



Structural Morphology and Optical Properties of the Activated Carbon Decorated in Rubber Type Buna- N Nanoparticles Used in Industrial Applications

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Abstract

Potential uses for nanomaterials in light-emitting diodes, solar cells, polarizers, light-stable color filters, optical sensors, optical data communication, and optical data storage have led to the rise of interest in this field. Because they mix the qualities of two or more different materials and may exhibit unique mechanical, electrical, or chemical behaviors, nanomaterials are of special interest. Comprehending and adjusting these impacts may result in hybrid gadgets built from these nanocomposites that possess enhanced optical characteristics. In this work prepared polymer Buna-N with Activated carbon nanocomposites of well-defined compositions and studied the optical properties of powders and their thin films. The UV-visible light absorption spectrum was employed to describe the optical properties of industrial rubber – activated carbon composites. These composites, consisting of Plastic polymer Buna-N revealed a novel UV-visible absorption band in the wavelength range of 226-235 nm. This distinctive feature is attributed to interchain interactions within the material. To assess the optical properties, a successful optical transmission method was employed, enabling the determination of crucial parameters such as dielectric constant, absorption coefficient (α), and energy gap. Four samples of industrial rubber – activated carbon composites were analyzed in this manner. The UV-Visible spectrophotometer served as the primary tool for the optical characterization. The results highlighted the strong dependence of these properties on both the material's nature and the type of radiation used. The primary objective of this research is to enhance the optical properties of the polymer Buna-N decorated with activated carbon. The aims to leverage these improved properties for the extraction of oil. The goal is to develop a material that exhibits the best-suited properties for the conditions involved in drilling and oil extraction processes.

Introduction

Nanocomposites have been developed to fulfill various industrial needs, include making processing simpler and broadening the range of attributes by adjusting the kind, proportional amount, or structure of every constituent [1]. Notably, using the carbon black as a filler in Plastic Buna composites, the composite's characteristics can transition from insulating to conductive [2]. However, a significant concern is that Plastic Buna polymer composites are susceptible to degradation caused by exposure to sunlight. The degradation process is primarily driven by the action of UV radiation, leading to oxidation and resulting in photooxidation. The extent of degradation varies depending on the location, influenced by the intensity of radiation present. Variation holds considerable importance in numerous applications, as the degree of degradation affects the properties of the composites. For transparent compositions, this degradation manifests as a yellowing effect and generally results in a loss of mechanical properties, such as reduced elongation at break and diminished impact strength [3].

Nanocarbon materials are utilized to enhance the electrical and mechanical properties of Buna polymer composites. Among these materials, activated carbon stands out as the most effective stabilizer for most Buna polymers. Effectiveness of activated carbon depends on the type, size of particles, and the degree of their dispersion within the polymer matrix. Interestingly, activated carbon surpasses its predicted weathering stabilization ability, as it not only screens the polymer from UV light but also efficiently traps radicals formed during photooxidative processes, which otherwise lead to chain degradation. Additionally, activated carbon stabilizes polymers by quenching the excited states induced in Buna polymer due to UV radiation absorption [3,4].

Investigation of impact of UV light on polymers has garnered significant attention over the years, and spectroscopy plays a crucial role in this research. Industrial rubbers containing pendant aromatic ring groups, for instance, exhibit a distinct fluorescence band at longer wavelengths when exposed to irradiation. This phenomenon arises from the interaction of excited with ground state aromatic groups, leading to intermolecular excimers formation. The observed fluorescence serves as a valuable tool for studying polymer structures [5].

Additionally, when polymers are subjected to ionizing radiation, they undergo a wide range of changes in their physicochemical properties, often attributed to rearrangements in the chemical structure of Buna polymer caused by energy deposition [6].

Natural or industrial rubbers are composed of large hydrocarbon particles with double bonds. Throughout the various manufacturing processes, different materials are added to improve their optical properties, facilitate kneading, reduce costs, or enhance rubber resistance to weather conditions. The study of Buna is not only crucial for its industrial significance but also serves as an example of a chain structure with minimal disruptive interactions within its basic string configuration. Activated carbon is therefore not a product of the modern era; rather, its significance for both humans and the environment has been recognised for thousands of years. Because

of its remarkable capacity to adsorb toxins and hazardous gases, or what is known as the phenomenon of adsorption, active carbon has found widespread applications in magazines, toothpaste, medicine preparation, mineral extraction, and many other industrial settings.

