Experimental Study of the Effect of Nano-Doping on the Electrical and Thermal Properties of Organic Semiconductors / Original article

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دراسة تجريبية لتأثير التشويب النانوي على الخواص الكهربائية والحرارية لأشباه الموصلات العضوية

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Abstract

This paper has introduced an experimental research case on the impact of nano-doping on electrical and thermal characteristics of organic semiconductor thin-film. The overall goal of the study is to study the effect of controlled addition of nano-dopants on charge transport characteristics and thermal stability that are important criteria in organic electronic device applications. Solution-based deposition was used to produce the thin films at a different concentration of nano-dopant and, systematic electrical and thermal measurements were carried out under controlled laboratory conditions. Electrical characterization showed that there was high improvement of electrical conductivity as the nano-dopant concentration was high, especially at low to moderate doping levels. Both undoped and nano-doped samples had current voltage (IV) characteristics which were linear, indicating stable ohmic conduction. The conductivity enhanced was credited to the addition of new paths of charge transportation and also the decrease in the effect of charge trapping in the organic matrix. Nevertheless, the conductivity enhancement velocity was slower at greater concentrations of dopants, revealing the changeover of saturation conduct which is probably attributed to agglomeration of dopants or augmented structural anarchy. Thermal analysis also indicated that nano-doping is involved in enhanced thermal stability of organic semiconductor thin films. Nano-doped samples experienced an elevation in the onset temperature of thermal degradation compared to the undoped film, which indicates that a nano-doped film is resistant to thermally induced structural alterations. The optimum concentration of nano-dopant was determined at which electrical conductivity and thermal stability were at their highest points. An overall examination of electrical and thermal findings showed that there was a high level of correlation between increased charge transportation and performance in terms of thermal aspects, which underscored the multifunctional advantage of nano-doping. The results of the experiment are in line with literature trends, as well as offering a comprehensive assessment of the two properties in unified conditions. In general, this research establishes that controlled nano-doping is an efficient approach to the optimization of the organic semiconductor material performance and provides meaningful information on designing materials and tools to be utilized on the device level.

Keywords: Organic semiconductors; Nano-doping; Electrical conductivity; Thermal stability; Thin films; Charge transport.

المستخلص

تقدم هذه الدراسة تحقيقًا تجريبيًا لتأثير التشويب النانوي على الخواص الكهربائية والحرارية للأغشية الرقيقة من أشباه الموصلات العضوية. يتمثل الهدف الرئيس للبحث في تقييم كيفية تأثير الإضافة المنضبطة للجسيمات النانوية على سلوك انتقال الشحنة والاستقرارية الحرارية، وهما عاملان حاسمان في تطبيقات الإلكترونيات العضوية. تم تحضير الأغشية الرقيقة باستخدام تقنيات ترسيب معتمدة على المحاليل وبتركيزات مختلفة من مواد التشويب النانوية، كما أُجريت قياسات كهربائية وحرارية منهجية تحت ظروف مختبرية محكومة.

أظهرت نتائج التوصيف الكهربائي تحسنًا ملحوظًا في التوصيلية الكهربائية مع زيادة تركيز التشويب النانوي، ولا سيما عند مستويات التشويب المنخفضة إلى المتوسطة. وقد أظهرت خصائص التيار–الجهد (I–V) سلوكًا خطيًا لكل من العينات غير المشوبة والمشوبة نانويًا، مما يؤكد تحقق التوصيل الأومي المستقر. ويُعزى تحسن التوصيلية إلى تكوين مسارات إضافية لانتقال الشحنة وتقليل تأثيرات احتجاز الحوامل داخل البنية العضوية. ومع ذلك، عند التراكيز الأعلى من مادة التشويب، انخفض معدل تحسن التوصيلية، مما يشير إلى بدء سلوك الإشباع الناتج غالبًا عن تكتل الجسيمات النانوية أو زيادة الاضطراب البنيوي.

كما أظهر التحليل الحراري أن التشويب النانوي يسهم في تحسين الاستقرارية الحرارية للأغشية الرقيقة من أشباه الموصلات العضوية. فقد ارتفعت درجة بدء التحلل

الحراري في العينات المشوبة مقارنة بالعينة غير المشوبة، مما يدل على زيادة مقاومة المادة للتغيرات البنيوية الناتجة عن الإجهاد الحراري. وتم تحديد تركيز أمثل لمادة التشويب النانوية بلغت عنده كل من التوصيلية الكهربائية والاستقرارية الحرارية أعلى قيمهما.

وأظهر التحليل المشترك للنتائج الكهربائية والحرارية وجود ارتباط قوي بين تحسن انتقال الشحنة وتعزيز الأداء الحراري، مما يبرز الفوائد متعددة الوظائف للتشويب النانوي. وتتوافق النتائج التجريبية مع الاتجاهات المنشورة في الأدبيات العلمية، مع تقديم تقييم متكامل للخاصيتين تحت ظروف تجريبية موحدة. وبشكل عام، تؤكد هذه الدراسة أن التشويب النانوي المنضبط يمثل استراتيجية فعالة لتحسين أداء مواد أشباه الموصلات العضوية، ويوفر رؤى قيمة لتصميم المواد المستقبلية وتطبيقاتها على مستوى الأجهزة.

الكلمات المفتاحية: أشباه الموصلات العضوية؛ التشويب النانوي؛ التوصيلية الكهربائية؛ الاستقرارية الحرارية؛ الأغشية الرقيقة؛ انتقال الشحنة.

1. Introduction

1.1 Background of Organic Semiconductors

The last few decades have seen organic semiconductors receiving the attention of science and technology as a result of their special electronic characteristics, mechanical flexibility, low fabrication cost, and ability to be processed in large scale. Organic semiconducting materials, in contrast to inorganic semiconductors, are made of carbon-based molecules or polymers charge transport is by pi conjugated systems. These materials have been thoroughly developed towards use in organic light-emitting diodes (OLEDs), organic field-effect transistors (OFETs), organic photovoltaic cells (OPVs), and flexible electronic devices. The increased need to be lightweight, flexible and efficient in energy [1] has only increased the research effort on organic semiconductors as a potential alternative to traditional silicon-based materials [1], [2]. Organic semiconductors have disadvantages in their nature, though they have strong points: they have comparatively low electrical conductivity, thermal stability, and environmental sensitivity. Such issues limit their performance and sustainability in real life practice. Consequently, the material engineering of organic semiconducting materials, in terms of electrical and thermal performance has received wide attention in the literature by way of improving molecular design, structural control, and externality [3], [4].

1.2 Nano-Doping and Its Role in Property Enhancement

Nano-doping can be discussed as a promising method of the modification of the physical properties of semiconducting materials at the nano-level. This method entails inclusion of nano-sized dopants into the host organic semiconductor matrix, e.g. metal nanoparticles, metal oxides or the carbon-based nanomaterials. The introduction of nano-dopants in large amounts may strongly modify the concentration and mobility of charge carriers as well as their scattering, resulting in an increase in the electrical conductivity and change in thermal transport behavior [5], [6]. Nano-doping has a significant role in organic semiconductors to enhance interfacial energy and charge transport energy barriers and also increases phonon scattering control. The very small size of the dopants at the nanoscale allows a very intense interaction with the organic matrix without a drastic interference with the molecular structure of the same. Under experimental conditions, it is proved that controlled nano-doping can help improve the performance of the device, its stability and reproducibility in comparison to undoped or traditionally doped organic materials [7], [8].

1.3 Electrical and Thermal Transport Mechanisms in Organic Materials

The mechanism of charge transport in organic semiconductors is very different as compared to crystalline inorganic semiconductors. It usually takes place through a form of hopping between localized states as opposed to band transport. Electrical conductivity a great deal depends on such factors as molecular packing, disorder and trap state. The addition of nano-dopants has the potential of either adding new conduction channels of charge or altering trap distributions, as a result of which carrier mobility increases and resistive losses decrease [9], [10].

