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MODELING AND FABRICATION OF P3HT/SWCNT HYBRID NANOSTRUCTURES FOR HIGH-PERFORMANCE OPTOELECTRONIC DEVICES

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Abstract

Single-wall carbon nanotubes (SWCNTs) offer outstanding electrical characteristics and are robust but flexible. As a result, they have a widespread range of electrical uses, involving semiconductors, RFID chips, effective field transistors (EFT), smart materials, data storage equipment, and CMOS batteries. Utilizing B3LYP-SDD/DFT (Density Functional Theory), a reduction in absorbance is observed with the incorporation of SWCNT nanocomposites, resulting in a broader absorption spectrum relative to pure P3HT. The incorporation of SWCNTs can extend the absorption spectrum into the near-infrared zone, enabling the solar cell to harness a broader spectrum of sunlight and potentially enhancing total energy conversion efficiency. The decrease in absorbance creates a phenomenon known as “nanotube aggregation”. The Poly(3-hexylthiophene) (P3HT): SWCNTs thin films, which are based on the solution, were prepared using the spin coating technique. UV-visible absorption spectroscopy has been utilized to evaluate the characteristics of nanocomposites. The findings demonstrated that adding SWCNTs to the P3HT matrix reduces absorption intensity without obviously changing the P3HT's band locations. The structural investigation was conducted using XRD, which showed that SWCNTs directly affected the crystallinity of P3HT. Using SEM pictures to investigate the

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ISSN 2760-4985 (Online) Volume 02, Issue 05, May 2026

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morphological features, it was possible to see that the transparent nanotubes on the P3HT surface were evenly distributed. Uses like light-emitting diodes (LEDs) and photo detectors might benefit from the development of new states of electronics inside P3HT brought about by the inclusion of SWCNTS. This is due to the possibility that the composite material's introduction of a new state of electronics might serve as a means of boosting the LED structure's capacity for charge carriers, such as holes and electrons.

Keywords: The Poly(3-hexylthiophene), carbon nanotube, DFT, Physical Properties, Nanocomposites.

Introduction

Polymer composites are a very interesting and extensively researched area within nanotechnology and composites, exhibiting great potential as versatile, high-performance materials.

A substance's constituents can determine whether it is an organic or inorganic substance. Many years ago, materials that came from living things were regarded as organic materials and were thought to contain an undefinable "living force." Due to their usage in electrical and optoelectronic devices, organic semiconductors have been the concentrate of extensive study in recent years [1,2-7].

Because of its adaptability, ease of manufacture, and changeable properties, conductive polymer composites (CPCs) are one of the most important and exciting subjects in polymer composite studies, which have been continuing for many years [3,4,8].

In the three decades since conducting polymers were discovered, the research of organic semiconductors has advanced remarkably [5-10]. Most of these natural compounds can be chemically treated from solution to be inks, particularly the polymers. This makes it possible to employ normal printing methods to produce

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Eureka Journal of Geoscience, Materials & Resource Engineering (EJGMRE)

ISSN 2760-4985 (Online) Volume 02, Issue 05, May 2026

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organic electrical devices in large quantities and at a reasonable cost on a variety of flexible substrates, including paper, fabric, and plastic foils [5,7,11]. This is in sharp contrast to the highly complex and costly techniques employed in the manufacture of conventional inorganic semiconductor devices.

Many toxic compounds and solvents are used in the inorganic electronics production process. The ability to adjust the chemical structure of organic semiconductors to alter their physical and chemical functioning is an additional advantage [5-10]. Organic semiconductor devices such as organic photovoltaics, organic thermoelectric, organic thin film transistors, and organic sensors are only a few examples of the many devices that have been produced. These devices are anticipated to open the door for future of electronics with energy-efficient security systems, spintronic memory, photonics, and sensors because of their inexpensiveness and simplicity of fabrication and processing [1,12]. Because of their special physical characteristics, carbon nanotubes (CNTs) become important nanofillers that can give polystyrene better mechanical, thermal, and electrical qualities, exceeding researchers' ever-expanding expectations [13-16] Organic photovoltaic devices are using SWCNTs more and more since they are readily available and have a low cost of production.

A carbon nanotube's diameter and length measured at the nanoscale are used to classify it as either multi-wall (MWCNT), double-wall (DWCNT), or single-wall (SWCNT). The formation of a conducting network or continuous channels may cause the composite's electrical conductivity to rise over time [17,18]. Conducting polymers with a carbon-based π-conjugated backbone have superior mechanical characteristics similar to conventional plastics and the electrical conductivity of metals as compared to inorganic or metallic thermoelectric materials. Conducting polymers have shown a lot of promise and useful uses thus far in many different areas. Bundles of nanotubes exfoliate as a result of chemical functionalization, improving solubility and processability. Functionalization modifies the physical and chemical characteristics of nanotubes, improving their

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ISSN 2760-4985 (Online) Volume 02, Issue 05, May 2026

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interaction with polymer [19]. The maximum efficiency of power conversion was attained by doping functionalized SWCNTs with P3HT. P3HT is a widely recognized conducting polymer with distinctive physicochemical features that can be used as a model system to investigate electronic/thermal correlations and create high-performing thermoelectric equipment [20-26].

Though the nature of electron or hole charge transport inside the nanotube continues to be a controversial topic, several theories have proposed an electron transfer in P3HT: SWCNTs hybrids. Although these hybrids have been suggested as hole transfer layers by previous investigators [27-30].

For use in printable or high-end electronics, SWCNTs must be synthesized on a large scale. SWCNTs are showing promise as a material for low-cost, large-area microelectronics made using additive manufacturing techniques like roll-to-roll printing, as well as high-performance, high-density devices. This article examined the impacts of various weight percentages of acid-treated SWCNTs added to the P3HT matrix in order to estimate the functional materials SWCNTs' impact on the organic P3HT and its attributes [29-32].

Computational details and Electronic properties

Gauss View 5.0.8 program was used to draw the underlying structure of the complex and give the database to its information document. The estimations were practiced by using the Gaussian 09 bundle of projects [30-40]. P3HT: SWCNTs nanocomposites were completely loose by using B3LYP-SDD/DFT (Density Functional Theory). The electronic excitation vitality was determined for the unwinding of test cases by using the TD-DFT/B3LYP technique with SDD premise sets [11,33,34]. The TD-DFT technique was proven dependable for ascertaining the spectral properties of composites.

The electronic energy divisions in DFT is clarified in the following relationship:

$E = E_T + E_V + E_J + E_{XC}$

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https://eurekaoa.com/index.php/9

Where E_T is the electronic kinetic energy, E_V is the attractive potential energy which binds the electron to the nucleus, E_J is the repulsive energy between the electrons. In DFT, the correlation of electrons is considered through the exchange-correlation term E_{XC}. The last term emerges due to the anti-symmetry of the wave function, the quantum mechanics term, and the dynamic correlation in the motion of the specific electron. Thus, DFT is predominant over conventional HF transactions.

