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The Prediction of Photoactive Semiconductor Potential of Bio-Activated Rice Husk Ash Using Analytical Method

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Keywords：Rice husk activated carbon, CuO, organic photosensitizer, analytical method.

ABSTRACT

This study investigates the photoactive potential of bio-activated rice husk ash (RHA) as a semiconductor using analytical methods for CuO and SiO2 extraction prediction. The study focuses on the enhancement of photoactive characteristics in RHA through bioactivation, utilizing pineapple peel juice as a natural activator. Analytical method based on UV-Vis spectroscopy peak frequency of RHA, sunked (SCNM), and floated (FCNM) products were utilized to determine CuO and SiO2 extraction potential. We employ modern physics theorem to determine photosensitizing capability of each sample based on CuO and SiO2 characterization results. The results indicate SCNM is the best material to extract CuO and SiO2 due to its lowest bandgap energy, Highest hole carrier concentration, highest electron-pair, and produce more photosensitive material. Hence, SCNM is the best RHA derivative for organic photoactive semiconducting material.

INTRODUCTION

The utilization of rice husk ash (RHA) as a precursor for semiconductor materials has gained significant attention due to its abundant availability and environmentally friendly characteristics. This study extends the understanding of RHA by exploring the bioactivation process with pineapple peel juice, aiming to enhance its photoactive potential.

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The introduction sets the stage by providing background information, outlining the significance of bioactivation, and establishing the need for predicting Copper Oxide (CuO) and silica (SiO2) extraction potential using advanced analytical methods.

RHA has gained attention as a potential source of semiconducting materials due to its unique composition and properties. RHA is primarily composed of SiO2 and silicon is a well-known semiconductor material. The silica content in RHA serves as the foundation for its semiconducting characteristics (Wu et al., 2014). Silicon is a semiconductor with a crystalline structure that allows for controlled electrical conductivity. In RHA, the silica component possesses a similar crystalline structure, and when appropriately processed or modified, it can exhibit semiconductor behavior (Roncali et al., 2007). Additionally, RHA may contain trace elements and impurities that can introduce additional semiconductor properties. The application of RHA as a semiconducting material involves various processes, such as purification, activation, or doping, to enhance its electrical and photoactive characteristics. Researchers may explore different methods, such as bioactivation with natural substances, to tailor RHA for specific semiconductor applications. The abundance of rice husks globally makes RHA an environmentally friendly and cost-effective potential source for semiconductor materials.

On the other hand, CuO serves as a compelling photosensitizer in the context of semiconductor materials due to its distinctive properties that facilitate efficient light absorption and electron transfer processes. As a photosensitizer, CuO harnesses its inherent semiconducting nature, characterized by a narrow bandgap, to absorb light in the visible and near-infrared regions of the electromagnetic spectrum (Hou et al., 2022). Upon absorption of photons, CuO generates electron-hole pairs, initiating photoexcitation (Mallik & Rath, 2022). The excited electrons can then participate in redox reactions, promoting charge separation and transfer processes crucial for various photoactive applications. Moreover, CuO has a unique electronic structure which includes multiple oxidation states. Consequently, the unique electronic structure enhances its capability to act as a versatile mediator in catalytic reactions, making it an ideal candidate for organic photosensitizers in diverse fields, ranging from solar energy conversion to photodetectors and environmental remediation (Mishra & Ahmaruzzaman, 2022). The distinctive attributes of CuO contribute to its effectiveness as a photosensitizer, fostering advancements in the development of efficient and sustainable semiconductor-based technologies.