Experimental Details

1. Chemicals Materials

We bought natural activated carbon from Aldrich that was 99.9% pure and had a particle size of 150 mm. The remaining compounds utilised in this investigation are all analytical-grade materials that were bought from Sigma Aldrich and didn't require any additional purification.

2. Synthesis of Activated Carbon (AC)

A 50 mm Nano activated carbon sample was taken and subjected to heat treatment in an oven at temperatures ranging from 50 to 100°C for 24 hours. Subsequently, it was further heated at 100°C for 7 hours, ground, and then passed through a 50 mm sieve. The particles retained under 50 mm were selected for subsequent experiments, including the preparation of activated carbon from date stones using the physical activation method. The preparation method involved impregnating the dried and crushed date stones with an activating agent, such as $ZnCl_2$. The impregnated stones were then subjected to carbonization at high temperatures. The aim of these investigations was to determine the optimal operating conditions for the process.

3. Preparation Buna Polymer

Transparent rubber polymer, specifically Buna, was utilized in this study. To dissolve the polymer, a 97% pure organic solvent called HEPTAN was employed. Various concentrations of polymer solutions were prepared by melting specific weights of Buna in 100 ml of the organic solvent. This approach was taken to expedite the dissolving process. The Buna polymer- activated carbon composites were then created, incorporating different percentages of activated carbon, ranging from 3 to 12 wt%. These composite samples, with a thickness of 0.15mm, were further cut into sizes measuring 2.6×2.8 cm². For further analysis, all the composite samples underwent UV-Visible transmission and reflection studies. A Shimadzu double-beam UV-VIS Spectrophotometer (UV-210 A) was employed for this purpose, covering the wavelength range of 190-800 nm. The measurement method used in this study was previously described elsewhere [6]. Additionally, the samples were annealed in air at a temperature of 30°C as part of the experimental process.

Optical Calculation

To correct for offsets caused by instrument baseline drift, temperature, scattering, and refractive effects, the ultraviolet-visible absorbance above 700 nm was considered negligible. Thus, the average sample absorbance

within the range of 700 to 800 nm was subtracted from the spectrum. This adjustment was made to ensure accurate measurements and reliable data analysis.

Absorbance units were converted to absorption coefficients follows [7]:

$$\alpha = 2.303 \frac{A}{d} \dots\dots\dots(1)$$

Where absorption coefficient (α) (m⁻¹) for the solutions, (A) is the absorbance for the solution, and (d) the thickness of samples.

The extinction coefficient is calculated by using the following equation [8]:

$$K = \alpha \lambda / 4 \pi \dots\dots\dots (2)$$

Ultraviolet-visible (UV/Vis) spectroscopy has emerged as a significant tool for estimating the optical gap energy (E_g) in polymers. The optical absorption edge can be linked to the optical gap energy (E_g) through Tauc's equation [9]. By extrapolating the spectrum and identifying its intersection with the abscissa, we can determine the optical gap energy (E_g). Tauc's equation, essential for this analysis, is provided below [6,8,9]:

$$\alpha h\nu = A (h\nu - E_g)^n \dots\dots\dots (3)$$

Results and Discussion

A distinct (002) peak is clearly visible at 26.4° in the XRD spectrum of activated carbon containing Buna polymer. This peak vanishes from the XRD pattern following the oxidation processes, and a new peak is seen at 44.6°, which suggests that the activated carbon is present and corresponds to the (101) carbon planes.

