The Role of Thermal Energy in Carrier Detrapping and Mobility in ITO/PPV-D/Al Devices

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Abstract: The effect of temperature on the electrical properties of organic based electroluminescent structures is examined. For this purpose, thin film of organic light-emitting semiconductor (polyphenylenevinylene derivative – PPV-D) is deposited between indium-tin oxide (ITO) anode and aluminum cathode. DC current-voltage (I-V) characteristics of the fabricated devices ITO/PPV-D/Al are measured at varying ambient temperatures, ranging from room temperature (25ºC) to 70ºC. The measured characteristics are explained on the basis of the trapped space-charge-limited current theory. The predominant conduction mechanism is determined as a space-charge-limited conduction with an exponential trap energy distribution and field independent mobility in broad range of the applied voltage. Several important electrical parameters like a trap factor, free charge carriers' density, trapped carriers density and effective mobility are estimated and discussed from observed temperature dependent I-V curves. It is shown that trap factor, effective mobility and free carriers density in the organic based structure increase non-linear with increasing the ambient temperature. Such analysis of the charge transport process in polymer devices may gives information needed for optimization of the existed structures.

Key words: Charge transport, Effective mobility, Traps distribution, OLED devices, Thin films.

1. INTRODUCTION

A great number of potential applications of organic semiconductor materials for use in electronics and optoelectronics devices such as organic field-effect transistors, solar cells, organic light emitting diodes and so on are found [1]. However, degradation of these devices with respect to temperature and the aging effect are still serious problems. To improve stability together with improved performance, it is very important to have a good understanding of the physical phenomena taking place in polymer based devices such as charge transport, density of traps, mobility and other factors with respect to the temperature [2].

Poly(9,9-di-(2-ethylhexyl)-9H-fluorene-2,7-vinyle-ne) (PPV-D) is a promising organic p-type semiconductor material [3] for luminescent applications. PPV-D has attracted research attention due to its ease synthesis and relatively good environmental stability. However a very limited amount of information is available in scientific literature about the electrical properties of PPV-D and especially as a function of temperature. The electrical behavior of PPV-D above room temperature does not seem to have been reported.

Various models are applied to explain the charge transport mechanism in organic semiconductors. Among them, two models are used most frequently to explain the I-V characteristics: a) the trapping model with space-charge-limited current (SCLC) and b) the field dependent mobility model [4]. The trapping model assumes that there a certain distribution of traps, called localized states, where the free charge carriers can be trapped. The trapped carriers may be released after some period due to either temperature or other excitation and to contribute to the polymer conduction. This model is applied for relatively low voltages, where only temperature dependence of the mobility is considered and field dependent mobility is ignored. The field dependent mobility model assumes exponential dependence of mobility μ_p on the square root of electric field F. According to the Poole-Frenkel law at high voltages μ_p could be expressed as in [5]:

$$ln\,\mu_p \sim \sqrt{F}. \quad (1)$$

In this study ITO (Iindium-Tin Oxide)/PPV-D/Al structures were fabricated and characterized by electrical measurements as a function of the temperature. The observed characteristics were explained on the basis of the trapped SCLC model by assuming that the traps are exponentially distributed in energy band gap of the PPV-D. This was made for estimation of the density of traps, free and trapped carrier concentration, trap factor and their variation at different temperatures in the prepared polymer films.

The primary novelty of utilizing PPV-D within this single-layer architecture stems from its hybrid molecular engineering. Traditional light-emitting polymers frequently studied in literature, such as pristine poly(p-phenylene vinylene) (PPV) or its alkoxy-substituted derivative poly(2-methoxy-5-(2'-ethylhexyloxy)-1, 4-phenylenevinylene) (MEH-PPV), suffer from intrinsic bottlenecks. Standard PPV requires high-temperature thermal conversion of a precursor film, which frequently introduces structural defects, carbonaceous impurities, and degradation to underlying transparent conductive oxides like indium-tin-oxide (ITO). On the other hand, MEH-PPV resolves solubility

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Received on 16-05-2026 Accepted on 07-07-2026 Published on 27-07-2026

E-ISSN: 3110-9772/26

issues but possesses a flexible backbone prone to interchain aggregation and phase segregation, driving severe efficiency roll-off and a high susceptibility to thermal oxidative degradation.