In general, RHA does not naturally contain CuO as a primary component. RHA is predominantly composed of silica (silicon dioxide) or SiO2 along with other trace elements and impurities, and copper is not typically one of them (Putranto et al., 2021). However, when studying the UV-Vis spectrum of a material after undergoing specific treatments or modifications, certain absorption peaks or features may suggest the presence of additional compounds or elements that were not initially part of the material (Sun et al., 2013). CuO has been found on RHA when it used to enhance the performance of mortar (Fapohunda et al., 2017). The experimental study on a new mixture scheme of mortar using CuO from RHA triggers the formation of microporosity on a microstructure makes the mechanical energy transfer more effective. The pore formation on a microstructure can be due to electrical resistivity reduction triggered by a conductor or semiconductor traces such as multi walled carbon nanotube (MWCNT) (Yuan et al., 2019). The organic photosensitive molecule traces such as curcumin also can enhance photoactivity of a tofu pore (Satrio et al., 2020). Therefore, we find the CuO trace on RHA through this study.

In semiconductor materials, the formation of electron-hole pairs is a fundamental process that indicates charge transfer and plays a crucial role in the material's electronic behavior. Semiconductors have an energy band structure with a valence band and a conduction band separated by a bandgap (Böer & Pohl, 2023). At absolute zero temperature, the valence band is fully occupied by electrons, and the conduction band is empty. When a semiconductor is exposed to energy in the form of photons (e.g., light), electrons in the valence band can absorb this energy and move to the higher energy state of the conduction band. This transition leaves behind a "hole" in the valence band, representing an unoccupied electron state. The electron in the conduction band and the hole in the valence band together form an electron-hole pair. The electron-hole pair serves as an indication of charge transfer because the movement of an electron from the valence to the conduction band leaves a positive charge (the hole) behind (Lewkowicz & Rosenstein, 2009). The electron and the hole are essentially mobile charge carriers within the semiconductor, and their movement contributes to the material's electrical conductivity. In applications such as photovoltaic devices (solar cells) or photodetectors, the separation and movement of electron-hole pairs are critical (Hofmann & Koch, 2023). When an external electrical field is applied or when the semiconductor is part of a device structure, the electrons and holes can be separated, creating an electric current. This separation of charges is the basis for the conversion of light energy into electrical energy in solar cells and the detection of light in photodetectors.

Understanding and controlling the generation and movement of electron-hole pairs are key aspects to synthesize semiconductor material. Therefore, this study provides a theoretical analysis to confirm the presence of CuO on RHA based on electron-hole pair. The theoretical analysis result is backed by the elemental and photo sensitivity characterization test results. The validated theoretical analysis of electron-hole answers the presence of CuO on RHA in study [8]. In this study, the possibility of CuO formation on RHA is discussed according to electron-hole pair semiconducting material.

METHOD

A multi-steering-axle tank vehicle with circular section tank is presented to study the influence of the liquid load shift on the directional dynamics of the vehicle. The tank vehicle is modeled as a quasi-steady state three-dimensional roll plane model of the tank, and is assumed at a constant forward speed. A schematic sketch of the tank truck model considered in this study is shown in Fig. 1. dd The methodology section details the experimental procedures undertaken to investigate the photoactive semiconductor potential of bio-activated RHA. It covers the preparation of RHA, bioactivation with pineapple peel juice, and the analytical methods employed, such as UV-Vis spectroscopy for peak frequency determination and the characterization of SCNM and FCNM products. The section ensures clarity in experimental design, allowing for reproducibility.

In this study, the grinding process of RHA to achieve a particle size of 200 mesh was executed as a key component of the experimental methodology. Initially, raw rice husk ash was collected and prepared through controlled combustion, ensuring the removal of impurities. Subsequently, a precision grinding approach was adopted using a ball mill equipped with appropriate grinding media. The RHA was loaded into the mill, and grinding media were introduced to facilitate the comminution process. The milling operation was conducted under controlled conditions to ensure consistency and reproducibility. Periodic sampling during the grinding process allowed for the monitoring of particle size distribution. The grinding duration was optimized to achieve the target particle size of 200 mesh. The resulting finely ground RHA was then carefully collected for subsequent characterization and analysis. This methodological approach ensures the production of RHA with the desired particle size.