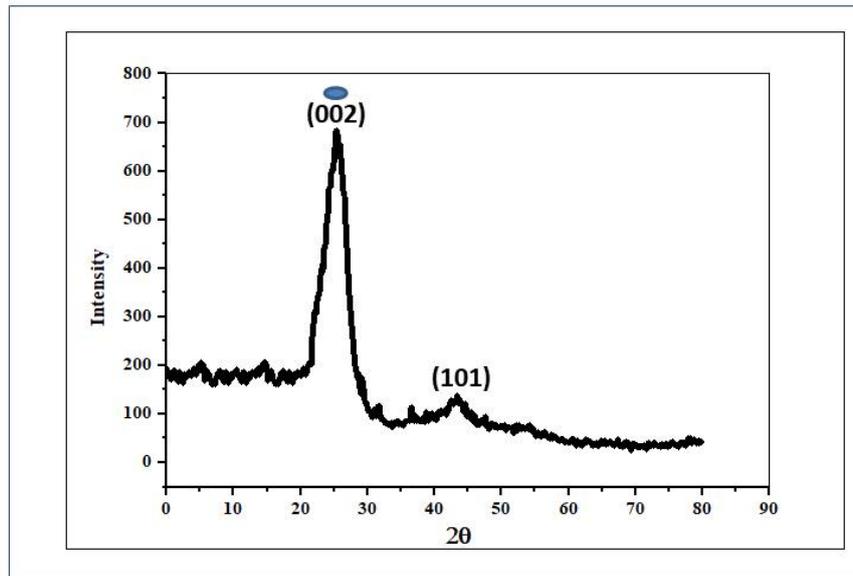


Fig (1) show XRD patterns of Activated Carbon – Buna polymer nanocomposite .

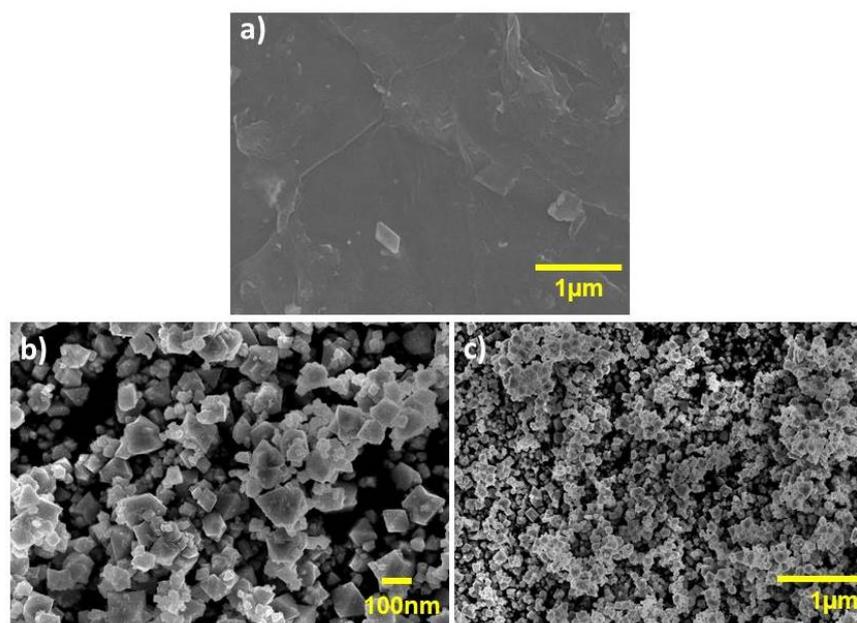


Fig. 2 High magnification FESEM images of (a) pure activated carbon and (b,c) Activated carbon decorated Buna polymer composite.

Using FE-SEM analysis, the morphologies of the as-prepared samples were studied. FE-SEM pictures of pure activated carbon and activated carbon embellished with composites made of buna polymer are displayed in Fig. 2. Figure 2(a,b, and c) displays the morphologies. The displays 30–100 nm thick activated carbon nanoparticles with a few tiny particles affixed to the surface. The morphology of activated carbon ornamented with composites

made of Buna polymers is shown in Fig. 2(b,c). The surfaces of these two samples displayed some irregular nanostructures along with regular nanoparticles.