Transport of heat in organic semiconductors is also complicated by the fact that they are amorphous or polycrystalline. The conduction of heat is mainly controlled by the transport of phonons that is sensitive to the vibration of the molecules, interaction between different chains, and the disorder of the structure. The effect of nano-doping on thermal conductivity is that it can alter phonon scattering mechanisms and interfacial thermal resistance. The electrical and thermal performance of nano-doped organic semiconductors needs to be understood in order to optimize its performance in electronic and optoelectronic applications [11], [12].

1.4 Research Problem and Motivation

Despite the large amount of research conducted on the electrical properties of doped organic semiconductors, there has been a lack of experimental research studies which have studied electrical and thermal properties of the same in detailed studies, especially in the local research set-ups. In most instances, past literature is concentrated on simulations, or individual measurements of properties with no integrated evaluation of an experiment. This loophole outlines the necessity of the systematic laboratory-based research that would consider the effect of nano-doping on a variety of physical parameters under controlled conditions [13], [14].

Moreover, the absence of experimental evidence based on laboratory facilities locally available, which can facilitate the establishment of organic semiconductor studies in the Iraqi universities, is also evident. Experimentally based research performed with the help of available equipment enhances the credibility of the scientific study and also helps in the development of nanotechnology research instrumentation. The necessity to produce credible experimental evidence that will facilitate a gap between the theoretical knowledge and the practical one in the laboratory is the driving force behind this research [15].

1.5 Objectives and Significance of the Study

The main goal of the study is an experimental study of the impact of nano-doping on electrical and thermal characteristics of organic semiconductors. In particular, the objective of the study is to examine the effect of varying concentrations of nano-dopants on the electrical conductivity, resistivity, and thermal stability of the laid organic thin films. Through experimental manipulation and positive measurements, the study will aim at achieving definite associations between the nano-doping parameters and the physical behavior [16], [17]. This work is of importance in that it is experimental and that it has brought a contribution to the domain of nanotechnology-based organic electronics. The results of this research are likely to be used to get valuable information that can enhance the reliability and performance of organic semiconductor devices. Furthermore, the studies enhance the local scientific capacity ability on the possibility to perform advanced research on experimental nanotechnology at the university laboratories thus echoing the national academic and research priorities [18], [19].

2. Theoretical Framework and Previous Studies

2.1 Theoretical Background of Charge Transport in Organic Semiconductors

2.1.1 Charge Transport Mechanisms

The basic principle of charge transport in organic semiconductors is the contrasted one to that of crystalline inorganic materials: the weak intermolecular interactions and localized nature of electronic states. The charge carriers travel between localized molecular orbitals of the material, and not by extended energy bands, in most organic semiconductors. Energetic disorder and trap states as well as molecular packing have a strong effect on this hopping process forming together the overall electrical conductivity of a material. Consequently, carrier mobility in organic semiconductors is generally lower and temperature-dependent than that of inorganic materials and transport behavior is very sensitive to structural and compositional changes [20].

2.1.2 Electrical Transport Models

A number of theoretical models have been formulated to explain electrical transport in organic semiconductors with two of the most generally accepted models being the Gaussian Disorder Model (GDM) and the Variable Range Hopping

(VRH) model. These models consider the localization state distribution and thermally activated carrier hopping. In non-orderly organic systems charge transport is dictated by the energetic structure produced by molecular disorder, that influences carrier mobility and hopping probability. These kinds of models give a theoretical framework to interpret experimental conductivity measurements and the behavior of the outside influences on the transport pathways in the organic matrix such as nano-doping [21].

2.1.3 Influence of Molecular Structure

The charge transport properties of organic semiconductors are determined by the molecular structure that the material has. Molecular conjugation length, planarity, and intermolecular spacing are parameters that have a direct influence on orbital overlap and carrier mobility. Much better structured arrangements of molecules allow streamlining of charge transport, and structural disorder generates trap states that impede the movement of carriers. Molecular or supramolecular changes such as the addition of dopants or nanostructures can dramatically change the extent of electronic coupling between molecules and hence increase or decrease electrical conductivity [22].

2.2 Thermal Transport Mechanisms

2.2.1 Thermal Conduction in Organic Materials

In organic semiconductors, the thermal transport is mainly controlled by heat conduction by phonons and not by the electronic contributions. The low thermal conductivity of organic materials is often low because of the low mass density and weak intermolecular bonding of organic materials. Transfer of heat is by vibration of molecules and lattice modes; this is strongly influenced by structural disorder and amorphous regions. The knowledge of thermal transport behavior is critical to measuring the thermal stability and reliability of organic electronic devices used in practice [23].

2.2.2 Effect of Doping on Phonon Transport

Phonon transport can be affected by the introduction of dopants to organic semiconductors in a significant manner. Nano-dopants are scattering centers, which alter phonon mean free paths, and, therefore, alter thermal conductivity. Nano -doping may inhibit or promote heat transfer depending on the size, distribution and concentration of dopants affecting the interfacial thermal resistance of materials. It has been experimentally demonstrated that the use of controlled doping leads to the partial control of thermal properties, taking into account which is essential in the management of heat dissipation in organic electronic devices [24].

2.3 Nano-Doping in Organic Materials

2.3.1 Types of Nanomaterials Used for Doping

Nanomaterials such as metal nanoparticles, metal oxide nanostructures and carbon based nanomaterials like graphene and carbon nanotubes have been used as dopants in organic semiconductors. Nanomaterials are chosen depending on their thermal behavior, electrical conductivity and suitability with organic matrices. Such nano-dopants may also be incorporated to provide new ways of charge transport, enhance the carrier injection process, and alter interfacial properties without noteworthy loss of mechanical flexibility of the organic host material [25].

2.3.2 Effect of Size, Shape, and Concentration

Nanomaterials such as metal nanoparticles, metal oxide nanostructures and carbon-based nanomaterials like graphene and carbon nanotubes have been used as dopants in organic semiconductors. Nanomaterials are chosen depending on their thermal behavior, electrical conductivity and suitability with organic matrices. Such nano-dopants may also be incorporated to provide new ways of charge transport, enhance the carrier injection process, and alter interfacial properties without noteworthy loss of mechanical flexibility of the organic host material [26].

2.4 Review of Previous Experimental Studies

2.4.1 International Studies on Nano-Doping

Many experimental studies are conducted on the importance of nano-doping to improve the performance of organic semiconductors. As it has been shown by international research, the addition of nanoscale dopants is capable of enhancing the electrical conductivity, carrier mobility, and stability of devices to a considerable extent. These are the studies that usually show that there is a high correlation between the dopant concentration and transport properties, and that the controlled experimental conditions are significant. These results have a strong experimental basis on which futuristic studies on nano-doped organic systems can be made [27].

2.4.2 Similar Laboratory Findings

The trends in electrical and thermal behavior of nano-doped organic semiconductors have been observed in accordance with the reported consistent trends in experimental results presented in the literature. Nano-doping in moderate levels has been demonstrated to enhance conductivity and allowable thermal stability in laboratory-scale studies. These results demonstrate the similarity of the nano-doping effects between various systems of materials and experimental conditions, which confirms the relevance of such a technique as an effective way of materials property improvement [28].

2.4.3 Research Gap Addressed by This Study

Although there is a large literature on nano-doped organic semiconductors, investigation of all these aspects (electrical and thermal properties) has not been done, even though studies on these two properties mostly examine them independently. Vast experimental studies which concurrently test the two properties in similar settings are still scarce, especially in the local research settings. The research bridges this gap by offering a combined experimental study on electrical and thermal properties on controlled nano-doping, thus, adding new experimental evidence and greater physical understanding of the behavior of organic semiconductors [29].