The Gaussian View 5.0 software tool characterizes both the HOMO (highest occupied molecular orbital) and LUMO (lowest unoccupied molecular orbital) of these structures using the B3LYP/SDD approach, as illustrated in Fig. 1-B and C [30,35,36]. The findings indicate a reduction in the Eg values. This indicates the proximity of the HOMO and LUMO values, suggesting the potential for electronic transitions between the valence and conduction bands, as illustrated in Fig. 1-B and C.. The distribution is symmetrical in the charges of P3HT: SWCNTs nanocomposites as well as in the charges of the three samples. This proves the high physical and chemical compatibility of the compound as shown in Fig. 1-D and E. TDDFT-based descriptors were computed to evaluate the composite materials' stability and reactivity. [9], [35,37].

$$\mu = \left(\frac{\partial E}{\partial N}\right)_{V(\vec{r}),T} \quad (1)$$

$$\eta = \frac{1}{2}\left(\frac{\partial^2 E}{\partial N^2}\right)_{V(\vec{r}),T} \quad (2)$$

$$S = \frac{1}{2\eta} \quad (3)$$

$$\omega = \frac{\mu^2}{2\eta} \quad (4)$$

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https://eurekaoa.com/index.php/9

Electron affinity and ionization potential are referred to as EA and IP in this context. The global attributes may be stated numerically as follows using a finite variation method. The formula that follows is utilized to determine the gap of energy [14,38,39]:

$$Eg = ELUMO - EHOMO \quad (5)$$

The electron affinity and ionization energy are represented by equation (6):

$$IP == -E_{HOMO}, \; EA == -E_{LUMO} \quad (6)$$

Fig.1-D and E show the 3-D electron density (TD) and electrostatic potential (ESP) surfaces of P3HT: SWCNTs nanocomposites obtained from the B3LYP/SDD level of theory. Through observing the TD and compounds' ESP surfaces, the pulling of potentials toward the fields of high electronegativity is clarified. One can understand that limiting the effective terminal positions of each compound in linkage with the surrounding species or molecules is to construct new nanocomposites.

Table 2, which demonstrates that the overall energy of the nanocomposite, P3HT: SWCNTS, rises in comparison to the energy of P3HT, supports this. The interactions that take place between the SWCNTS particles when they are integrated into the P3HT matrix are what cause this rise in energy. A composite system's overall energy is increased by these physical bonding, chemical bonds, electrostatic forces, potentials, and interactions. The energy needed to break up the P3HT bonds and disperse the particles during the SWCNTS combination process raises the system's overall energy. Instead of lowering the system's overall energy, other inter-particle interactions, such as electrostatic forces, van der Waals contacts, or bonds of chemistry with these particles, would provide forces that aid in bringing those particles to the matrix's interface [11,40,41].

Due to the enhancement of various surfaces in large nanocomposites, the HOMO and LUMO exhibit form affects as well as continuous fluctuation uncertainty.

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Eureka Journal of Geoscience, Materials & Resource Engineering (EJGMRE)

ISSN 2760-4985 (Online) Volume 02, Issue 05, May 2026

https://eurekaoa.com/index.php/9

Fermi level, ionization liveliness, and electron liking are all related to the different quantities that may be determined from the HOMO and LUMO energies. Ionization potential and electron fondness are generally associated with the LUMO and HOMO energies independently when the sign is negative [18,42,43]. The Fermi level is the normal of the LUMO and HOMO energies. The LUMO and HOMO energies are affected by these three quantities in a similar way as a result of these relationships. Figure 1 also displays the energy levels of the LUMO and HOMO of P3HT and P3HT: SWCNTS structures. These energy features suggest that P3HT: SWCNTS has a higher electron-accepting capacity, making it more stable than pure P3HT [44].

Because each atom's electron configuration stability in the creation of P3HT: SWCNTS is marginally greater than that of the base P3HT, they are less reactive than the base material. As a result, our study shows that the P3HT modified with SWCNTS has improved optical absorption and emission properties that may improve the optical sensor, photovoltaic systems, and design of light-emitting diodes uses. The composite material may now be used in a wider range of technical fields because of these enhanced properties [36,45,46].

Table 2 demonstrates that adding SWCNTS to pure P3HT has the impact of Alphabets, which causes the band gap (Eg) width to decrease from 1.866 eV to 0.977 eV. The reduction in Eg suggests that the existence of SWCNTS has reorganized or changed the energy levels in P3HT by introducing new energy levels between the energy levels or gap. As a result, the charge transport characteristics are enhanced to meet the requirements of certain applications, including electrical conductivity. Additionally, the modified P3HT might show a number of advantageous properties, such as improved emission and absorbance [31,47]. The performance of various sensing applications may be enhanced by the addition of SWCNTS, which may result in improved characteristics [20,39]. P3HT-based catalysts may become more active and selective as a result [9,40]. These characteristics suggest that SWCNTS are

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ISSN 2760-4985 (Online) Volume 02, Issue 05, May 2026

https://eurekaoa.com/index.php/9

useful in situations where controlling electrical conductivity is necessary. In sectors like electronics, this flexibility is crucial for the production of circuits and conductive layers [48, 49].

The IP and EA were obtained from table 2; the findings indicate that the former is more than the IP of pure P3HT and the latter is likewise greater than the EA of pure P3HT. In terms of EA, the magnitudes fluctuate according to the fluctuation of the electronic of the particular molecule owing to structural changes and bonding; higher magnitudes of IP imply a stronger electron-donating propensity is less. Interfaces, electrical properties, electron affinity and ionization potential, may all be altered by adding SWCNTS particles. These particles may participate in electron transfer activities with the P3HT host, altering P3HT's features including electron affinity and ionization potential. This supports the idea that adding SWCNTS changes the system's electronic profile, necessitating a study of conductivity and other electronic features [31,50,51]. Particularly for opto-electronic applications, the incorporation of SWCNTS may result in the creation of new or altered state of electronics inside the material. These modifications to the electrical characteristics have an impact on the material's sensitivity to light and may be helpful in devices like photodetectors or light-emitting diodes (LEDs) due to the possibility that adding a new electronic state to the composite material might improve the charge carriers movement, such as holes and electrons, inside the LED structure. The recombination electron-hole pair formation process inside the LED junctions may be improved by this increased transport efficiency, which would increase the device's efficiency [4,52,53].