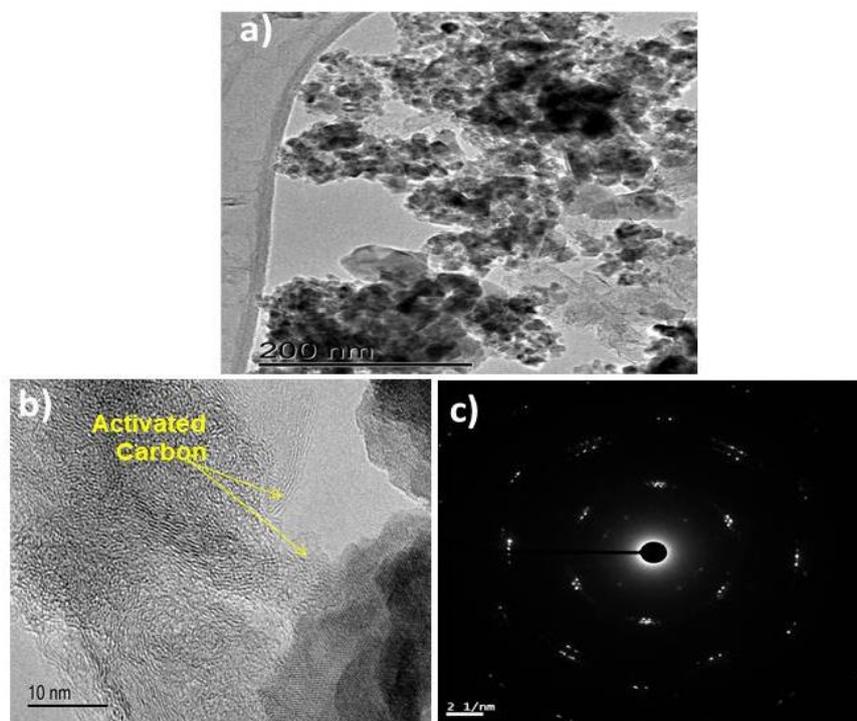


Fig. 3 (a,b) TEM images of Activated carbon decorated with Buna polymer , (c) corresponding SAED pattern.

Buna polymer composites embellished activated carbon morphologies. In figure 3(a-c), it was further investigated by TEM and HRTEM. The activated carbon-Bona nanostructure is depicted in a TEM picture in Figure 3(a), where the surface morphology indicates the presence of molecules. The link between the activated carbon and the Buna polymer structure is depicted in the HRTEM image in Figure 3(b), which is a crucial component for enhancing the electronic conductivity of the polymer and activated carbon HRTEM system. The accompanying selected area electron diffraction (SAED) pattern, shown in Figure 4(c), indicates that the porous activated carbon is crystalline. The rings that make up this electron diffraction pattern are clearly defined.

Figure 4 exhibits the typical UV-Vis spectra of Buna polymer - Nano activated carbon composites, illustrating the normalized spectra for different levels of activated carbon content (3 w%, 6 w%, 9 w%, 12 w%). Noteworthy, the addition of the filler to the polymer results in an intensified peak. Upon in-depth analysis of the UV-Vis spectra, a significant shift in absorption wavelength is observed, particularly within the 226-235 nm range, indicating the carbonization of polymeric materials when subjected to irradiation. This shift, moving absorption edge from the UV to the visible region, can be attributed to an increase in conjugation length. In this case, for a

linear structural polymer, there is a correlation between the optical band gap energy and the number of carbon atoms per conjugation length. [6,7,11].