The RHA samples were subjected to High-Energy Milling (HEM) over the course of one million cycles. The HEM process involved the utilization of specialized milling equipment with high-energy input to systematically refine the RHA particles. Initially, raw RHA was carefully collected and prepared through controlled combustion. Subsequently, the samples underwent the HEM treatment, which encompassed repeated cycles of intense milling, effectively reducing particle size and promoting homogeneity. The milling duration of one million cycles was chosen based on preliminary optimization studies to achieve the desired nanoscale characteristics while avoiding potential agglomeration.

RHA samples underwent a bioactivation process through immersion in pineapple peel juice. The bioactivation was carried out at a controlled temperature of 60̊C for duration of 4 hours. This specific treatment aimed to enhance the photoactive characteristics of the RHA by leveraging the natural activating properties found in pineapple peel juice. The choice of temperature and duration was based on preliminary optimization studies to ensure effective bioactivation while minimizing potential side effects. The immersion process allowed for the interaction of the RHA with the bioactive compounds present in pineapple peel juice, facilitating the incorporation of these compounds into the RHA matrix. This bioactivation step is crucial in tailoring the RHA for potential applications as a semiconductor or photosensitizer, and the optimized conditions provide a basis for reproducible and controlled bioactivation in subsequent investigations. The immersion process produces sunked (SCNM) and floated (FCNM) RHA. Both SCNM and FCNM samples were separated and rinsed until dried.

The semiconducting carbon nanomaterial obtained was thoroughly examined using scanning electron microscopy (SEM) to assess its structural and morphological properties. This technique provides detailed insights into the effectiveness of the bioactivation process in inducing semiconducting characteristics. The SEM was performed for RHA, SCNM, and FCNM samples with 30000X magnification. Another characterization was UV-Vis spectroscopy which was utilized to examine the optical properties of the synthesized semiconducting carbon nanomaterial. The absorption spectra obtained through UV-Vis spectroscopy provided valuable information regarding the electronic transitions and bandgap characteristics, offering insights into the material's semiconducting behavior.

$$E = hf\,(J) \tag{1}$$

$$N = \frac{I}{E}(Cd.\ J^{-1}) \tag{2}$$

$$A = \log\left(\frac{I_0}{I}\right) = \in cl(\%) \tag{3}$$

$$c = \frac{mass}{volume}(kg.\ m^{-3}) \tag{4}$$

$$I = A.\ q.\ p.\ \mu_p.E(A) \tag{5}$$

$$n_h = \frac{1}{q.\ B} \cdot \frac{|V_H|}{I}(m^{-3}) \tag{6}$$

$$J = q \cdot p \cdot \mu_p \cdot E(A \cdot m^{-2}) \tag{7}$$

The investigation of electron-hole-pair in RHA, SCNM, and FCNM was accomplished through an analytical method. The determination of the number of electron-hole pairs was carried out employing the Beer-Lambert law (equation (2)) where the number of absorbed photons based on UV-Vis spectroscopy data (equation (3)) was correlated with the energy derived from incident photon energy (equation (1)). The concentration, essential for these calculations, was determined through the mass to volume ratio of each sample (equation (4)). The number of hole carrier was determined by equation (6) with electric current obtained from equation (5). The magnetic field (B) was assumed 2.5T, with hole velocity (VH) 1.5x10-3 V.m-1, the charge (q) was 1.6x10-19 C, and the average ion mobility (μ) was 1.4 cm2 s-1. The current density (J) on cathode was determined by equation (7).

RESULT AND DISCUSSION

Presenting the results of the study, this section discusses the findings in detail. The emphasis is on the comparison of photoactive characteristics among different RHA derivatives. Analytical results, including UV-Vis spectroscopy data and characterization of SCNM and FCNM products, are analyzed and correlated with the photosensitizing capabilities. The discussion interprets the implications of the results in the context of organic photoactive semiconducting materials, providing insights into the factors influencing CuO extraction potential.