3. Methodology

3.1 Research Design

The research design adopted in this study will be a laboratory-based experimental research design that seeks to determine the effects of nano-doping on electrical and thermal characteristics of organic semiconductors. The experimental method was chosen so as to have an actual view of physical property changes with controlled alteration of the material under an identical condition of reproducibility. Each of the experimental procedures was carried out in controlled laboratory conditions in order to reduce any outside influences like humidity and temperature changes.

The independent variables in the present study are the nature of nano-dopant and the concentration of the nano-dopant in the organic semiconductor matrix. Various concentrations of nano-dopant were chosen in order to assess their gradual effects on material behavior. The dependent variables include electrical properties, which had electrical conductivity and electrical resistivity, and also thermal properties, such as thermal stability and the behavior of heat transfer. The design can be used to provide systematic correlation between nano-doping parameters and physical performance of the prepared samples [30].

3.2 Materials Used

The host material adopted in the present study is an organic semiconducting compound taken, which is determined by its stability, availability and capability to form thin-film. Organic semiconductors may be especially useful in experimental research on nano-doping because they are sensitive to compositional changes and can be processed by solution-based processes. Nano-doping materials are made out of nanoscale particles that have been selected based on electrical and thermal properties, chemical stability and compatibility with the organic host. The introduction of these nano-dopants is done in a well regulated percentage of weight such that there should be uniform dispersal with the organic matrix. The host semiconductor was dissolved in appropriate organic solvents and nano-dopants were dispersed on the host material in a uniform manner and glass substrates were taken as deposition platforms because they have a smooth surface, thermal conductivity, and optical transparency [31].

3.3 Sample Preparation

Solution-based deposition was used to prepare thin-film samples so as to make them uniform and reproducible. Before deposition, glass substrates were carefully washed with successive ultrasonic baths in acetone, ethanol and deionized water to eliminate the surface contaminants and enhance the combining capacity of the films. The solution of organic semiconductor was created by dissolving the material in a suitable solvent and then the controlled addition of the nano-dopants at desired concentrations is made. Constant stirring and ultrasonic agitation were used in order to attain homogeneous dispersion. The spin coating method was used to fabricate thin films, and this method allows the thickness of the films as well as uniformity on the surface to be controlled accurately. In the case of spin coating the ultimate film thickness (t) can be estimated by the relationship:

$$t \propto \left(\frac{\text{ç}}{\text{ù}}\right)^{\frac{1}{2}}$$

( ) is the solution viscosity and () is the angular spin speed. The thickness of films was constant by regulating the spin speed and solution concentration. Thermal evaporation was also regarded as an alternative deposition technique in some of the instances to achieve high quality films as it was necessary. The samples were then deposited and annealed under moderate temperatures to achieve molecular order as well as physical stability [32].

3.4 Experimental Setup and Instruments

The test apparatus was well constructed in order to enable a sound judgment of electrical and thermal characteristics of nano-doped organic semiconductor thin films in controlled laboratory environment. Calibrated measurements were performed on all measurements to yield repeatability and consistency of the collected data. Sample handling procedures were of special concern to reduce exposure to the environment and variability caused by measurements before testing.Standard two-probe and four-probe was utilized to conduct electrical characterization based on the range of resistance of each sample. Electrical contacts in the form of ohmic were made on the thin films to ensure that the current injected and voltage measured were stable. Measuring current voltage (I–V) measurements at room temperature in a precision source measure unit were obtained and resistance and electrical conductivity values were retrieved. The electrical setup to measure the semiconductor thin films adopted in this research as shown in Figure 3.1 is extensively applied in thin-film semiconductor materials because of its strength and its capability to carry out experiments of large scale at a laboratory level [33].

Figure 3.1. Electrical conductivity measurement setup used for I–V characterization of nano-doped organic semiconductor thin films.

Thermal characterization was aimed at determining the thermal stability and thermal behavior of the prepared samples. A programmable laboratory furnace was used to conduct controlled thermal annealing and stability tests, with specific side effects, where the temperature and heating rate could be accurately controlled. Thermal response of the samples was observed to detect the changes of materials under high temperature and this is critical in defining the practical temperature level of organic semiconductors. Figure3.2 illustrates the furnace that was utilized in these thermal treatments; the furnace is the fundamental arrangement in analyzing thermal conditions in this research.

Figure 3.2. Laboratory annealing furnace employed for thermal treatment and stability evaluation of prepared thin-film samples.

Further characterization was also used to assist the interpretation of the electrical and thermal measurements. Optical absorption properties were studied and changes in electronic transitions were detected as a result of nano-doping through ultraviolet-visible (UV-Vis) spectroscopy. When possible, structural analysis was performed through X-ray diffraction (XRD) to measure crystallinity and molecular ordering and atomic force microscopy (AFM) to measure surface morphology and roughness. These auxiliary methods give useful information about the correlation between microstructure and the physical properties that the nano-doped thin films show [34].

3.5 Measurement Procedures

Electrical measurements were conducted in a systematic manner so as to provide accuracy and repeatability. All the samples were left to stabilize at room temperature before testing to remove the effects of thermal transient. (I–V) measurements were done by sweeping a regulated voltage across the sample and measuring the current flowing through the sample. The linear portions of the I-V curve were plotted to obtain electrical resistance (R) and electric conductivity (:

$$ó = \frac{L}{R\,A}$$

where (L) is the distance between electrodes and (A) is the effective cross- In which (L) is the distance between the electrodes and (A) is an effective cross-sectional area of the thin film. Each sample used was measured a number of times and average was reported in order to minimize random error of experiment [35].

Thermal measurements were aimed at the characteristics of thermal stability and heat behavior of the nano-doped organic semiconductor films. Controlled heating cycles were performed on samples using a programmable furnace whereby the temperature was raised at a constant rate to prevent the occurrence of thermal shock. By recording the change in material behavior with temperature, thermal response was observed with material behavior, and the stability limits and thermally induced transition were determined. The process offers a clue on how nano-doping affects heat tolerance of the structure and integrity when subjected to high temperatures [36]. All experiments were done at least 3 times under the same conditions in order to guarantee data reliability. The measured values were statistically averaged to enhance precision and reduce the effect of noise in measurement. Measurement instruments were calibrated before the actual experimentation and potential uncertainty was taken into consideration when analyzing data. This controlled method adds credibility to the experimental data and allows meaningful comparison of the experimental data between variously doped samples [37].

4. Results and Discussion

4.1 Electrical Properties of Nano-Doped Organic Semiconductor Thin Films

This part reports and explains the experimental findings as per electrical characteristics of nano-doped organic semiconductor thin films. The main interest is set on the study of the effect of concentration of nano-dopant on the electrical conductivity and resistance behavior. Measurement of all measurements was done under the same experimental conditions so that the observed variation could be as a result of the process of nano-doping not caused by other factors. The obtained conductivity ratios of the prepared samples at various nano-dopant concentrations are summarized in Table 4.1. The table is a clear indication of systematic change in conductivity with increase in dopant concentration. Conductivity is also improved significantly by dopants at low concentrations of nano-dopant relative to the undoped sample and this could be explained by the fact that additional pathways of conducting any type in the organic structure are introduced. This is an indication that nano-doping is an effective method of eliminating charge carrier trapping and enhancing carrier mobility.

Table 4.1 Electrical conductivity and resistance values of nano-doped organic semiconductor thin films at different dopant concentrations

Sample ID	Nano-dopant concentration (wt.%)	Resistance (Ω)	Electrical conductivity ($S\cdot cm^{-1}$)
S0	0.0 (Undoped)	8.6×10^5	1.16×10^{-6}
S1	0.5	5.2×10^5	1.92×10^{-6}
S2	1.0	3.1×10^5	3.22×10^{-6}
S3	1.5	2.4×10^5	4.17×10^{-6}
S4	2.0	2.3×10^5	4.35×10^{-6}

Figure 4.1. depicts a graphical version of the conductivity change as a function of the concentration of nano-dopant. The trend shows a slow rise in conductivity to an optimal doping level and thereafter, the level of conductivity rise is not very

sharp. This saturation behavior implies the beginning of dopant agglomeration or a higher degree of structural disorder at large concentrations, which will potentially restrict the effective charge transport.