PPV-D overcomes these constraints by structurally merging the highly resilient, rigid-rod polyfluorene backbone with conjugated vinylene units and long, branched 2-ethylhexyl solubilizing side-chains. The 9,9-dialkyl substituted fluorene moieties provide excellent thermal resilience, while the rigid vinylene linkage maintains a continuous π-conjugation length with highly localized, predictable HOMO-LUMO energy states. This targeted molecular functionali-zation prevents the tight, disordered π -π stacking typical of pristine PPV, drastically reducing structural trapping defects and optimizing the material for high-purity, solution-processed thin-film deposition via spin-coating. While previous research on alternative PPV derivatives focuses primarily on room-temperature photoluminescence tuning or general chemical synthesis pathways, the specific charge-transport physics of PPV-D under elevated temperatures has remained entirely unmapped. This work delivers a scientific contribution by identifying the exact conduction and detrapping boundaries of a single-layer ITO/PPV-D/Al device operating at temperatures up to 70°C.

Single-layer organic structures are notorious for charge injection imbalances, as holes typically face a much lower energy barrier than electrons when entering from the ITO anode. By performing a rigorous temperature-dependent current-voltage evaluation using the trapped Space-Charge-Limited Current (SCLC) theory, this study successfully separates field-driven transport from thermally activated transport.

2. PREPARATION OF THE ORGANIC STRUCTURES

In this work a highly pure form of commercially available yellow-orange emitting color PPV-D was used for the fabrication of the films. Fig. (**1**) shows its molecular structure. The solution with concentration 8 mg/ml was prepared in chloroform at room temperature (25°C). The polymer film was deposited on spin-coater at angular speed 1100 reverses per minute for spinning time of 40 seconds onto ITO covered glass. ITO film with thickness of approximately 180 nm was grown by vacuum reactive RF sputtering. Finally, aluminum cathodes were deposited on organic layers by vacuum thermal evaporation via shadow mask, which results in the formation of light-emitting areas 2mm×3mm. Details for the electrodes deposition conditions are given in [6]. The PPV-D thickness was about 100 nm measured by profilometer. Before measuring, copper wires (Cu) were led out from the two electrodes by using high conductive silver (Ag) adhesive. Cross-section view of a finished structure is shown on Fig. (**2**).

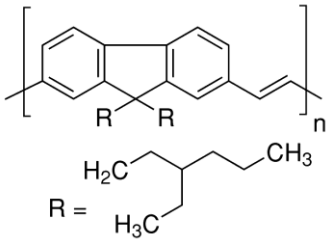

Figure 1: Molecular structure of the used light-emitting polymer.

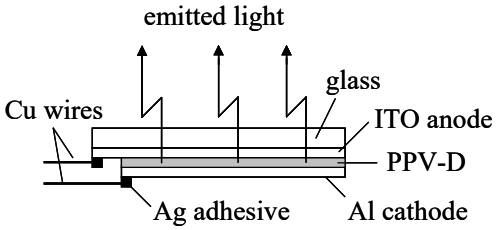

Figure 2: Cross-section view of the ITO/PPV-D/Al structure.

3. METHODS FOR INVESTIGATION OF THE PREPARED ORGANIC STRUCTURES

The exponential trap distribution model was first proposed by Mark and Helfrich [7]. It was assumed that the free carrier concentration p_o is much less than the trapped carrier concentration p_t and the trap distribution h as a function of energy E is given as:

$$h(E) = \frac{N_t}{E_c} exp\left(-\frac{E_t}{E_c}\right), \quad (2)$$

where N_t is the density of traps, E_t is energy of discrete local level and E_c is the characteristic constant expressed as characteristic temperature T_c, $E_c=kT_c$, where k is the Boltzmann constant. Traps are locations arising from damaged chain bonds in the polymer or impurities and are called localized states that very often capture free charge carriers, playing a very important role in the conduction process of a polymer [8]. Photoluminescence and electroluminescence spectroscopies are commonly used to determine the trap presence in organic materials. Based on the exponentially distributed traps theory, at given voltage V the current I through a polymer layer having thickness d, relative permittivity ε_s and density of states in the valence band N_v is given [9] by

$$I = q^{1-l}.\mu_p.N_v.\left(\frac{2l+1}{l+1}\right)^{l+1}.\left(\frac{l\varepsilon_s}{(l+1)N_t}\right)^{l}.\frac{V^{l+1}}{d^{2l+1}}, \quad (3)$$

where $l = T_c/T$ and T is absolute temperature, q is electrical charge. With other words I-V characteristics may follow the dependence $I \sim V^m$, where $m = l+1$. Thus, the experimental I-V characteristics may be used to

determine the electrical parameters of a conducting polymer by employing (3) to its different regions of operation.