This is fully consistent with the results of the electron density and electrostatic potential, where we notice a symmetrical distribution of charges and electrostatic efforts, resulting in increased liberation of the electrons that leads to an increase in conductivity. And this perfectly agrees with the reached practical results. The configured geometrical properties of homojunction structures (Angstrom bond

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Eureka Journal of Geoscience, Materials & Resource Engineering (EJGMRE)

ISSN 2760-4985 (Online) Volume 02, Issue 05, May 2026

https://eurekaoa.com/index.php/9

distances) ascertained by the B3LYP/6-31G -SDD procedure are demonstrated in Table 1. Table (1) clearly displays that the experimental results for DLC (donor) strongly agree with the geometrical features measured by the current method. The difference in atomic numbers for the conjugated atoms is what determines the bond length for these atoms [44,54].

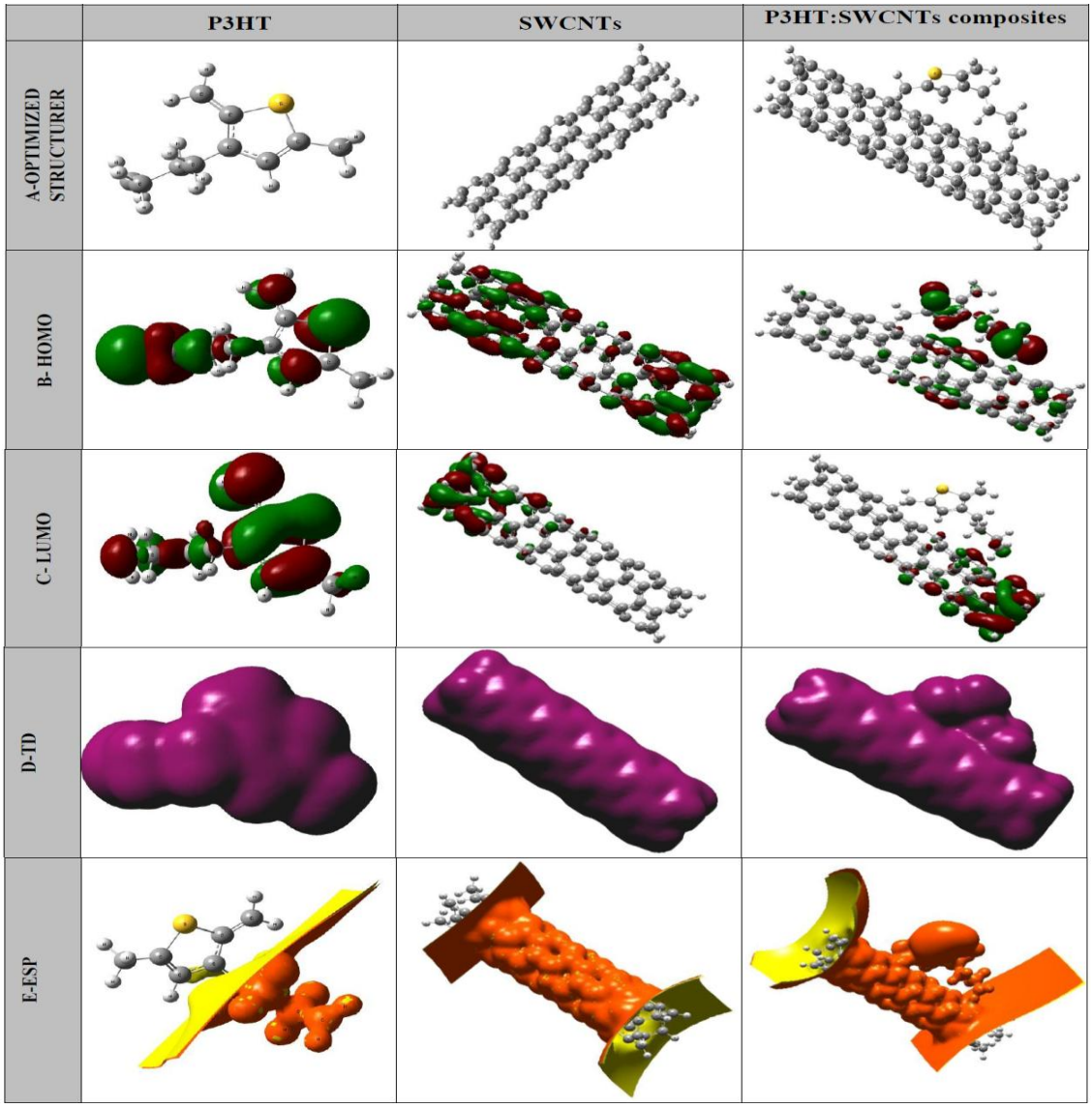

Fig. 1. Optimized Computational structures (Theoretical calculations) of study molecules.

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Eureka Journal of Geoscience, Materials & Resource Engineering (EJGMRE)

ISSN 2760-4985 (Online) Volume 02, Issue 05, May 2026

https://eurekaoa.com/index.php/9

Table.1 optimized parameters of atoms in P3HT, SWCNTS and P3HT: SWCNTS.

Molecule	P3HT	P3HT:SWCNT
ET(a.u)	-7658.34	-6894.17
HOMO(eV)	-5.3240	-17.3240
LUMO(eV)	-3.4576	-16.3475
E_g(eV)	1.866	0.977
IE(eV)	5.324	17.324
EA(eV)	3.458	16.348

Table 2. Illustrate electronic features of the nanostructures via utilizing TD-DFT B3LYP/6-311G(d,p).

Species	P3HT	SWCNTS	P3HT: SWCNTS
Bond Length (A^0)	C-C 1.4204 C=C 1.4473 C-C 1.4351 C-S 1.5196 C-H 1.0742	C-C 1.5424 C=C 1.4371 C-H 1.0173	C-C 1.4228 C=C 1.4437 C-C 1.4729 C-S 1.5178 C-H 1.0834

We notice from Fig. 2 a decrease in absorbance with the addition of SWCNT nanocomposites, and accordingly, a broader absorption spectrum appears compared to pure P3HT. The presence of SWCNTs can broaden the absorption band into the near-infrared region, allowing the solar cell to capture a wider range of sunlight and potentially increasing the overall energy conversion efficiency. The decrease in absorbance creates a phenomenon known as “nanotube aggregation”. The effective surface area available for light absorption may be

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Eureka Journal of Geoscience, Materials & Resource Engineering (EJGMRE)
ISSN 2760-4985 (Online) Volume 02, Issue 05, May 2026

https://eurekaoa.com/index.php/9

decreased when SWCNTs are added to a polymer matrix like P3HT because they have a tendency to form aggregates or bundles [15,46,55]. When compared to the pure polymer, this aggregation effect may cause the nanocomposite to absorb less total energy. Moreover, the scattering or reflection of light caused by SWCNTs may possibly be a factor in the observed decrease in absorption. The scattering effect, which occurs when light interacts with single-walled carbon nanotubes and deviates from its intended route, causes decreased absorption by the polymer matrix.