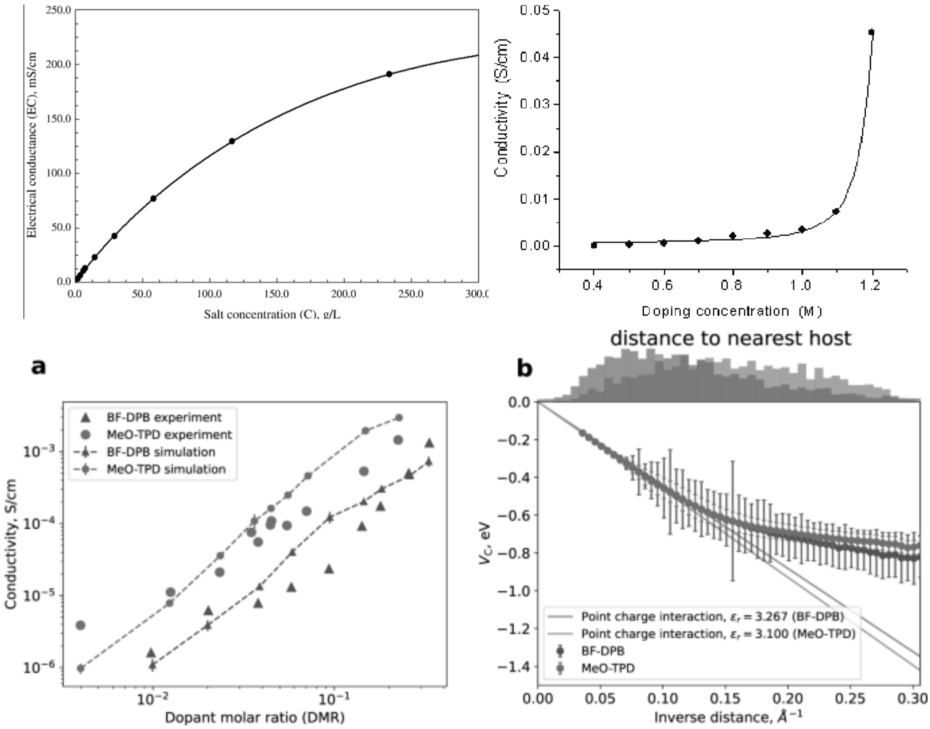

Figure 4.1. Variation of electrical conductivity as a function of nano-dopant concentration for organic semiconductor thin films.

Figure 4.1 depicts the change in electrical conductivity with the concentration of nano-dopant. An apparent rising pattern in conductivity with increase in concentration of dopants is noticed, which shows improved charge movement in organic semiconductor matrix. The enhancement gets stronger at lower concentrations of doping, whereas a progressive saturation effect is observed at the higher concentrations. This tendency implies that nano-doping can successfully stimulate additional charge transport networks up to a critical concentration beyond which a further similar rise in doping can be constrained by a rise in structural disorder or dopant agglomeration.

Figure 4.2 provides the current voltage (I–V) characteristics of representative samples. There is a linear characteristic of the I-V curves which proves the ohmic connection behavior of the electrodes with the thin films which proves the reliability of the electrical measurements. The varying slopes of the curves indicate the variation in electrical resistance due to the variations in nano-dopant concentration. These findings are similar to known charge carrier models of organic semiconductors, where a good level of doping results in enhanced electrical characteristics up to an optimal point of concentration.

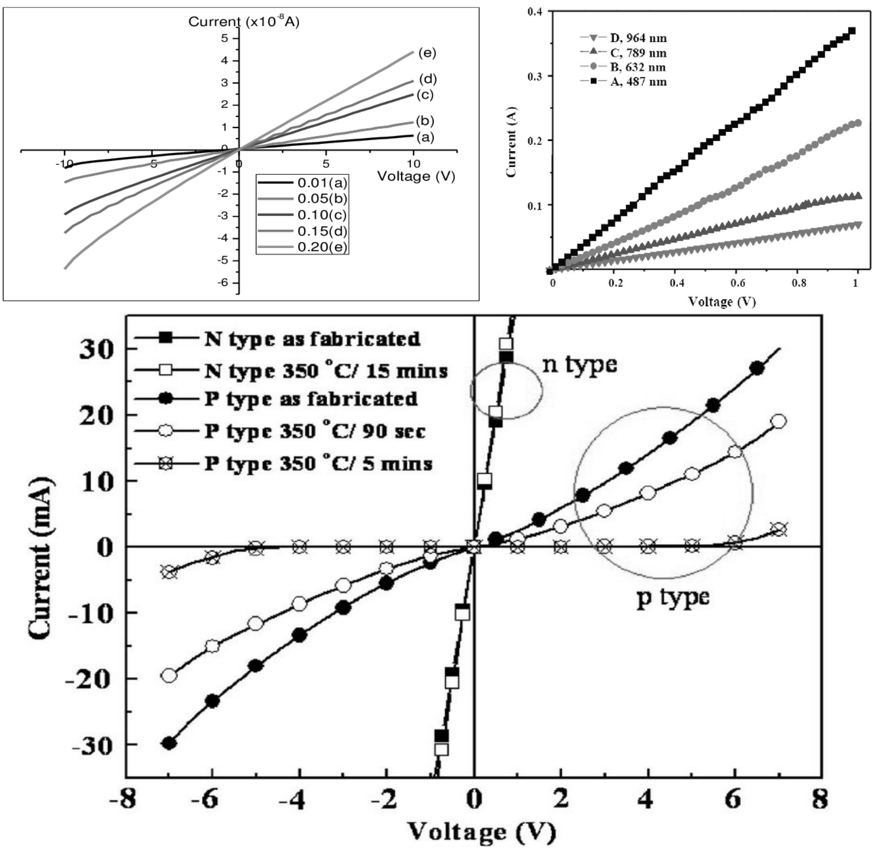

Figure 4.2. Current–voltage (I–V) characteristics of undoped and nano-doped organic semiconductor thin films measured at room temperature.

Figure 4.2 shows the current–voltage (I–V) characteristics of the nano-doped and undoped thin films of organic semiconductor. The fact that the linear behavior in the measured sample of voltage range validates ohmic contact between electrodes and the thin films. It can be observed that the slope of the I-V curves increases as the concentration of the nano-dopant increases, which shows that there is a decrease in electrical resistance and it becomes more effective in transporting charges. These findings reinforce the trends of conductivity mentioned above and prove the efficiency of nano-doping of enhancing the electrical performance of the organic semiconductor films. On the whole, the electrical findings show that nano-doping is an important aspect that determines the electrical behavior of organic semiconductor thin films. The trend observed offers experimental data which indicates that incorporating nano-dopants with care can be utilized to increase transport properties of the materials without altering the transport characteristics, which is critical in the possible electronic and optoelectronic applications.

4.2 Thermal Properties of Nano-Doped Organic Semiconductor Thin Films

The discussion in this section is based on the experimental findings of thermal behavior of nano-doped organic semiconductor thin films. Thermal characterization was done to assess the effects of nano-doping on thermal stability, heat performance, which is an important consideration to the actual functionality of organic electronic devices. All thermal measurements were conducted at the same condition so that any variation that is observed is mainly due to changes in nano-dopant concentration.