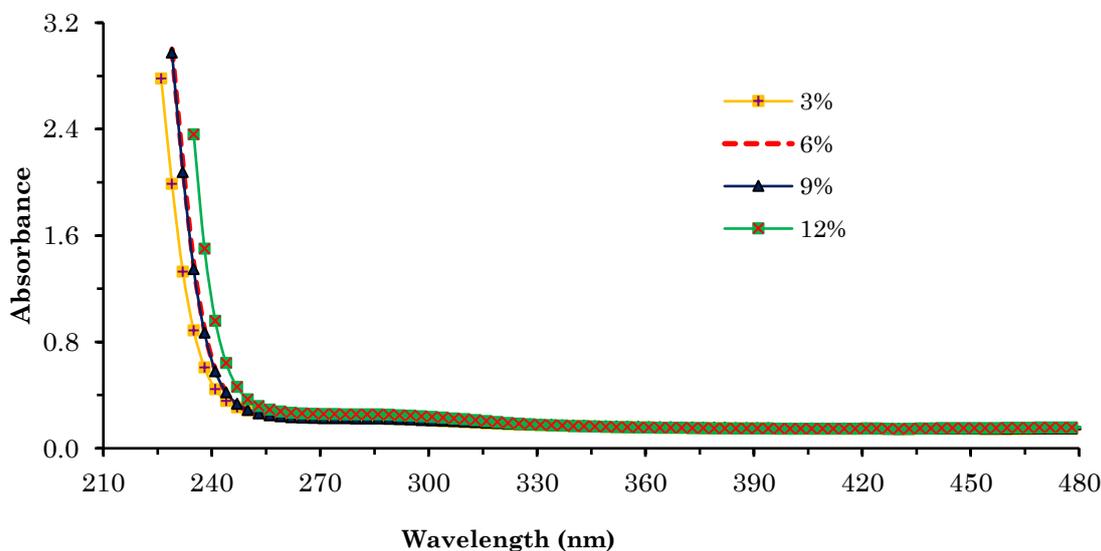


Fig. 4. UV/Vis spectra of Buna polymer- activated carbon composites

When light energy in the UV and visible spectrums is absorbed by polymeric materials, electrons in the n to π^* orbital shift from their ground state to higher energy states. The molecule's unsaturated groups, which supply electrons, make this possible. [6].

Figure 5 illustrates the absorbance value plotted against the concentrations of activated carbon in the Buna polymer. The observed results can be attributed to interchain interactions occurring outside the polymer coils. There is a slight increase in absorbance as the polymer coils get closer to each other due to the interchain interaction on their outer surfaces. With an increase in Buna polymer concentration, the concentration of Nano activated carbon groups increases linearly. Furthermore, it's expected that the microviscosity will gradually rise. [11,6].

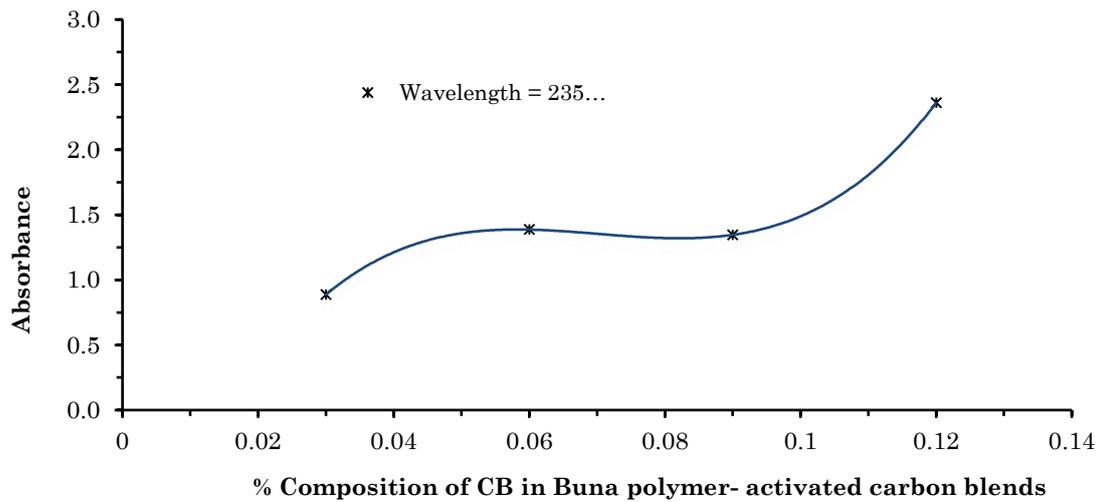


Fig. 5 The absorbance as function of CB content in (Buna polymer - activated carbon) composites

The absorption coefficient for each sample was determined using equation (1). It is evident that the absorption coefficient is strongly dependent on the energy (E) of the photons. Figure 6 demonstrates that when the energy of the photons (E) is less than the optical energy gap (Eg), no electron-hole pairs can be created, making material transparent and resulting in a small absorption coefficient. On the other hand, when E is greater than or equal to Eg, strong absorption occurs [10,12].