3. EXPERIMENTAL RESULTS AND DISCUSSIONS

The prepared structures were investigated by measurement of I-V characteristics at different ambient temperatures. For this purpose, the samples (OLEDs) were put in thermostat chamber. The temperature regulation circuit consists of contact thermometer (CT) and circuit closer (K1), which switch over the heater in the chamber. The range of the controlled temperatures is from room temperature (25°C) only to +70°C, because the polymer degrada-tion temperature is approximately 80°C. The prepared ITO/PPV-D/Al structures were attached to the apparatuses with Teflon wires, holding out against high temperatures and don't allowing inducting of disturbances. The temperature-dependent current-voltage characteristics were measured in the thermostat chamber evacuated to a base pressure of 10^{-3} mbar to prevent oxygen and moisture degradation of the PPV-D layer. The sample temperature was regulated using a PID-controlled heating element with a Pt100 temperature sensor, ensuring a thermal stability of ±1.5°C during each measurement sweep. Prior to the experimental runs, the measurement setup was calibrated using a standard reference resistor, and the open-circuit leakage current of the system was verified to be below 10^{-13} A, which is well below the minimum experimental current levels reported here.

The block diagram of the test circuit is shown on Fig. (**3**). For measurement of the I-V characteristics was used regulating voltage source with working range from 0V to 12V. The adjustment of the voltage applied to the device electrodes was realized by voltage attenuator consist of reference voltage source E_G, multi-turn trimer - potentiometer R_p and voltage follower with precise operational amplifier OP177 (from Analog Devices). The voltage and current measurement was realized, respectively with digital voltmeter VC820 (from Voltcraft) with accuracy 4 ½ digits and precise picoampermeter BM545 (from Tesla).

The obtained I-V characteristics as a function of temperature for ITO/PPV-D/Al devices are shown on Fig. (**4**). They considered a forward bias operation, since light-emission, which is on interest arises in forward turn-on state. It is evident from the figure that the electrical response strongly varies with tempera-ture. In the low voltage Region 1 under 80mV (R1), a negligible amount of current is flowing. A zoomed view of R1 showed that the characteristics are almost linear. At higher voltages (above ~ 100mV) the current follow $I \sim V^2$ (square law in Region 2 (R2)), indicating presence of space-charge-limited conduc-tion [10]. Lampert's theory of SCLC predicts that valuable information could be obtained from I-V characteristics of organic semiconductors while opera-ted in R2 [11]. For this region equation (3) is transformed to

$$I = \frac{9}{8}\varepsilon_s \theta \mu_p \frac{V^2}{d^3}, \quad (4)$$

where θ represents the trap factor, which is defined as the ratio of free hole/electron concentration p_o/n_o to the total carrier concentration (p_o+p_t) or (n_o+n_t) and for a p-type polymer film is

$$\theta = \frac{p_o}{p_o+p_t}, \quad (5)$$

where p_t is concentration of trapped charge carriers.

The defects in the films influence the overall device operation, by acting as luminescent quenching centers [12]. They also could cause charge misbalance and moving of the recombination zone out of bulk of the electro-luminescent polymer.

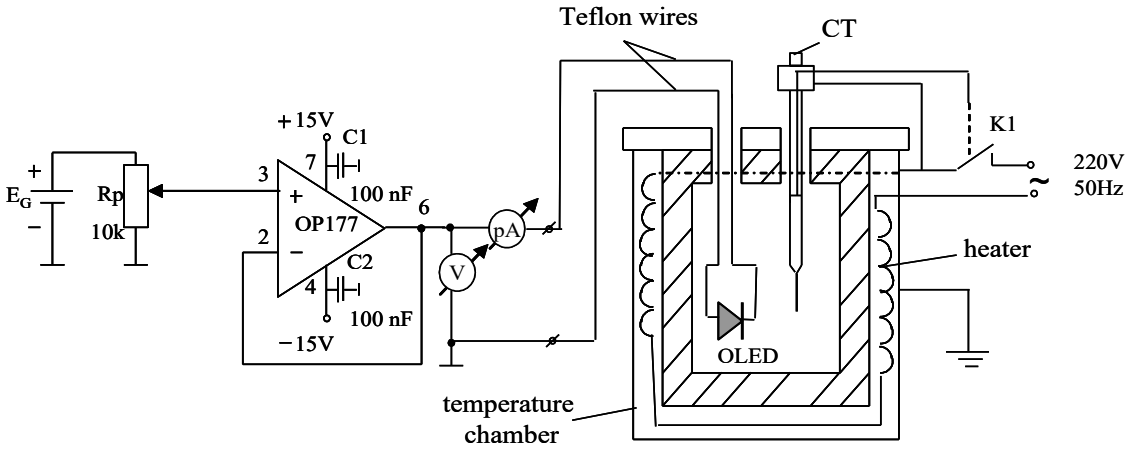

Figure 3: Block diagram of the test circuit for I-V characteristics measurement as a function of the temperature.