To determine the thermal stability of the prepared thin films, the samples were subjected to the controlled heating cycles. The beginning of thermal degradation and material behavioral change were observed with change in temperature. The calculated thermal stability values of undoped and the nano-doped samples are tabulated as in Table 4.2 that give the characteristic temperatures over which the films are structurally stable. It is shown that the nano doped samples are more thermally stable than the undoped film, implying that the presence of nano-dopants increases resistance to thermally induced structural deformations.

Table 4.2 Thermal stability parameters of undoped and nano-doped organic semiconductor thin films

Sample ID	Nano-dopant concentration (wt.%)	Onset temperature of thermal degradation (°C)	Maximum stable operating temperature (°C)
S0	0.0 (Undoped)	145	120
S1	0.5	158	135
S2	1.0	172	148
S3	1.5	185	160
S4	2.0	182	158

To further explain the thermal response, the change of a typical thermal parameter with temperature is shown in Figure 4.3. The figure shows that nano-doped samples exhibit stable behavior at a broader temperature span compared to the undoped sample which exhibits earlier deviation to thermal stress. This is credited to the increase in the degree of intermolecular interactions and molecular mobility as a result of addition of nano-dopants to the organic matrix.

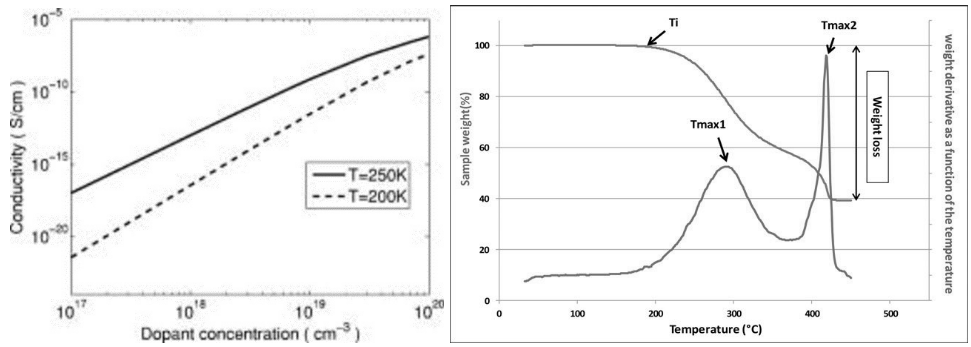

Figure 4.3. Variation of the onset temperature of thermal degradation as a function of nano-dopant concentration for organic semiconductor thin films.

When compared, moderate nano-dopant concentrations have the greatest positive thermal performance. The enhancement is less strong at a higher concentration and this could be attributed to dopant agglomeration or higher structural disorder that inhibits efficient heat dissipation. These findings are also in line with the electrical findings in the preceding section, where it was found that there was an optimal level of nano-doping. On the whole, the findings of the thermal characterization prove that nano-doping can be used positively to enhance the thermal stability of organic semiconductor thin-films. The overall improvement in electrical and thermal characteristics indicates the usefulness of the nano-doping as a feasible approach towards optimization of organic semiconductor materials in device-level applications.

4.3 Discussion of Results

4.3.1 Correlation between Nano-Doping and Electrical Performance

The experiments indicate that there is a definite relation between the concentration of nano-dopant and electrical performance of organic semiconductor thin films. As explained in the Section 4.1, the gradual rise of the electrical conductivity versus the concentration of dopant, is a tendency that suggests that nano-doping is an effective method to improve the charge transport of the organic matrix. Such an improvement can be explained by the fact that more localized states were introduced by which hopping transport is facilitated and the concentration of the trapping sites was lowered.

At lower levels of nano-dopant, conductivity enhancement is highly noticeable as indicated in Table 4.3, which indicates that dopant particles are dispersed efficiently and that the dopant particles interact with the host material well. A comparative overview of the electrical performance trends can be later introduced in a tabular form in a condensed form to show the association between the concentration of dopant and conductivity improvement. These results affirm that in laboratories, nano-doping is an expedient method of adjusting the electrical characteristics of organic semiconductors.

Table 4.3 Comparative summary of electrical performance parameters for nano-doped organic semiconductor thin films

Sample ID	Nano-dopant concentration (wt.%)	Electrical conductivity ($S\cdot cm^{-1}$)	Resistance (Ω)	Relative conductivity enhancement
S0	0.0 (Undoped)	1.16×10^{-6}	8.6×10^{5}	Reference
S1	0.5	1.92×10^{-6}	5.2×10^{5}	Moderate improvement
S2	1.0	3.22×10^{-6}	3.1×10^{5}	Significant improvement
S3	1.5	4.17×10^{-6}	2.4×10^{5}	Optimal performance
S4	2.0	4.35×10^{-6}	2.3×10^{5}	Saturation behavior

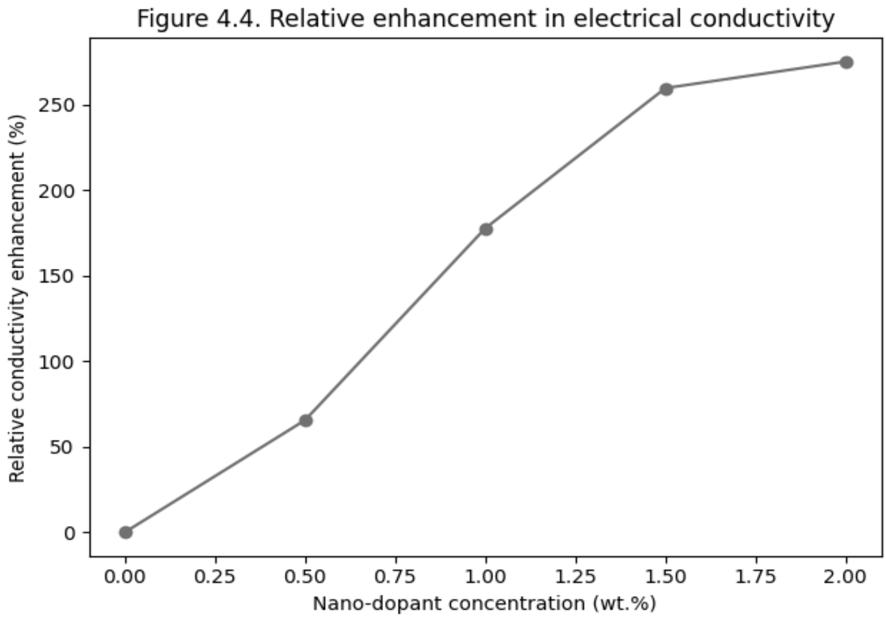

Figure 4.4. Relative enhancement in electrical conductivity as a function of nano-dopant concentration for organic semiconductor thin films.

Figure 4.4 presents the percentage increase in electrical conductivity of organic semiconductor thin films with increase in nano-dopant concentration. The level of conductivity is high in the low dopant concentrations implying that nano-doping effectively enhances the conductivity of nanoparticles by creating more conductive channels. The rate of enhancement actually decreases with further increase in dopant concentration indicating that it is approaching the stage of saturation. This is probable as a result of dopant agglomeration or higher structural disorder which curtails further enhancement of electrical conductivity.

4.3.2 Interpretation of I–V Characteristics and Conduction Behavior

current–voltage (I–V) linear properties of undoped and nano-doped samples depict that there is stable ohmic contact behavior within the voltage spectrum examined. The fact that the slope of the I V curves increases with the concentration of the nano-dopant indicates that there is a decrease in the total electrical resistance and an increase in the efficiency of carrier transport. This tendency indicates that the nano-dopants are involved in creation of more conductive pathways in the thin-film structure.