The SEM imaging outcomes reveal discernible structural distinctions among the materials: RHA, SCNM, and FCNM. The micrographs illustrate distinctive morphologies, highlighting variations in surface topography and particle arrangements. These structural variances signify the diverse synthesis processes and treatment approaches employed, emphasizing the customized characteristics of each material. In Figure 1(a), the RHA sample exhibits a single large microstructure with attached smaller microstructures, while Figure 1(b) illustrates the SCNM's dense structure featuring irregular surfaces characterized by wrinkles and bumps. In contrast, the microstructures of FCNM, as depicted in Figure 1(c), appear smoother in comparison to SCNM.

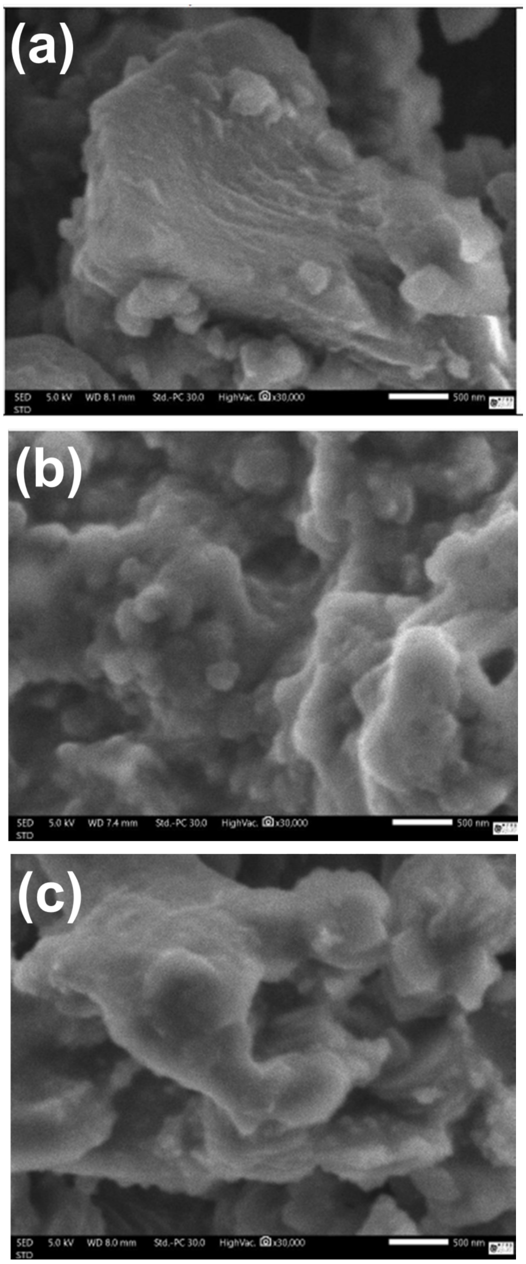


Fig. 1. The 30000x magnification SEM imaging results of (a) RHA, (b) SCNM, (c) FCNM.

The surface irregularities, serving as indicators of sample density, are prominently exhibited through the presence of wrinkles, particularly evident in the SCNM and FCNM samples. Increased wrinkles signify higher density, a characteristic observed in both SCNM and FCNM. Notably, the higher weight of SCNM compared to FCNM enables it to penetrate the liquid film, causing it to sink, while the lighter FCNM remains buoyant on the surface. Furthermore, the smaller contact surface area due to wrinkles in the denser SCNM generates higher pressure in water compared to FCNM, contributing to its sinking behavior.

EDS characterization results elucidate the atomic composition of each sample's surface. In Figure 2(a), the RHA sample predominantly comprises carbon (C) with a lower silicon (Si) content, presenting a 10:3 carbon-silicon ratio and Zn. Conversely, Figure 2(b) demonstrates that the SCNM sample contains more Si than carbon in a 5:9 ratio, additionally featuring Ferrous (Fe) and a trace amount of Aluminum (Al). The FCNM, illustrated in the same figure, exhibits a carbon to silicon ratio of 9:4, along with the presence of copper (Cu) atoms.