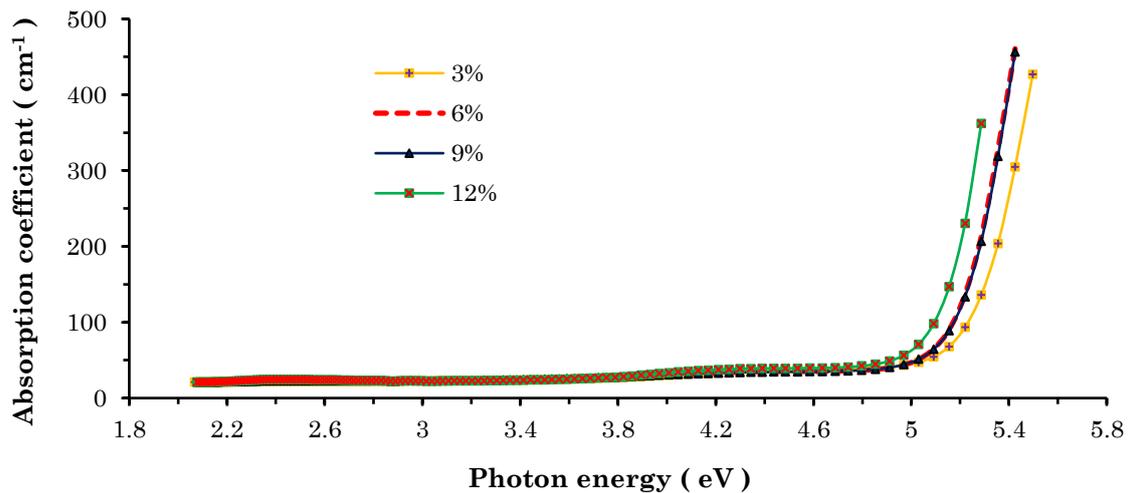


Fig. 6 . The Absorption Coefficient for Buna polymer-Activated carbon blnction of photon energy

To estimate the optical energy gap, optical measurements are analyzed using the expression for optical absorbance and photon energy (E) with equation 3. The optical band gap is obtained by extrapolating the linear portion of the plot of the absorbance versus E to $E=0$. Figure 4 illustrates a straight line representing direct transitions with a value of $n=2$ [9-13]. Figure 7 displays the optical gap values of Buna polymer – Nano activated carbon composites, which are measured at 5.1 eV, 5.02 eV, 4.99 eV, and 4.9 eV for CB concentrations of 3%, 6%, 9%, and 12%, respectively. This trend of decreasing optical gap values with increasing CB content in the polymer can be attributed to the reduction in packing density as the CB content rises [14-15].