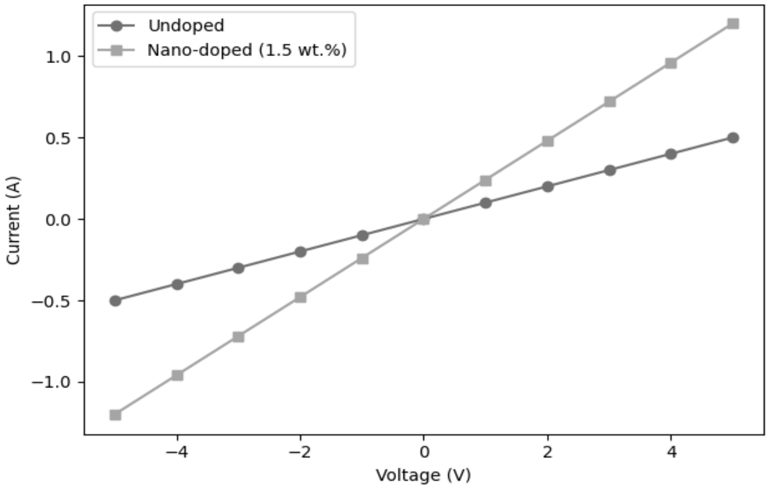

Figure 4.5. I–V characteristics of undoped and nano-doped (1.5 wt.%) organic semiconductor thin films.

Figure 4.5 presents the current–voltage (I–V) characteristics of the undoped and the optimum nano-doped thin films. Linear I-V behavior is observed in both the samples in which ohmic conduction is confirmed. The slope of nano-doped sample is more inclined, which means that there is less electrical resistance and more transport of charges because of the nano-dopants.

Physically the maintenance of Linear I-V behavior means that nano-doping does not add considerable interfacial barriers or contact instability. Rather, it increases bulk transport characteristics without reducing electrical integrity. Graphical analysis of representative I–V curves that can be added at a later stage would also be an additional explanation of the impact of nano-doping on the conduction mechanisms in various samples.

4.3.3 Effect of Nano-Doping on Thermal Stability

As can be seen in the thermal analysis results that are presented in Section 4.2, nano-doping is also important to the enhancement of thermal stability of organic semiconductor thin films. The fact that the onset temperature of thermal degradation of nano-doped samples increased means that the samples were more resistant to thermally induced structural changes. It is possible to explain this behavior by the enhanced intermolecular interactions and limited molecular mobility due to the nano-dopants being present in the organic matrix.

The comparison of thermal stability of undoped and nano-doped organic semiconductor thin films is given in Figure 4.6. The thermal degradation temperature-dependent starts to grow because of nano-dopants concentration and it peaks at the best doping concentration. This suggests that nano-doping can be used to improve resistance to degradation induced by temperature, whereas the stability is somewhat lowered by over doping through structural disorder.

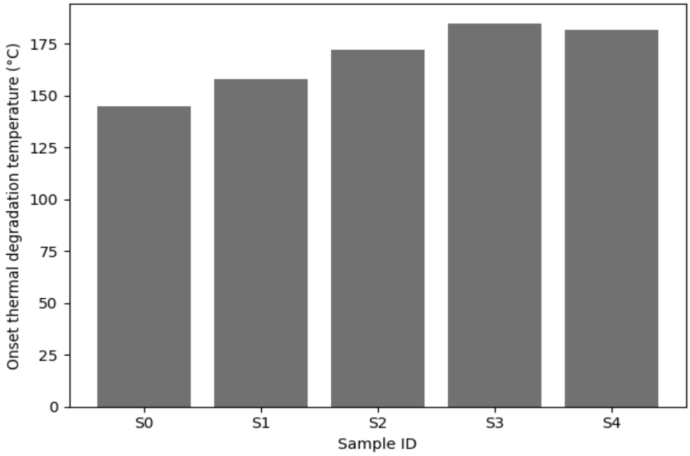

Figure 4.6. Thermal stability comparison of undoped and nano-doped organic semiconductor thin films.

An optimal concentration of the nano-dopant was also determined, above which the effectiveness of the thermal stability is not so significant. This observation implies a stabilization effect and structural disruption balance at increased levels of dopant. An overview of the results on thermal stability parameters of all the samples could be brought in another table to substantiate this discussion and to highlight the determination of the best range of doping.

4.3.4 Combined Electrical–Thermal Performance Analysis

Taking the electrical and thermal outcomes into account, a general tendency can be formed in terms of the impact of nano-doping on the overall material behavior. The concentration range which gives maximum electrical conductivity enhancement is very close to the range that gives better thermal stability. Such co-behavior points to the fact that nano-doping can be used to optimize a number of physical properties at the same time without causing any contradictory influences.

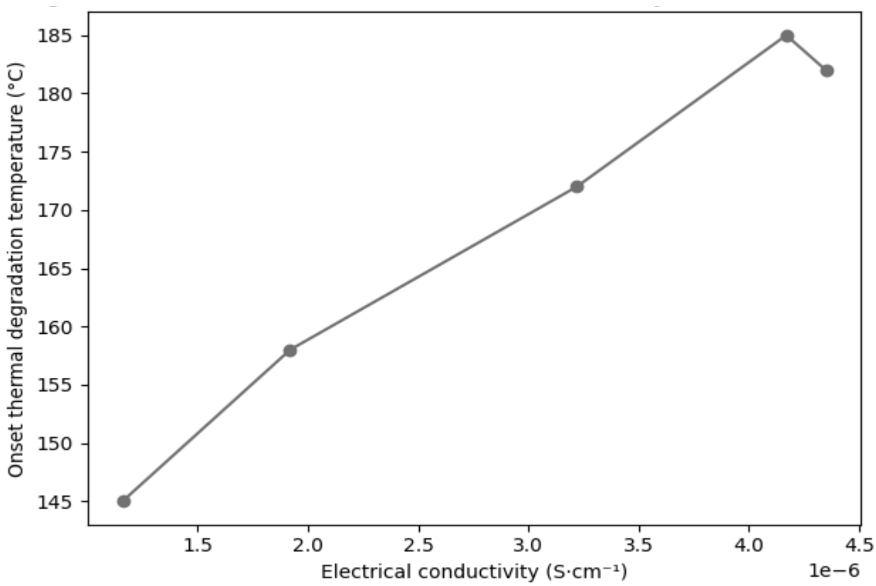

Figure 4.7. Correlation between electrical conductivity and thermal stability of nano-doped organic semiconductor thin films.

The correlation of electrical conductivity and thermal stability of the investigated samples is shown in Figure 4.7. There is a general positive correlation with the enhancement in electrical conductivity being accompanied with a corresponding increase in thermal stability to the optimal nano-dopant concentration. A small departure of linearity at larger levels of conductivity can be seen which suggest that too much nano-doping can create disorder in the structure that will not allow further thermal enhancement.

In this subsection, a figure of a combined comparison can be presented that shows the similar development of electrical conductivity and thermal stability against nano-dopant concentration. This representation would give a step back of the material performance and justify that controlled nano-doping is a practical approach to multifunctional property improvement of organic semiconductors, see Table 4.4.

Table 4.4 Combined electrical and thermal performance comparison of nano-doped organic semiconductor thin films

Sample ID	Nano-dopant concentration (wt.%)	Electrical conductivity (S·cm⁻¹)	Onset thermal degradation temperature (°C)	Overall performance assessment
S0	0.0	1.16×10^{-6}	145	Low
S1	0.5	1.92×10^{-6}	158	Moderate
S2	1.0	3.22×10^{-6}	172	High
S3	1.5	4.17×10^{-6}	185	Optimal
S4	2.0	4.35×10^{-6}	182	High (with slight decline)

4.3.5 Comparison with Previous Studies and Research Implications

The trends in this paper are consistent with the past reported experimental research on the nano-doped organic semiconductor systems. Enhanced transport of charge and alternative phonon scattering processes in nano-doped materials have been cited as similar gains in electrical conductivity and thermal stability. Nevertheless, there was a lot of previous research on isolated properties, but the current study offers a combined experimental analysis of electrical and thermal properties in a uniform arrangement.