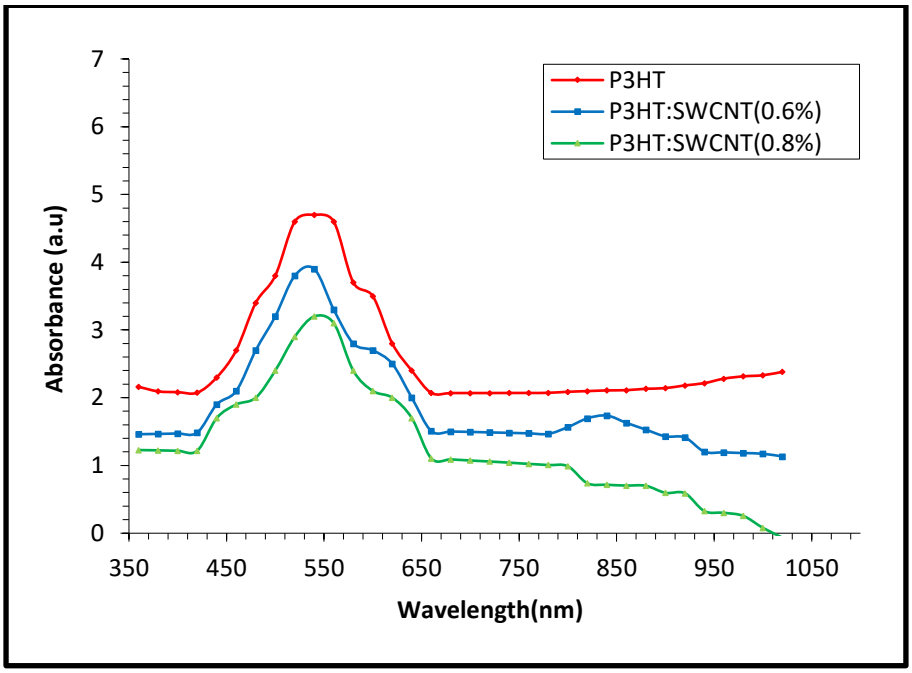

Fig. 2. Absorbance for pristine P3HT and P3HT:SWCNT hybrids.

Additionally, as we examine the optical characteristics, we find that the addition of SWCNT nanocomposites reduces the absorption coefficient of pure P3HT polymer (Fig.3). This is because the concentration of the P3HT polymer drops in relation to the total compound when SWCNT nanocomposites are added to the P3HT polymer matrix, causing a dilution effect. The absorption coefficient may

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ISSN 2760-4985 (Online) Volume 02, Issue 05, May 2026

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decrease as a result of this drop in polymer concentration. The optical characteristics of the surrounding P3HT polymer, such as its refractive index, light scattering, or changes in its electronic structure close to the interface, are similarly impacted by the presence of CNTs at the nanocomposite's interfaces. The observed drop in the absorption coefficient may be attributed to these interfacial effects. This is further explained by the possibility that CNTs will cause scattering and reflection events to arise inside the nanocomposite [37,46,56]. When light interacts with the nanocomposite, the carbon nanotubes can scatter or reflect a portion of the incident light, reducing the overall amount of light absorbed by the pure P3HT polymer. This scattering and reflection effect could contribute to the observed decrease in the absorption coefficient.

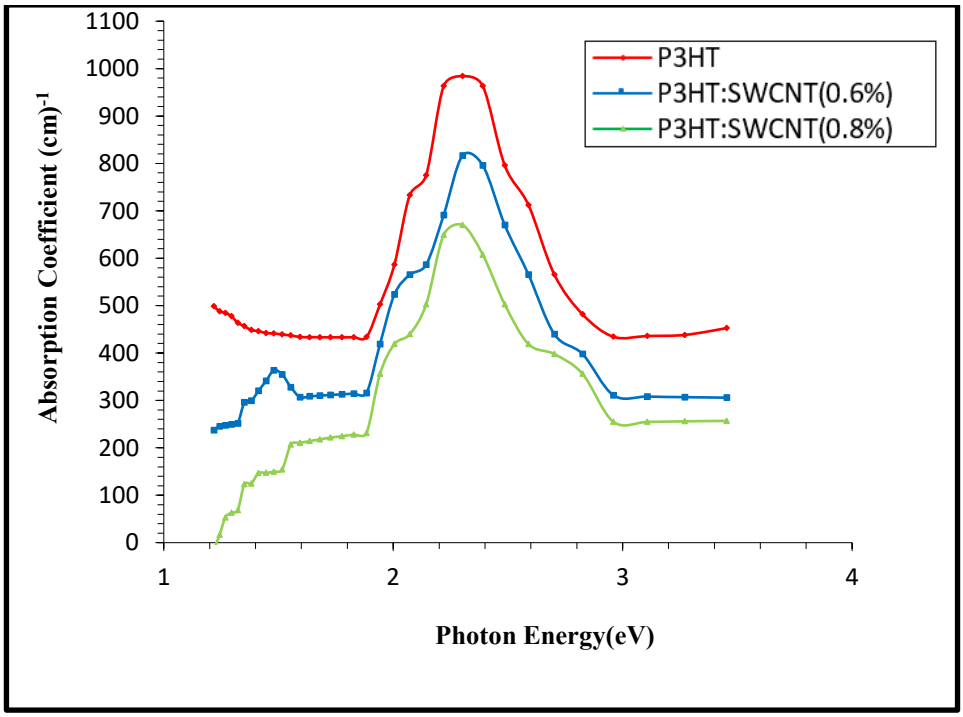

Fig.3. Coefficient of absorption for pristine P3HT and P3HT:SWCNT hybrids.

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ISSN 2760-4985 (Online) Volume 02, Issue 05, May 2026

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Experimental methods

P3HT and DCB were utilised without any additional purification after being provided by Sigma Aldrich. As previously indicated, SWCNTs (Sigma Aldrich) were functionalized using an acid treatment [19]. P3HT was dissolved in 12 mg/ml DCB solution, mixed for 150 minutes at 50 °C. Additionally, 0.75 mg/ml of functionalized SWCNTs were distributed throughout DCB. After 50 minutes of sonication in an ultrasonic bath, the P3HT and SWCNTs solutions were mixed at two different volume ratios (0.6 and 0.8); the pure P3HT solution was taken into consideration to examine the impact of the SWCNTs on these hybrids. The P3HT: SWCNTs solutions were then sonicated for a duration of 50 minutes.

View of the nanocomposites' properties through their morphology and structure.

(Fig. 4) presents the findings of X-ray diffraction in terms of crystalline structure information of the materials under investigation. Analysis of the XRD patterns showed that all three samples of pure P3HT, P3HT: SWCNT (0.6%), and P3HT: SWCNT (0.8%) had crystalline behavior as evidenced by clear and distinct peaks observed at specific angles (2θ values). The peaks observed at $2\theta = 5.492$, $2\theta = 5.507$, and $2\theta = 5.601$, respectively, correspond to the distinct crystal features of the samples and to the arrangement of atoms or molecules in the crystal lattice [18,57,58].