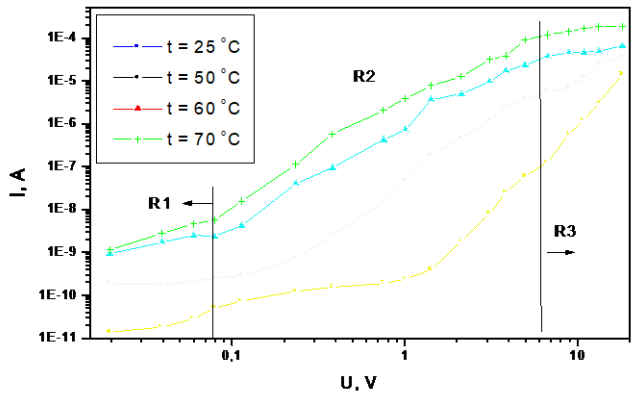

Figure 4: I-V characteristics of ITO/PPV-D/Al organic electro-luminescent structure at different temperatures from 25 °C to 70 °C.

The temperature sweeps in this work were restricted to a maximum of 70°C to prevent irreversible thermal degradation of the polymer light-emitting structures. While the purely chemical decomposition of PPV-based polymers typically occurs well above 300°C, the practical operational limit of the device is dictated by its glass transition temperature T_g, which lies in the range of 80°C - 100°C. Approaching or exceeding it triggers severe morphological relaxation of the spin-coated PPV-D matrix, leading to polymer chain rearrangement. Furthermore, at temperatures above 70°C, literature indicates that degradation is accelerated via thermally activated diffusion of aluminum atoms from the top cathode into the organic layer and accelerated oxidation. Therefore, 70°C represents the safe upper threshold for maintaining stable, reproducible, and non-destructive SCLC characterization cycles without inducing device failure.

Experimentally, the value of trap factor θ could be calculated from the ratio of currents I_1 and I_2 at the beginning and end of square law regions respectively for each characteristic. The results for θ obtained at different temperatures are summarized in Table **1** and are illustrated on Fig. (**5**).

Table 1: Calculated Trap Factor θ Refer to ITO/PPV-D/Al Structures at Different Temperatures

T, °C	I_1,m A	I_2,m A	$\theta.10^{-3}$
25	2.10^{-7}	2.10^{-3}	0,1
50	4.10^{-7}	3.10^{-3}	0,15
60	2.10^{-6}	1.10^{-2}	0,2
70	6.10^{-5}	7.10^{-2}	0,85

The initial value of the trap factor increases gradually with the temperature and after that there is a steep increase (occurring at about 60°C). This may be attributed to the fact that at higher temperatures more trapped charge carriers released from their localized states and play a role in the conduction process as free carriers in the PPV-D film.

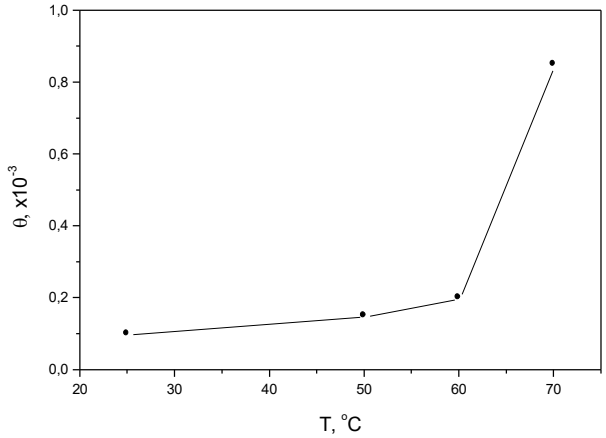

Figure 5: Variation of the trap factor with the temperature for ITO/PPV-D/Al device.