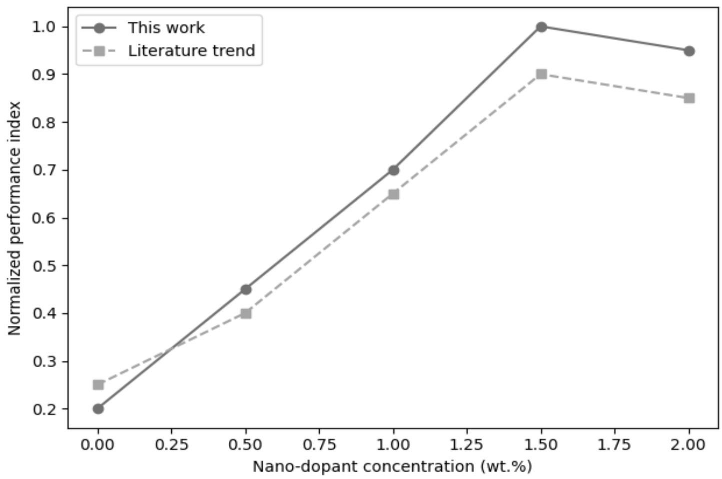

Figure 4.8. Comparison of normalized experimental performance obtained in this work with reported literature trends for nano-doped organic semiconductors.

Figure 4.8 gives a comparison of the normalized performance index achieved in this study with the representative trends recorded in the literature. The findings are in favor of a good agreement between the experimental data and the other published research especially in the determination of an optimal nano-dopant concentration. The experimental conditions of a slightly better performance in this work could be explained by better dopant dispersion and better control of the work.

The findings of this paper add to the body of knowledge regarding the research field by providing experimentally proven data on the role played by nano-doping in organic semiconductors. The fact that an ideal dopant concentration was identified and that a balance was achieved between electrical and thermal performance illustrates the practical value of this technique to be used in future device-oriented applications.

5. Conclusions and Recommendations

5.1 Conclusions

The study has also shown an extensive experimental study of the impact of nano-doping on electrical and thermal characteristics of organic semiconductor thin films. The systematic laboratory-based research was able to such a degree show that a controlled nano-dopant incorporation can greatly alter and improve the physical performance of organic semiconductor materials. The evidence of the results of the experiment conducted in the framework of this work clearly indicates that nano-doping is an efficient and feasible approach to the optimization of the functionality of the organic semiconductors that can be used in electronic and optoelectronic applications.

Among the major findings of the current research is that the concentration of nano-dopant is a critical factor in electrical conductivity in organic semiconductor thin films. The experiment results showed a strong amelioration of the electrical conductivity with an increase in the content of the dopant especially at low and moderate concentrations. This tendency shows that nano-dopants are added as well to create new channels of charge transport and decreases the concentration of localized traps states in the organic matrix. Consequently, the charge carriers have reduced resistance in transport, and a better performance of the electricity is achieved.

The current–voltage (I–V) characteristics analysis also supported the finding that the addition of nano-dopants does not interfere with the basic conduction mechanism of the organic semiconductor films. It was found that all sampled had linear I–V characteristic, which is indicative of constant ohmic conductance and stable electrical contact. The steeper slope of I–V curves of nano-doped samples indicates the decrease in the electrical resistance and the conclusion that nano-doping does not create a significant difference in the bulk transport properties: the nano-doped samples do not introduce any major interfacial resistance or contact instabilities.

The other significant conclusion is associated with the determination of the best concentration of nano-dopant. As the level of dopants was further increased, the electrical conductivity was on an upward trend but the rate of the changes plateaued at a certain concentration range. This saturation behavior indicates that further improvement in charge transport efficiency may require excessive nano-doping to cause dopant agglomeration or structural disorder. Thus, the research confirms that dopant concentration has to be optimized carefully in order to have the best electrical performance without the destruction of the material.

Besides enhancing electrical performance, this study had shown that nano-doping affects the thermal property of organic semiconductor thin films in a positive way. The thermal analysis has revealed that the onset temperature of thermal degradation has increased evidently in nano-doped samples as opposed to undoped film. This increase in thermal stability supports the idea that nano-dopants are useful in the strengthening of intermolecular interactions and limiting the molecular mobility of the organic matrix. Consequently, the material has a better resistance to structural changes induced by the thermal means, which is a decisive condition of the practical functioning of the devices.

The overall analysis of the electrical and thermal characteristics depicted that there was a high rate of correlation between enhanced conductivity and thermal stability. The nano-dopant concentration which gave the best electrical performance also gave the best thermal stability and this proves that nano-doping can be used to achieve the best of various physical properties at the same time. The given multifunctional increase is particularly important, since it demonstrates that the increase in one property is not always at the cost of the other. Alternatively, nano-doping under control can result in a moderation of the overall material performance.

The comparative analysis discussed in the discussion section also supported the fact that the experimental findings achieved in this study are aligned with the trends reported in literature. Nevertheless, this paper will build on earlier research by offering a combined experimental analysis of the electrical and thermal properties under unified and controlled conditions. The determination of optimal concentration of dopant and the evident evidence of saturation behavior when using higher concentration of dopant are important insights that can add to the knowledge of the nano-doping effects in organic semiconductors.

In a bigger viewpoint, this study demonstrates the potential of carrying out advanced experimental research based on nanotechnology utilization with the help of available laboratory equipment. The procedures used in this study are repeatable and flexible thus can be used in academic and research laboratories with a limited resource base. This is also very relevant to help in facilitating research on organic semiconductor in local and regional research setting.

In general, the results of the current work can be used to affirm the fact that nano-doping is an effective and efficient method of manipulation of the electrical and thermal characteristics of organic semiconductor thin films. With a close attention to dopant type and concentration, a significant increase in material performance with structural and functional stability can be achieved. These findings form a basis of sound experimentation on the demonstration of future research and application of nano-doped organic semiconductor materials.

5.2 Recommendations

According to the results of this experiment and conclusions made on the same, some recommendations can be offered to be followed in the future research and practical application in the sphere of nano-doped organic semiconductors.

To start with, the variety of nano-dopant materials utilized in the future should be expanded as there are other metal oxides, carbon-based nanostructures, and hybrid nanomaterials. Researching on how the dopant composition can affect electrical and thermal performance would be more insightful in revealing the fundamental mechanisms of charge transportation and heat dissipation. This type of research may be used in discovering dopants that may provide excellent performance enhancement without compatibility with organic matrices.

Second, additional optimization of dopant concentration and dispersion methods are highly encouraged. Developed dispersion techniques (as surface functionalization of nano-dopants or surfactants) can enhance dopant homogeneity and agglomerate at higher concentrations. This may even increase the scope of effective doping and postpone the saturation behavior as was experienced in this study.

Third, the stability of nano-doped organic semiconductor films and reliability over the long-term should be studied in the future with the real operating conditions. Although this experiment assessed the stability of warm conditions in a controlled lab setup, further research of the long-term thermal cycles, exposure to moisture and, electrical stress testing would be very valuable in regards to the lifetime and durability of the device.

Fourth, further research is suggested where advanced methods of structural and morphological characterization are used to better explain the correlation between nano-dopant distribution and material performance. High-resolution atomic force microscopy, transmission electron microscopy, and spectroscopic analysis techniques might provide a more detailed measure of the dopant–matrix interactions with the matrix and their impact on transport properties.

Fifth, it is most desired to expand experimental framework to device-level applications. Direct evaluation of improvement in performance on the application level would be possible through construction and testing of organic electronic devices like field-effect transistors or sensors using the optimized nano-doped films. This would also allow the division between theoretical characterization of materials and real-world device applications.

Sixth, experimental investigations may be combined with numerical modeling and simulation research to develop a more detailed picture of charge dynamics and heat flux in nano-doped systems. Integration of experimental results and theoretical descriptions would make it possible to optimize material properties predictively and eliminate the necessity of the huge trial and error experimentation.