The increase in crystallite size and degree of crystallinity with increasing SWCNT concentration indicates that the presence of SWCNTs affects the structure of the P3HT thin film. Successful grafting of the polymer to single nanotubes indicates that the P3HT chains have attached to the surface of the single-walled carbon nanotubes. This grafting process can improve the arrangement and crystallinity of P3HT chains. Moreover, the interaction between P3HT and SWCNTs could also contribute to the observed changes in the crystal structure. SWCNTs may provide nucleation sites for P3HT chains,

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ISSN 2760-4985 (Online) Volume 02, Issue 05, May 2026

https://eurekaoa.com/index.php/9

promoting their alignment and organization into a more ordered structure. This interaction between the polymer and carbon nanotubes can facilitate charge transfer within the film, leading to improved carrier mobility, and it plays an essential role in determining the carrier mobility of organic thin films[40,44,59].

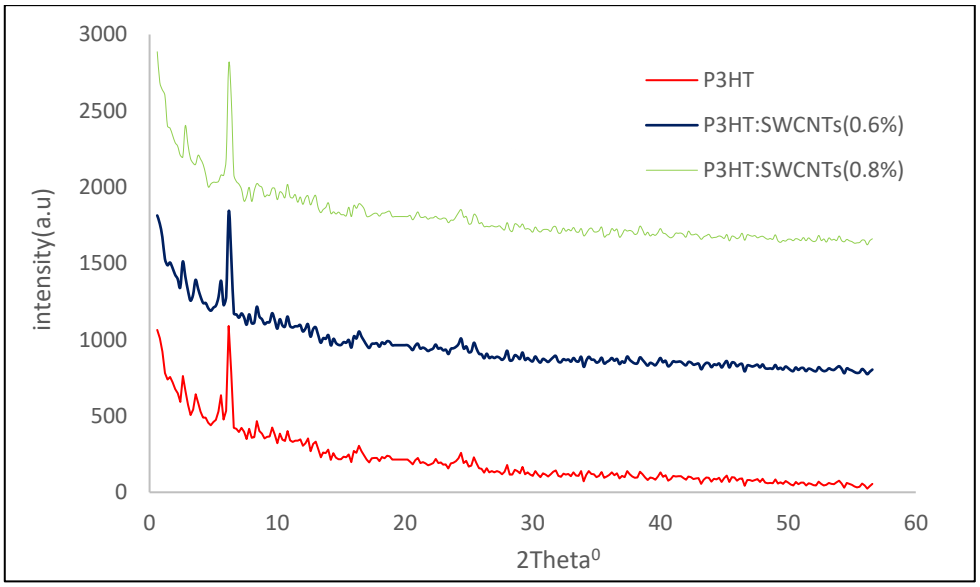

Fig. 4. XRD pattern for pristine P3HT and P3HT:SWCNTs hybrids.

SEM was used to examine the morphological characteristics of the thin films under study (Fig. 5). The P3HT thin film showed no obvious aggregation and a smooth surface. The surface morphology of the P3HT was altered by the addition of SWCNTs. On the surface of the thin film, distinct characteristics of nanotubes were evenly distributed. The latter spoke of using acid-treated nanotubes rather than untreated ones.

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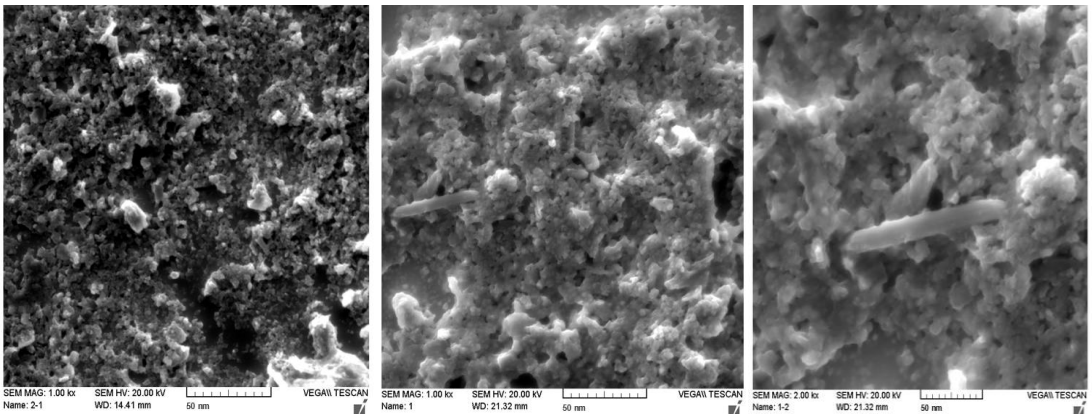

P3HT P3HT:SWCNT(0.6%) P3HT:SWCNT(0.8%)

Fig. 5. SEM images for pristine P3HT and P3HT: SWCNTs hybrids.

Conclusions

Based on the findings of the spin coating technique's X-ray diffraction analysis of the thin P3HT: SWCNTs films. The membranes were found to be extremely homogeneous. This suggests that the P3HT crystallinity is directly impacted by SWCNTs. The UV-visible absorption and fluorescence spectroscopy results demonstrate that the addition of SWCNTs to the P3HT matrix resulted in a drop in absorption intensity and no discernible change in the P3HT's band locations. SEM photographs showed that clear and evenly distributed nanotubes were visible on the P3HT surface. As a result, for instance, values decrease. This makes them interesting materials for a variety of electrical devices, including EFTF and organic solar cells, by bringing the HOMO and LUMO values more closely together and enabling electronic transitions between the valence and conduction bands. Uses including light-emitting diodes (LEDs) and photo detectors may benefit from the incorporation of SWCNTS, which might produce new or modify existing electronic states inside the material. This is due to the

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Eureka Journal of Geoscience, Materials & Resource Engineering (EJGMRE)

ISSN 2760-4985 (Online) Volume 02, Issue 05, May 2026

https://eurekaoa.com/index.php/9

possibility that adding a new electronic state to the composite material might increase the charge carrier's mobility, such as holes and electrons, in the LED structure.