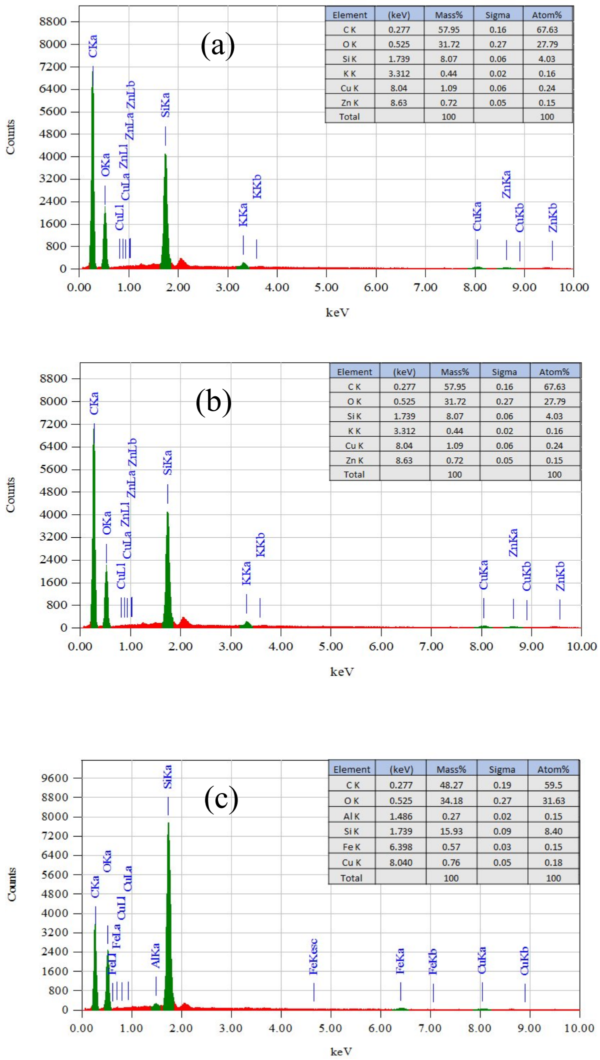


Fig. 2. The EDX spectrum shows the element of (a) RHA, (b) SCNM, (c) FCNM.

The elemental ratios play a pivotal role in dictating the functional characteristics of the materials. Consequently, we assess the Cu and Si ratios of each sample, visually represented in a bar chart in Figure 3. The presence of Copper (Cu) and Silicon (Si) signifies the semiconducting properties of the materials [8]. All samples exhibit the coexistence of Copper oxide (CuO) and Si, suggesting the potential extraction of both semiconducting materials. The likelihood of extraction is highest in SCNM, followed by RHA, and then FCNM. Moreover, the Cu to Si ratio serves as a determinant of the photoactivity of a material [9]. Silicon-based materials, like silicon wafers or silicon-based compounds, demonstrate photoactive behavior in the near-infrared (nIR) region (800-2500 nm wavelength), while CuO-based materials exhibit activity in the ultraviolet (UV) region (200-400 nm wavelength) with different bandgap characteristics [10].

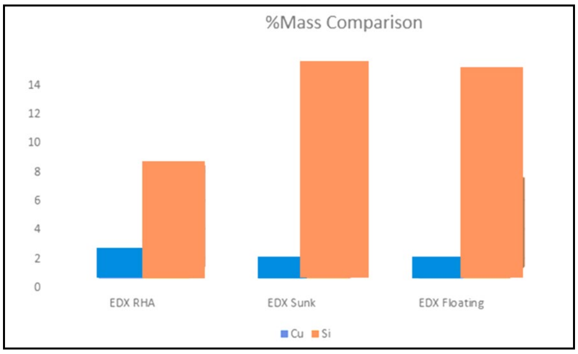


Fig. 3. The mass percentage comparison of Cu and Si content of RHA, SCNM, and FCNM.