Using (4) and assuming θ=1, the variation in μ_p as a function of temperature was evaluated from the observed characteristics and plotted in Fig. (**6**). A dielectric constant ε_s=3 was used for PPV-D in the calculations [13]. The voltage was chosen in the SCLC region. A value of 4V was used, as all characteristics at the different temperatures are in SCLC regime for this voltage. Figure (**6**) also shows the variation of effective mobility μ_{eff} obtained by incorporation the trap factor. All numerical results are summarized in Table **2**. The effective mobility, which include the trap factor is less than mobility of a pristine (trap free) organic semiconductor. The effective mobility can be expressed as [9]

$$\mu_{eff} = \mu_p \theta = \mu_p \left[\frac{p_o}{p_o + p_t}\right]. \quad (6)$$

Table 2: Calculation of Mobility and Effective Mobility for PPV-D Film

T, °C	I, mA	μ_p, cm²/V.s	μ_{eff}, cm²/V.s
25	2.10^{-3}	$5,37.10^{-2}$	$0,537.10^{-5}$
50	3.10^{-3}	$43,89.10^{-2}$	$6,58.10^{-5}$
60	1.10^{-2}	$329,21.10^{-2}$	$65,84.10^{-5}$
70	7.10^{-2}	1024.10^{-2}	$870,40.10^{-5}$

The field-dependent mobility effects, typically described by the Poole-Frenkel model, were neglected in the calculations. This assumption is justified because the maximum electric field reached in the experiments does not exceed 1.2×10^5 V/cm. In this moderate field regime, the observed steep increase in current density $I \infty V^m$, where $m > 2$, is heavily dominated by the rapid filling of exponential trap states rather than a field-activated change in charge carrier drift velocity. Therefore, the standard trap-limited SCLC model remains highly accurate for these operating parameters.

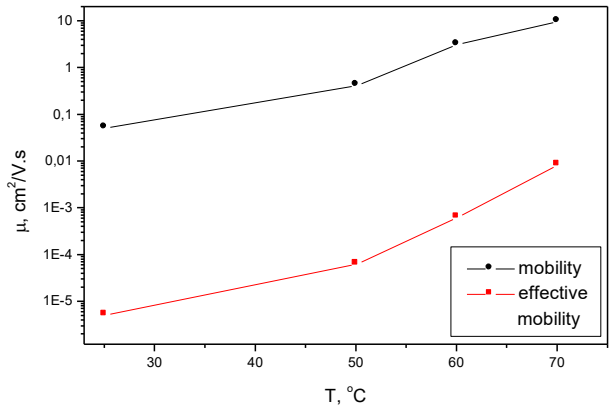

Figure 6: Variation of effective mobility and trap-free mobility with respect to temperature for PPV-D film.

The hole mobility in the organic semiconductors at room temperature is lower than those at inorganic, because of the intra- and intermolecular bonds and conductivity mechanism. Charge transport process in organic semiconductors is dependent on π-bonding orbitals and their overlap and is referred to hopping transport [14].

To ensure statistical reliability and evaluate device-to-device reproducibility, a batch of 5 identical structures was fabricated and tested under identical conditions. The relative standard deviation of the measured current among different devices did not exceed 5.5%. The results are summarized in the Table **3**.

Table 3: Error analysis and standard deviation averaged from 5 identical devices.

T, °C	$\theta\times10^{-3}$	SD ($\theta\times10^{-3}$)	$\mu_{eff}\times10^{-5}$ (cm²/V.s)	SD ($\mu_{eff}\times10^{-5}$)
25	0.10	±0.0055	0.537	±0.0295
50	0.15	±0.0083	6.580	±0.3619
60	0.20	±0.0110	65.840	±3.6212
70	0.85	±0.0468	870.4	±47.8720

Fig. (**7**) shows the variation of p_o and p_t as a function of the temperature. These variables were calculated using the transition voltage V_{tr} [15] between linear region R1 and square law region R2 (represented on Fig. (**4**)) and the trap factor.