References

1. Gao C., Guo M., Liu Y., Zhang D., Gao F., Sun L., Li J., Chen X., Terrones M., Wang Y. Surface modification methods and mechanisms in carbon nanotubes dispersion. Carbon. 2023;212:118133. doi: 10.1016/j.carbon.2023.118133.
2. Liew K.M., Pan Z., Zhang L.-W. The recent progress of functionally graded CNT reinforced composites and structures. Sci. China Phys. Mech. Astron. 2020;63:234601. doi: 10.1007/s11433-019-1457-2
3. A. S. Hasan, F. Q. Mohammed, and M. M. Takz, "Design and synthesis of graphene oxide-based glass substrate and its antimicrobial activity against MDR bacterial pathogens," J. Mech. Eng. Res. Dev., vol. 43, no. 1, 2020.
4. Hussam Mohammad, Andrey A. Stepashkin and Victor V. Tcherdyntsev, Formation of Conductive Networks in Polysulfone Filled with Graphite-Derived Materials. Appl. Sci. 2024, 14, 2756. https://doi.org/10.3390/app14072756.
5. Hongfu Li,Guangfei Wang, Ying Wu, Naisheng Jiang, and Kangmin Niu, Functionalization of Carbon Nanotubes in Polystyrene and Properties of Their Composites: A Review, 16(6): 770, 2024. doi: 10.3390/polym16060770
6. Mohammed K. Al Hashimi , Buraq T. SH. AL-Mosawi , Burak Y. Kadem, and Yaqub Rahaq, Using SWCNTs to Enhancing the Performance of P3HT:PCBMBased Organic Solar Cells. 2022; 12(4):948-958. DOI: 10.22052/JNS.2022.04.016
7. Hamid, Hamood Shehab, Chisab, Raad Farhood, Mnati, Mohannad Jabbar and Q.A. Al-Jarwany Design a New Smart Monitoring Micro-Grid Photovoltaic System Network Based on Mobile Technology, ICASEA 2021, DOI:10.1109/ICASEA53739.2021.9733067

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Eureka Journal of Geoscience, Materials & Resource Engineering (EJGMRE)

ISSN 2760-4985 (Online) Volume 02, Issue 05, May 2026

https://eurekaoa.com/index.php/9

8. Gao, C.; Guo, M.; Liu, Y.; Zhang, D.; Gao, F.; Sun, L.; Li, J.; Chen, X.; Terrones, M.; Wang, Y. Surface modification methods andmechanisms in carbon nanotubes dispersion. Carbon 2023, 212, 118133.
9. Zhang, P.; Su, J.; Guo, J.; Hu, S. Influence of carbon nanotube on properties of concrete: A review. Constr. Build. Mater. 2023, 369, 130388.
10. Liew, K.M.; Pan, Z.; Zhang, L.-W. The recent progress of functionally graded CNT reinforced composites and structures. Sci. China Phys. Mech. Astron. 2020, 63, 234601.
11. Wang, R.; Sun, L.; Zhu, X.; Ge, W.; Li, H.; Li, Z.; Zhang, H.; Huang, Y.; Li, Z.; Zhang, Y.F. Carbon nanotube-based strain sensors: Structures, fabrication, and applications. Adv. Mater. Technol. 2023, 8, 2200855.
12. Tao, Z.; Zou, H.; Li, M.; Ren, S.; Xu, J.; Lin, J.; Yang, M.; Feng, Y.; Wang, G. Polypyrrole coated carbon nanotube aerogel composite phase change materials with enhanced thermal conductivity, high solar-/electro-thermal energy conversion and storage. J. Colloid Interface Sci. 2023, 629, 632–643.
13. Derbal-Habak H, Bergeret C, Cousseau J, Nunzi JM. Improving the current density Jsc of organic solar cells P3HT:PCBM by structuring the photoactive layer with functionalized SWCNTs. Sol Energy Mater Sol Cells. 2011;95:S53-S56.
14. Derval-Habak H, Bergeret C, Cousseau J, Nunzi JM. Improving the efficiency of polymer solar cells by incorporation of functionalized SWCNTs in organic photovoltaic cells based on P3HT:PCBM photoactive layer. 2009 3rd ICTON Mediterranean Winter Conference (ICTON-MW); 2009/12: IEEE; 2009.
15. Li, M.; Wang, T.; Liu, X.-L.; Bao, Z.-L.; Qian, P.-F.; Liu, K.; Shi, Y.; Ming, X.; Geng, H.-Z. Highly stable phosphotungstic acid/Au dual doped carbon nanotube transparent conductive films for transparent flexible heaters. Carbon 2023, 207, 219–229
16. M. Akraa, A. S. Hasan, and M. J. H. Kadhim, “Spectroscopy

Eureka Open Access Journals
Open Access | Peer Reviewed | International Journals | Multidisciplinary Areas
OPEN ACCESS JOURNALS

Eureka Journal of Geoscience, Materials & Resource Engineering (EJGMRE)

ISSN 2760-4985 (Online) Volume 02, Issue 05, May 2026

https://eurekaoa.com/index.php/9

Characterization of Ethylene Vinyl Acetate Degradation by Different Kinds of Accelerated Aging," Baghdad Science Journal, vol. 17, no. 3, p. 0795, Jul. 2020, doi: 10.21123/bsj.2020.17.3.0795.

17. S. F. A. AL-Abass, A. J. Braihi, and Ali. S. Hasan, "Oil spill cleaning up by polymeric sorbents using salt leaching method," 2023, p. 020024. doi: 10.1063/5.0171315.
18. Mallajosyula AT, Sundar Kumar Iyer S, Mazhari B. Role of single walled carbon nanotubes in improving the efficiency of P3HT:PCBM solar cells - impedance spectroscopy and morphology studies. 2010 35th IEEE Photovoltaic Specialists Conference; 2010/06: IEEE; 2010.
19. Derbal-Habak H, Bergeret C, Cousseau J, Nunzi JM. Improving the current density Jsc of organic solar cells P3HT:PCBM by structuring the photoactive layer with functionalized SWCNTs. Sol Energy Mater Sol Cells. 2011;95:S53-S56.
20. Derval-Habak H, Bergeret C, Cousseau J, Nunzi JM. Improving the efficiency of polymer solar cells by incorporation of functionalized SWCNTs in organic photovoltaic cells based on P3HT:PCBM photoactive layer. 2009 3rd ICTON Mediterranean Winter Conference (ICTON-MW); 2009/12: IEEE; 2009.
21. Mohammed Jawad H. Kadhim, Ali Salah Salah, Qassim Al-Jarwany, Electronic, Spectral and Structural Characteristics of Carbon Nanotubes Gallium nitride as an optoelectronic Applications, Vol. 5 (2022): EJPCM
22. Q.A. Al-Jarwany et al. , Realization of a sub-wavelength dimple using a 193 nm wavelength photonic nano jet. Volume 750, July 2020, 137400
23. Adam J. Clancy et al. Charged Carbon Nanomaterials: Redox Chemistries of Fullerenes,Carbon Nanotubes, and Graphenes, DOI: 10.1021/acs.chemrev.8b00128Chem. Rev. 2018, 118, 7363−7408This is an open access article published under a Creative Commons Attribution (CC-BY)License, which permits unrestricted use, distribution and reproduction in

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ISSN 2760-4985 (Online) Volume 02, Issue 05, May 2026

https://eurekaoa.com/index.php/9

any medium,provided the author and source are cited.