The UV-Vis characterization, depicted in Figure 5, unequivocally verifies the photoactivity of each sample, namely RHA, SCNM, and FCNM. Evidently, all samples exhibit a peak in the light absorption region at the UV range, specifically around 200 nm, as evident from the consistent positioning of the curve formations in Figure 5(a), 5(b), and 5(c) for RHA, SCNM, and FCNM, respectively. This consistent absorption pattern substantiates the presence of CuO in each sample. Furthermore, the intensity of light absorption serves as a direct indicator of the concentration of CuO semiconducting material. Remarkably, SCNM and FCNM demonstrate comparable concentrations of CuO, as inferred from the similarity in their respective absorption intensities, highlighting the potential similarity in their photoactive characteristics.

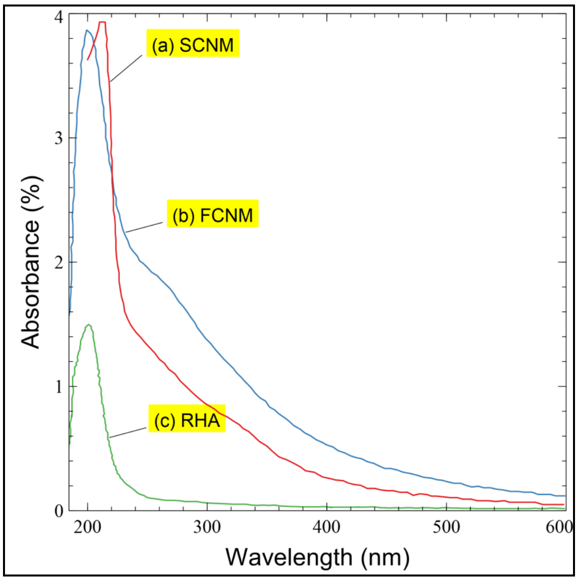
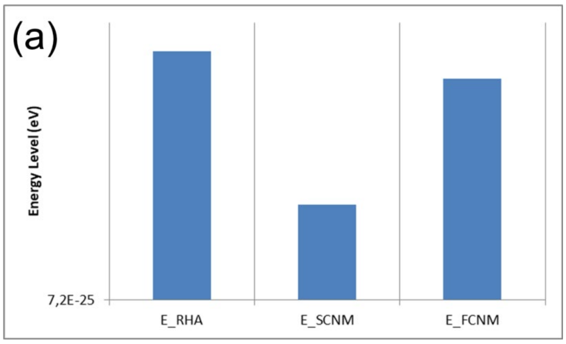
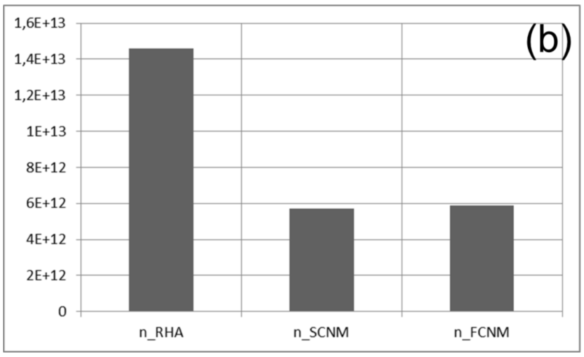


Fig. 4. The UV-Vis spectra of (a) SCNM, (b) FCNM, (c) RHA.

The analytical results based on UV-Vis characterization can be used to track the semiconducting material content. Figure 5(a) shows SCNM has the lowest bandgap energy while FCNM just slightly lower than RHA. The bandgap energy represents the amount of energy required to excites the electron on a certain orbital (Sofi'i et al., 2020). Therefore, the electron on SCNM valence orbital can jump to conduction band with lower energy. The electron population can be tracked by calculating the amount of hole-carrier concentration. In figure 5(b) the hole-carrier concentration of SCNM and FCNM are fewer almost half of untreated RHA. According to those results and the UV-Vis peak on UV range, the CuO mass can be predicted which shown in figure 5(c). The trace of CuO on low hole-carrier concentration samples was higher than the RHA. The CuO mass content of SCNM and FCNM are comparable.





