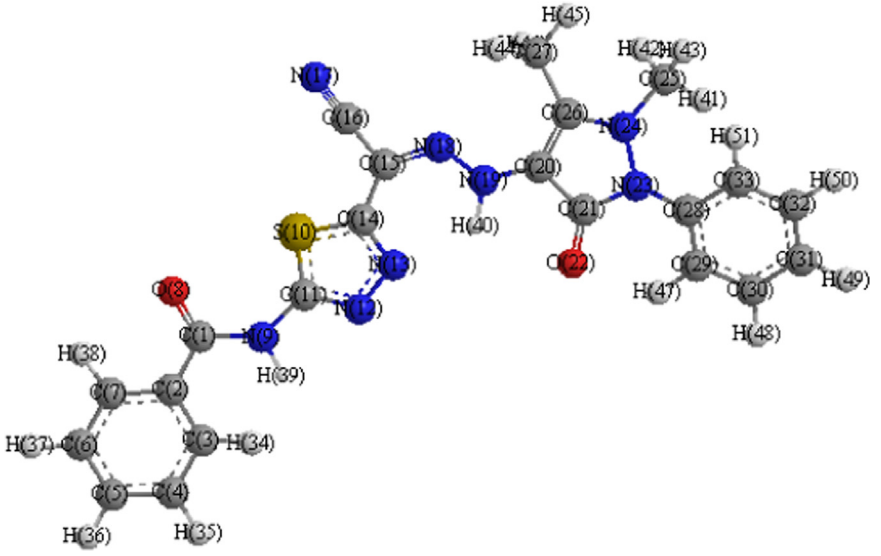

Fig. 1. The optimized structure of compound within numbering of atoms.