24. Liew, K.M.; Pan, Z.; Zhang, L.-W. The recent progress of functionally graded CNT reinforced composites and structures. Sci.China Phys. Mech. Astron. 2020, 63, 234601
25. Tao, Z.; Zou, H.; Li, M.; Ren, S.; Xu, J.; Lin, J.; Yang, M.; Feng, Y.; Wang, G. Polypyrrole coated carbon nanotube aerogel composite phase change materials with enhanced thermal conductivity, high solar-/electro-thermal energy conversion and storage. J. Colloid Interface Sci. 2023, 629, 632–643.
26. S. A. Habeeb, A. S. Hasan, Ţălu, and A. J. Jawad, "Enhancing the properties of styrene-butadiene rubber by adding borax particles of different sizes," Iran. J. Chem. Chem. Eng., vol. 40, no. 5, 2021, doi: 10.30492/ijcce.2020.40535.
27. A. A. Ati, A. H. Abdalsalam, and A. S. Hasan, "Thermal, microstructural and magnetic properties of manganese substitution cobalt ferrite prepared via co-precipitation method," Journal of Materials Science: Materials in Electronics, vol. 32, no. 3, pp. 3019–3037, Feb. 2021, doi: 10.1007/s10854-020-05053-4.
28. M. H. Al-Maamori, A. N. Al-Jamal, S. A. Habeeb, A. S. Hassan, and H. S. Majdi, "Al 3+ -modified ZnO thin film sensor fabricated by the sputtering method: Characterization and a carbon monoxide gas detection study," J Chem Res, vol. 48, no. 1, Jan. 2024, doi: 10.1177/17475198231221453.
29. F. Q. Mohammed, M. S. Edan, A. S. Hasan, and A. J. Haider, "Synthesis and Theoretical Concepts of Boron Nitride Nanowires Grown on Nitrides Stainless Steel Surface by Hybrid Gas Phase Process," Key Eng Mater, vol. 886, pp. 97–107, May 2021, doi: 10.4028/www.scientific.net/KEM.886.97.
30. S. H. Abud, A. S. Hasan, M. Almaamori, and N. Bayan, "Enhancement the ability to pump crude oil using rubber solutions," J Phys Conf Ser, vol. 1818, no. 1, p. 012235, Mar. 2021, doi: 10.1088/1742-6596/1818/1/012235.
31. S. Ren, M. Bernardi, R. R. Lunt, V. Bulovic, J. C. Grossman, and S. Gradecak, Toward efficient carbon nanotube/P3HT solar cells: Active layer morphology, electrical, and optical properties. Nano letters, 11: 5316-5321

Eureka Open Access Journals
Open Access | Peer Reviewed | International Journals | Multidisciplinary Areas
OPEN ACCESS JOURNALS

Eureka Journal of Geoscience, Materials & Resource Engineering (EJGMRE)

ISSN 2760-4985 (Online) Volume 02, Issue 05, May 2026

https://eurekaoa.com/index.php/9

(2011).

32. A. S. Hasan, A. H. Mousa, and A. R. A. Hussein, "Molecular Dynamics Simulation of SWCNT / PYA in sensors application," in 2022 Muthanna International Conference on Engineering Science and Technology (MICEST), IEEE, Mar. 2022, pp. 83–88. doi: 10.1109/MICEST54286.2022.9790266.
33. G. Jianxin, K. Byung-Seon, B. Seung, C. Sang, P. Sohyun, J. Taiha and J. Hee-Tae, Effect of SWNT Defects on the Electron Transfer Properties in P3HT/SWNT Hybrid Materials, Adv. Funct. Mater., 18, 2659–2665 (2008).
34. K. S. Rajiv, K. Jitendra, K. Amit, K. Vikram, K. Rama and S. Ramadhar, Poly(3-hexylthiophene): Functionalized single-walled carbon nanotubes: (6,6)-phenyl-C61-butyric acid methyl ester composites for photovoltaic cell at ambient condition, Solar Energy Materials & Solar Cells 94:2386–2394 (2010).
35. B. Y. Kadem, M. Al-Hashimi, A. S. Hasan, R. G. Kadhim, Y. Rahaq, and A. K. Hassan, "The effects of the PEDOT:PSS acidity on the performance and stability of P3HT:PCBM-based OSCs," Journal of Materials Science: Materials in Electronics, vol. 29, no. 22, pp. 19287–19295, Nov. 2018, doi: 10.1007/s10854-018-0055-4.
36. H. B. Hassan, A. S. Hasan, and A. Hashim, "Fabrication and advanced optical and electronic characteristics of PVA/SiC/CeO2 hybrid nanostructures for augmented nanoelectronics and optics fields," Opt Quantum Electron, vol. 56, no. 3, p. 309, Mar. 2024, doi: 10.1007/s11082-023-05940-0.
37. S. Yue, L. Jian-gang, D. Yan and H. Yan-chun, controlling the surface composition of PCBM in P3HT/PCBM blend films by using mixed solvents with different evaporation rates, Chinese Journal of Polymer Science, 31(7), 1029−1037 (2013).
38. M. H. Kadhim, A. S. Hasan, M. A. Akraa, and A. Y. Layla, "Preparation and optimization of heterojunction donor(DLC) – acceptor(SI) as a solar cell by

Eureka Open Access Journals
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Eureka Journal of Geoscience, Materials & Resource Engineering (EJGMRE)

ISSN 2760-4985 (Online) Volume 02, Issue 05, May 2026

https://eurekaoa.com/index.php/9

DFT and PLD," Journal of Ovonic Research, vol. 17, no. 3, pp. 273–281, May 2021, doi: 10.15251/JOR.2021.173.273.

39. Z.H. Ali, A. S. Hasan and, A.J. Braihi, "Synthesis, Characterization, and Infrared Blocking Efficiency of Polyvinyl Alcohol Composites Filled with Cadmium Sulfide and Zinc Sulfide NPs", Annales de Chimie: Science
40. H. B. Hassan, A. S. Hasan, and A. Hashim, "Synthesis and boosting the structural, optical and electronic characteristics of PS/SiC/In2O3 promising nanohybrid structures for tailored optoelectronics applications," Opt Quantum Electron, vol. 56, no. 2, p. 272, Feb. 2024, doi: 10.1007/s11082-023-05904-4.
41. O. Oklobia and T.S. Shafai, A study of donor/acceptor interfaces in a blend of P3HT/PCBM solar cell: Effects of annealing and PCBM loading on optical and electrical Properties, Solid-State Electronics 87:64–68 (2013).
42. A. S. Hasan, H. B. Hassan, and A. Hashim, "Synthesis and unraveling the optical and electronic characteristics of PVA/Co2O3/Fe2O3 hybrid nanostructures for promising nanoelectronics and photonics applications," Opt Quantum Electron, vol. 56, no. 4, p. 634, Feb. 2024, doi: 10.1007/s11082-023-06039-2.
43. Rathore, P., Negi, C. M. S., Verma, A. S., Singh, A., Chauhan, G., Inigo, A. R., & Gupta, S. K. (2017). Investigation of the optical and electrical characteristics of solution-processed poly (3 hexylthiophene)(P3HT): multiwall carbon nanotube (MWCNT) composite-based devices. Materials Research Express, 4(8), 085905.
44. A. S. Hasan, B. Y. Kadem, M. A. Akraa, and A. K. Hassan, "PVA:PEDOT:PSS:Carbon based nano-composites for pressure sensor applications," Dig. J. Nanomater. Biostructures, vol. 15, no. 1, 2020, doi: 10.15251/djnb.2020.151.197.
45. M. D. Shirsat, T. Sarkar, J. Kakoullis, N. V. Myung, B. Konnanath, A. Spanias, and A. Mulchandani, Porphyrins-Functionalized Single-Walled Carbon Nanotubes Chemiresistive Sensor Arrays for VOCs. J. Phys. Chem. C