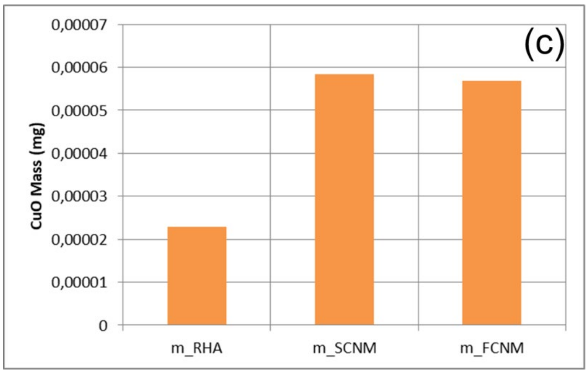


Fig. 5. The analytical results of (a) Bandgap energy, (b) Hole-Carrier Concentration, (c) Predicted CuO mass.

The hole-carrier concentration has a direct relation with electron concentration. Hole-carrier concetration determines the type of a semiconducting material (Kinzel et al., 2016). On high hole-carrier concentration, a semiconductor categorized as P-type (Positive type). Meanwhile, the N-type semiconductor contains more electrons than hole. When a semiconductor absorbs energy, typically through exposure to light or electrical excitation some electron-hole pairs are generated (Kim et al., 2018). A hole, created by the absence of an electron in the valence band, behaves as a positively charged carrier. Actually the hole itself is not positively charged but a neutral vacant region. However, the distribution of fermion such as electrons on a certain surface area or volume following the principle of energy minima (Coleman, 1963). The principle of energy minima is the similar principle to center of gravity (COG) on continuum mechanics. The balance state of a quantum system is achieved when the divergence of the energy vector is 0 (Dyadyusha & Kryachko, 1981). The dynamics of hole carriers involve their movement through the crystal lattice, a process influenced by external electric fields or thermal energy. Under the influence of an electric field, holes attracts electrons to migrate contributing to electrical conductivity (Dyadyusha & Kryachko, 1981). The movement of electrons to hole generates electric current.

SCNM has a potential as a good candidate for P-Type semiconductor. Figure 6 shows the amount of electron-hole pair in SCNM is the highest followed by FCNM and the untreated RHA. The presence of an electron-hole pair alters the electron density distribution within the material. Initially, electrons are concentrated in the valence band, contributing to a higher electron density in that region (Wang et al., 2023). When an electron is excited to the conduction band, it leaves the valence band, leading to a reduction in electron density in that band. Simultaneously, the generated hole in the valence band contributes to an increased hole density. Overall, the net effect is a redistribution of electron and hole densities across the semiconductor.

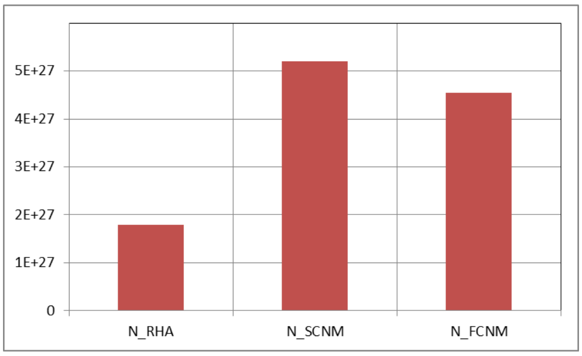


Fig. 6. The number of electron-hole pairs of each sample.