Region 1, shown on the I-V characteristic (Fig. **4**) is mainly associated with p_o, having linear behavior. The current in that region is therefore defined by taking $l = 0$ in (3), which was reduced to

$$I = q\mu_p p_o \frac{V}{d}. \quad (7)$$

Different conduction mechanism may arise, because of the energy states available in the conjugated organic semiconductors. It is a known fact that the charge transport mechanism in organic materials and devices depends on localized and extended states (or shallow and deep traps) [4]. Both of these states are involved in defining of the current flow through the sample. At higher temperature, the free carriers trapped in the localized energy states may acquire sufficient energy to leave the localized traps and enter into extended energy states, thus contributing into the current. As it is shown on Fig. (**7**), the concentration of free charge carriers increases considerably at higher temperatures, resulting in a corresponding decrease in trapped carrier concentration in the localized states. The traps, which could be present due to impurity or structural defects restrict the charges inside the energy band gap and hence affect the overall hopping process. When temperature increases, it is assumed that the charge is exited and may jump from a localized to an extended state. This could explain the observed higher current at high temperatures in PPV-D based structure depicted in Fig. (**4**). As the trap factor is a ratio between p_o and (p_o+p_t) it therefore also increase with the temperature as is shown in Fig. (**5**). The mobility of free carriers decreases in the presence of traps and the effective mobility is smaller than the ideal case for certain organic materials. Increasing of the mobility by increasing the temperature may be associated to the energy of the carriers, which is now high enough to allow them to move without falling into a trap.

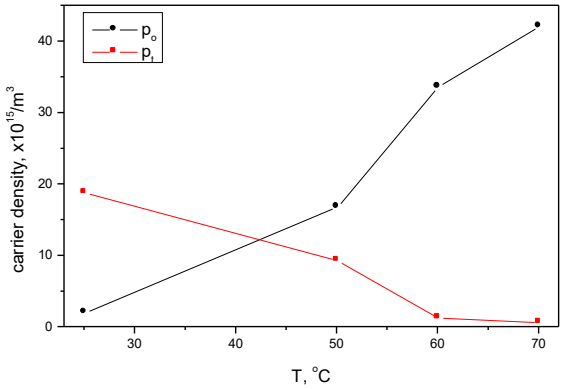

Figure 7: Variation of free carrier density p_o and trapped carrier density p_t for PPV-D film as a function of temperature.

4.CONCLUSIONS

The presence of defects in organic based structures modifies their electrical properties. The identification of the mechanisms that dominate charge transport processes in polymer devices may provide the necessary background for the development of new device structures or the improvement of the existing ones. It was applied here a practical approach for analysis of the experimental results obtained from DC conductivity measurements that makes possible the

determination of the parameters, characterizing the charge transport in polymers light-emitting devices. The carrier detrapping from the traps is stimulated by thermal energy supply in the range 25 ÷ 70°C. It was observed that these devices are nonlinear and the measured characteristics were explained assuming a hopping of free carriers between the energy states presented in the organic film. By applying the trapped space-charge-limited current model on the received I-V curves, the conduction mechanism and different electrical parameters such as trap factor, effective mobility, free carrier density and trapped carrier density were determined and their temperature dependence was investigated. The data showed that trap factor, effective mobility and free carrier density increase with the temperature increasing. This may be associated with increased rate of detrapping of carriers after acquiring sufficient thermal energy, which allows them to hop from one state to another while moving towards opposite electrodes.

In conclusion, this work provided a comprehensive analysis of the temperature-dependent charge transport mechanisms in ITO/PPV-D/Al thin-film structures using the space-charge-limited current (SCLC) model. The effective charge carrier mobility was found to be strongly temperature-dependent, increasing by more than three orders of magnitude. Ultimately, these major quantitative findings deliver crucial parameters required for numerical device modeling. By identifying the exact energetic distribution of traps and thermal detrapping thresholds, this study provides actionable baselines for optimizing charge injection balance, reducing power consumption, and mitigating trap-induced efficiency roll-off in next-generation organic optoelectronic and thin-film memory devices.

The observed temperature- and field-activated carrier detrapping behavior holds significant promise for specific thin-film electronic applications. In organic non-volatile memory devices (such as charge-trap transistors and memristors), controlling the detrapping threshold voltage and thermal activation energy is critical for adjusting data retention times and programmatic rewrite cycles. Additionally, the high sensitivity of the detrapping process to external thermal stimuli makes these PPV-D layers viable candidates for low-cost, flexible organic temperature sensors or thermal switches. Finally, in the context of OLEDs and organic photovoltaics (OPVs), a deep understanding of detrapping mechanisms allows engineers to model and mitigate long-term efficiency roll-off and device aging, which are traditionally caused by charge accumulation in deep electronic traps over prolonged operational periods.

FUNDING STATEMENT

This research received no specific grant from any funding agency in the public, commercial, or not-for-profit sectors.

CONFLICT OF INTEREST

The author declares no conflict of interests.

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https://doi.org/10.66000/3110-9772.2026.02.05