Eureka Open Access Journals
Open Access | Peer Reviewed | International Journals | Multidisciplinary Areas
OPEN ACCESS JOURNALS

Eureka Journal of Geoscience, Materials & Resource Engineering (EJGMRE)

ISSN 2760-4985 (Online) Volume 02, Issue 05, May 2026

https://eurekaoa.com/index.php/9

116, 3845 (2012).

46. Sura. K. Jebur, A. J. Braihi, and A. S. Hassan, "Graphene effects on the structural, morphological and optical properties of PEDOT:PSS thin films," Mater Today Proc, vol. 49, pp. 2733–2740, 2022, doi: 10.1016/j.matpr.2021.09.255.
47. Hasan, A. S., Hassan, H. B., Hashim, A., Hasan, N. B., & Al-kawaz, Y. A. (2024). Modeling, Fabrication and Characteristics of Novel (PVA-SiC-In2O3) Nanohybrid Structures for Optoelectronic Applications. Silicon, 1-14, doi: 10.1007/s12633-024-02991-0.
48. Mbarek, M., Ltayef, M., Almoneef, M., & Alimi, K. (2025). A Deeper Investigation of New Organic Nanocomposite System MEH-PPV-P3HT/SWCNT for Optoelectronic Applications. Journal of Applied Polymer Science, 142(9), e56541.
49. Hasan, A. S., and Hashim, A. (2024). Design, Optimization, Structural and Electronic Properties of PVA/ZnO/SnO2 Nanostructures for Nanoelectronics Fields. Nanosistemi, Nanomateriali, Nanotehnologii, 22(3), pp. 643–654, https://doi.org/ 10.15407/nnn.22.03.643.
50. Hasan, A. S., Hashim, A., and Hasan, Z. S. (2024). Design and Exploring the Structure and Electronic Characteristics of PS/MnO2/NiO Nanosystem for Optics and Electronics Nanodevices. Nanosistemi, Nanomateriali, Nanotehnologii, 22(3), pp. 713–726, https://doi.org/ 10.15407/nnn.22.03.713.
51. Sari, D. S. P., Salim, A. A., Chamidah, N. L. F., Yuliana, E. S., Taufiq, A., Pujiarti, H., ... & Mufti, N. (2025). Performance enhancement of silicon heterojunction solar cells using ethylene glycol-doped PEDOT: PSS/SWCNT interlayers. Journal of Materials Science, 1-17.
52. Ali S. Hasan, Ahmed Hashim, Ahmed Ehsan Jassem, Mohammed H. Al-maamori, Yasir A. Alkawaz and Zahraa S. Alameer. Tuning and Ameliorating the Microstructure and Electronic Features of SiC/PtSi Promising Nanostructures Doped Optical Material for Multifunctional Optoelectronics

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Eureka Journal of Geoscience, Materials & Resource Engineering (EJGMRE)

ISSN 2760-4985 (Online) Volume 02, Issue 05, May 2026

https://eurekaoa.com/index.php/9

Applications. Silicon (2025). https://doi.org/10.1007/s12633-025-03328-1.

53. Al-Zanganawee, J., Al-Timimi, M., Pantazi, A., Brincoveanu, O., Moise, C., Mesterca, R., ... & Enachescu, M. (2016). Morphological and optical properties of functionalized SWCNTs: P3OT nanocomposite thin films, prepared by spincoating. Journal of Ovonic Research, 12(4), 201-207.
54. Ali S. Hasan, Mohammed H. Abbas, Ahmed Hashim, Ahmed Ehsan Jassem, Mohammed H. Al-maamori, Hussein. M. Khalid, Zinah S. Hasan and Zahraa S. Alameer. Ameliorating and Tuning the Microstructure, Electronic and Optical Features of PMMA-SiC-ZnO Futuristic Nanostructures for Tailored Nanoelectronics Applications. Silicon (2025). https://doi.org/10.1007/s12633-025-03344-1.
55. Abdullah, N., Nurazzi, N. M., Silverwood, I. P., Matam, S. K., Demon, S. Z. N., Sa'aya, N. S. N., and Baharin, K. W. (2025). Structural and morphological studies of non-covalent functionalization carbon nanotubes wrapped poly (3-hexylthiophene-2, 5-diyl) nanocomposites. Next Nanotechnology, 7, 100111.
56. Hasan, A.S., Hashim, A. & Khalid, H.M. Synthesis and Ameliorating the Features of PMMA/CdS-SiO2 Futuristic Nanomaterials for Nanoelectronics and Optical Applications. Trans. Electr. Electron. Mater. (2025). https://doi.org/10.1007/s42341-025-00620-0.
57. Mahakul, P. C., Sa, K., Subramanyam, B. V. R. S., Patra, K. C., & Mahanandia, P. (2018). Investigation of optical and electrical properties of MWCNT/rGO/poly (3-hexylthiophene) ternary composites. Journal of Materials Science, 53(11), 8151-8160.
58. Hadi, A., Salman, S. R., Al Maimuri, N. M., Hashim, A., Rashid, F. L., & Hasan, A. S. (2025). Synthesis and Tailoring the Optimization and Dielectric Properties of PMMA/PEG/Barium Titanate Hybrid Nanostructures for Energy Storage and Electronics Applications. Chemistry, 19(2), pp. 277–285, https://doi.org/10.23939/chcht19.02.277.

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Eureka Journal of Geoscience, Materials & Resource Engineering (EJGMRE)

ISSN 2760-4985 (Online) Volume 02, Issue 05, May 2026

https://eurekaoa.com/index.php/9

59. Saini, V., Li, Z., Bourdo, S., Dervishi, E., Xu, Y., Ma, X., ... & Biris, A. S. (2009). Electrical, optical, and morphological properties of P3HT-MWNT nanocomposites prepared by in situ polymerization. The Journal of Physical Chemistry C, 113(19), 8023-8029.