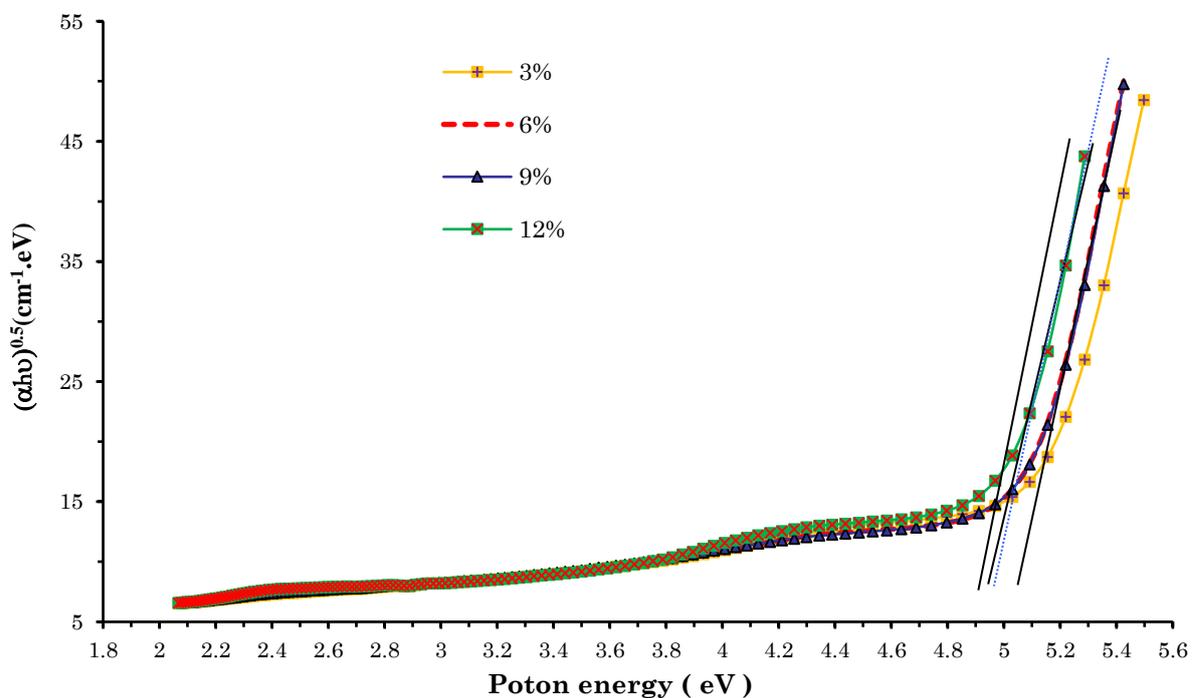


Fig. 7 . Plot of $(\alpha hu)^{0.5} \cdot hu$ for Buna polymer-activated carbon composites

Figure 8 shows how the extinction coefficient (k) for composites made of Buna polymer and activated carbon varies with wavelength. The graph shows that the extinction coefficient falls with increasing incident wavelength and rises with higher weight percentages of added activated carbon in the Buna polymer. The high absorption coefficient explains this behaviour of the extinction coefficient. The findings show that the host polymer's structure is altered by the doping atoms of activated carbon. [16-20].

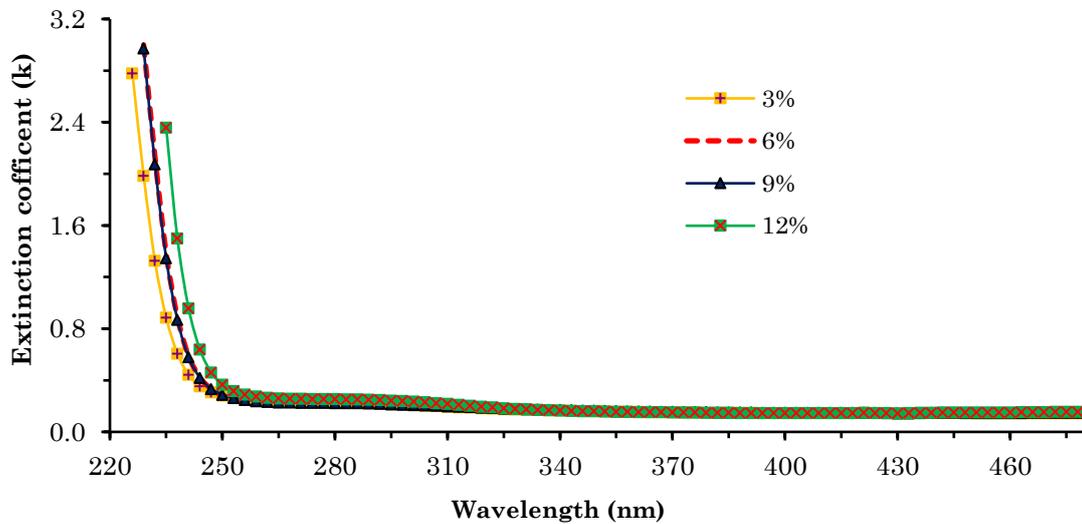


Fig. 8. UV/Vis spectra of Buna polymer – activated carbon composites

Conclusion

In summary, the study examines various parameters that influence the structure and properties of Buna polymer–Nano activated carbon composites. An optical method is employed to measure these composites, utilizing total reflectance at a wavelength range of 190-800 nm. The results demonstrate that the optical properties of the composites can be effectively altered by modifying the content of activated carbon.

Specifically, the absorption coefficient increases with higher filler wt.% content, while the optical energy gap decreases with increasing CB concentration in the Buna polymer. Furthermore, the extinction coefficient (k) shows an increase with the weight percentage of added activated carbon to the polymer and decreases as the incident wavelength increases.

The progress activated carbon –Buna nanocomposite development has given rise to novel materials with distinct properties, dependent on the type of nano-modified material and the manufacturing method used. Polymer and nanocomposites are gaining momentum in numerous applications across various industries, such as petroleum, food packaging, biomedicine, wastewater treatment, and materials with enhanced physical and chemical properties. These compounds hold great promise for large-scale applications in diverse fields.

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