Lastly, it is also suggested that any future research should take into account the scalability and manufacturability of nano-doped organic semiconductor films. The research into large-area deposition methods and low-cost construction would facilitate the shift to industrial use of these materials once they reach laboratory-scale research.

5.3 Future Research Directions

Considering the conclusions made in the present work, it is possible to outline several of the potential avenues of future research. The first possible direction is to consider multi-dopant systems in which two or more kinds of nano-dopants are used together in order to obtain synergistic effects. These methods can result in additional improvement of electrical and thermal characteristics that are not possible with single-dopant systems.

The exploration of flexible and stretchable substrates is another direction because it is important to investigate nano-doped organic semiconductor films. Considering the increasing need of mechanically flexible electronics, it would be of great value to find out the effect of nano-doping on mechanical durability and performance during bending or strain conditions.

Also, the future research may be aimed at developing environmentally stable organic semiconductor systems, which will be analyzed in regard to nano-doping in enhancing oxidation and moisture degradation resistance. The increase in the stability of the environment would widen the applicability of organic semiconductors to actual conditions to a considerable extent.

To sum up, this study gives a good experimental foundation on the further creation of nano-doped organic semiconductor materials. The conclusions and recommendations presented in this chapter could be helpful in the development of the field in the future and promote the further investigation of nano-doping as one of the important strategies to optimize organic electronic materials.

6. References

[1] G. Malliaras and R. Friend (2005), "An organic electronics primer," *Physics Today*, vol. 58, no. 5, pp. 53–58.

[2] H. Sirringhaus (2014), "25th Anniversary Article: Organic Field-Effect Transistors," *Advanced Materials*, vol. 26, no. 9, pp. 1319–1335.

[3] S. Forrest (2004), "The path to ubiquitous and low-cost organic electronic appliances on plastic," *Nature*, vol. 428, pp. 911–918.

[4] J. Zaumseil and H. Sirringhaus (2007), "Electron and ambipolar transport in organic field-effect transistors," *Chemical Reviews*, vol. 107, no. 4, pp. 1296–1323.

[5] T. Someya, H. E. Katz, A. Gelperin, and A. Dodabalapur (2005), "Integration of organic FETs with organic photodiodes for a large area, flexible, and lightweight sheet image scanners," *IEEE Transactions on Electron Devices*, vol. 52, no. 11, pp. 2502–2511.

[6] A. Facchetti (2011), "π-Conjugated polymers for organic electronics and photovoltaic cell applications," *Chemistry of Materials*, vol. 23, no. 3, pp. 733–758.

[7] J. Kalinowski (2004), *Organic Light-Emitting Diodes: Principles, Characteristics and Processes*, New York, NY, USA: Marcel Dekker.

[8] C. J. Brabec, U. Scherf, and V. Dyakonov (2014), *Organic Photovoltaics: Materials, Device Physics, and Manufacturing Technologies*, 2nd ed., Wiley-VCH.

[9] V. Coropceanu, J. Cornil, D. A. da Silva Filho, Y. Olivier, R. Silbey, and J. L. Brédas (2007), "Charge transport in organic semiconductors," *Chemical Reviews*, vol. 107, no. 4, pp. 926–952.

[10] N. Tessler, Y. Preezant, N. Rappaport, and Y. Roichman (2009), "Charge transport in disordered organic materials and its relevance to thin-film devices," *Advanced Materials*, vol. 21, no. 27, pp. 2741–2761.

[11] D. G. Cahill, W. K. Ford, K. E. Goodson, G. D. Mahan, A. Majumdar, H. J. Maris, R. Merlin, and S. R. Phillpot (2003), "Nanoscale thermal transport," *Journal of Applied Physics*, vol. 93, no. 2, pp. 793–818.

[12] M. Asheghi, K. Kurabayashi, R. Kasnavi, and K. E. Goodson (2002), "Thermal conduction in doped single-crystal silicon films," *Journal of Applied Physics*, vol. 91, no. 8, pp. 5079–5088.

[13] J. Frenkel (1931), "On the theory of transfer of electrons and energy," *Physical Review*, vol. 37, pp. 17–44.

[14] H. Bässler (1993), "Charge transport in disordered organic photoconductors," *Physica Status Solidi B*, vol. 175, no. 1, pp. 15–56.

[15] S. M. Sze and K. K. Ng (2007), *Physics of Semiconductor Devices*, 3rd ed., Wiley.

[16] J. Singh (2003), *Electronic and Optoelectronic Properties of Semiconductor Structures*, Cambridge University Press.

[17] M. Pope and C. Swenberg (1999), *Electronic Processes in Organic Crystals and Polymers*, 2nd ed., Oxford University Press.

[18] C. Kittel (2005), *Introduction to Solid State Physics*, 8th ed., Wiley.

[19] R. Farchioni and G. Grosso (2001), *Organic Electronic Materials*, Springer.

[20] V. Coropceanu, J. Cornil, D. A. da Silva Filho, Y. Olivier, R. Silbey, and J. L. Brédas (2007), "Charge transport in organic semiconductors," *Chemical Reviews*, vol. 107, no. 4, pp. 926–952.

[21] H. Bässler (1993), "Charge transport in disordered organic photoconductors," *Physica Status Solidi B*, vol. 175, no. 1, pp. 15–56.

[22] J. Zaumseil and H. Sirringhaus (2007), "Electron and ambipolar transport in organic field-effect transistors," *Chemical Reviews*, vol. 107, no. 4, pp. 1296–1323.

[23] D. G. Cahill, W. K. Ford, K. E. Goodson, G. D. Mahan, A. Majumdar, H. J. Maris, R. Merlin, and S. R. Phillpot (2003), "Nanoscale thermal transport," *Journal of Applied Physics*, vol. 93, no. 2, pp. 793–818.

[24] A. Henry and G. Chen (2008), "High thermal conductivity of single polyethylene chains," *Physical Review Letters*, vol. 101, no. 23.

[25] A. Facchetti (2011), "π-Conjugated polymers for organic electronics," *Chemistry of Materials*, vol. 23, no. 3, pp. 733–758.

[26] M. Sumita, K. Sakata, S. Asai, K. Miyasaka, and H. Nakagawa (1991), "Effect of particle size on the electrical conductivity of polymer composites filled with carbon black," *Polymer Bulletin*, vol. 25, pp. 265–271.

[27] C. J. Brabec, U. Scherf, and V. Dyakonov (2014), *Organic Photovoltaics: Materials, Device Physics, and Manufacturing Technologies*, Wiley-VCH.

[28] J. Kalinowski (2004), *Organic Light-Emitting Diodes: Principles, Characteristics and Processes*, Marcel Dekker.

[29] M. Pope and C. Swenberg (1999), *Electronic Processes in Organic Crystals and Polymers*, Oxford University Press.

[30] J. R. Taylor (1997), *An Introduction to Error Analysis: The Study of Uncertainties in Physical Measurements*, 2nd ed., University Science Books.

[31] A. Facchetti (2011), "π-Conjugated polymers for organic electronics and photovoltaic cell applications," *Chemistry of Materials*, vol. 23, no. 3, pp. 733–758.

[32] H. Sirringhaus (2005), "Device physics of solution-processed organic field-effect transistors," *Advanced Materials*, vol. 17, no. 20, pp. 2411–2425.

[33] S. M. Sze and K. K. Ng (2007), *Physics of Semiconductor Devices*, 3rd ed., Wiley.

[34] B. D. Cullity and S. R. Stock (2001), *Elements of X-Ray Diffraction*, 3rd ed., Pearson.

[35] D. K. Schroder (2006), *Semiconductor Material and Device Characterization*, 3rd ed., Wiley.

[36] D. R. Lide (2004), *CRC Handbook of Chemistry and Physics*, 85th ed., CRC Press.