The CuO content in RHA is a critical aspect that directly influences the photoactive potential of the material, especially when considering its application as a semiconductor or photosensitizer. The CuO content refers to the concentration or amount of copper oxide present in the RHA after a specific treatment or activation process. During the bioactivation process, pineapple peel juice was utilized as a natural activator to enhance the photoactive characteristics of RHA. The analytical methods employed, such as UV-Vis spectroscopy and characterization of sunked (SCNM) and floated (FCNM) products, were crucial in determining the CuO content in different RHA derivatives. The results indicated that SCNM exhibited the highest CuO content, making it the most promising RHA derivative for organic photoactive semiconducting materials. In the absence of CuO in RHA, the appearance of distinctive peaks in the UV-Vis spectrum could indicate the introduction of copper or related compounds during a specific treatment process. This might occur through external factors like contamination, deliberate addition of copper-containing substances, or interactions with the environment.

The CuO content is pivotal because it directly correlates with the material's ability to generate electron-hole pairs upon exposure to light. Higher CuO content generally implies increased photoactive potential, as it enhances the semiconductor's capability to absorb and utilize light energy efficiently. This information is crucial for understanding and optimizing the photoactive properties of bio-activated RHA for potential applications in solar energy conversion and other photoactive technologies.

The generation of electron-hole pairs in a semiconductor material holds significant importance and can provide several key functionalities in various applications. Electron-hole pairs generated by absorbing photons of sunlight in semiconductors contribute to the photovoltaic effect. This phenomenon forms the basis of solar cells, where the separation and flow of these charge carriers result in an electric current, converting light energy into electrical energy (Dyadyusha & Kryachko, 1981). In photodetectors, the creation of electron-hole pairs upon exposure to light trigger an electric current or voltage change. This property is harnessed for light detection in devices such as photodiodes and phototransistors (Koc, 2020). Electron-hole pairs are essential in the operation of semiconductor devices like transistors and diodes. By controlling the movement and recombination of these carriers, electronic components can be manipulated to perform specific functions in integrated circuits (Koc, 2020). In light-emitting diodes (LEDs), the recombination of electron-hole pairs results in the emission of photons, producing visible light. This property is crucial for applications in lighting, displays, and optical communication (Chen et al., 2005). In photocatalytic materials, electron-hole pairs participate in redox reactions when exposed to light, leading to the degradation of pollutants or the activation of chemical processes. This has implications for environmental remediation and sustainable energy applications (Siavash Moakhar et al., 2021). In the emerging field of quantum computing, manipulating electron-hole pairs at the quantum level is explored for qubit operations, offering potential advancements in computing power and information processing (Manousakis, 2002).

As we advance our understanding of electron-hole pair dynamics in semiconductors, future improvements in theoretical analysis hold promising avenues for enhanced precision and predictive capabilities. Development of advanced computational models, incorporating quantum mechanical effects and sophisticated first-principles calculations, can provide a more accurate representation of electron-hole interactions in SCNM and FCNM. Integration of machine learning techniques offers an opportunity to extract nuanced patterns from vast datasets, enabling the discovery of subtle correlations that influence carrier dynamics. Additionally, multi-scale modeling approaches, linking atomic-scale behavior to macroscopic phenomena, can yield comprehensive insights into complex semiconductor systems. Addressing the challenges of carrier recombination and transport mechanisms through theoretical frameworks will contribute to the design and optimization of semiconductor materials for diverse applications, including more efficient solar cells, advanced electronic devices, and quantum computing technologies. The continuous refinement of theoretical analyses will propel innovations in semiconductor science, opening new frontiers for materials engineering and device design.

CONCLUSION

The conclusion summarizes the key findings of the study and their implications for the field of photoactive semiconductors. It reiterates the significance of SCNM as the optimal RHA derivative for CuO extraction, emphasizing its potential application in organic photosensitizers. Additionally, the conclusion may suggest avenues for future research, such as exploring other natural activators or optimizing the bioactivation process for further enhancement. In conclusion, this comprehensive examination of the photoactive potential of bio-activated RHA using advanced analytical methods contributes to the growing body of knowledge in the field of semiconductor materials. The findings not only showcase the efficacy of bioactivation but also identify a promising RHA derivative, SCNM, for organic photoactive semiconducting applications.

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