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Development of phenolic-modified activated carbon for reduced energy band gap and improved semiconductor performance

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Abstract

This study aims to develop more efficient activated carbon-based semiconductor materials through modification with phenolic compounds to reduce the energy gap and increase adsorption capacity. Activated carbon was modified by adding phenolic compounds, then characterized using FTIR, UV-Vis, SEM, and EDS to analyze structural, morphological, and electronic changes. The UV-Vis characterization results showed that the AC 70 + F 30 sample experienced a wavelength shift towards the x-axis, which indicates a decrease in energy gap and is confirmed by Tauc plot analysis from 3.60 eV to 2.98 eV. SEM-EDS results revealed changes in pore morphology and a decrease in carbon content due to the interaction between activated carbon and phenolic compounds. These findings indicate that phenolic modification effectively reduces the energy gap and improved charge-transfer characteristics, thereby contributing to the development of more environmentally friendly and efficient activated carbon-based semiconductor materials.

Keywords:
Activated carbon, phenolic compounds, and energy gap.

1 Introduction

Activated carbon, a form of amorphous carbon with a broad pore structure, is widely used as a key component in various industrial sectors. Activated carbon can adsorb solutes, gases, and liquids, making it a very valuable material in environmental technology and waste treatment. The development of carbon-based materials, such as activated carbon, continues to be enhanced along with its abundant availability, low production cost, and environmentally friendly properties [1], [2]. Activated carbon (AC), which is obtained from biomass [3] such as coconut shells, has a high surface area and pore structure that supports the adsorption process and enhances photocatalyst activity, and has honeycomb-like cavities that can adsorb and enhance photocatalyst activity [4], [5]. Along with the advancement of industrialization and efforts to reduce environmental impact, activated carbon has become a major choice in environmentally friendly semiconductors [6].

Current research focuses not only on improving the adsorption efficiency of activated carbon, but also on optimizing its functionality through surface modification techniques and incorporation with other materials. These efforts aim to reduce the energy gap between adsorption and desorption processes, which often hinders the performance of activated carbon in semiconductors, especially on an industrial scale. Too wide an energy gap can reduce process efficiency, increase energy consumption, and reduce the ability of activated carbon in continuous adsorption. However, in the quest to develop more functional and efficient activated carbons, a number of significant challenges have been faced. Research combining activated carbon with other materials, such as phenolic resins, shows the potential to produce composite materials with higher performance. Such composites are expected to increase adsorption capacity, as well as reduce the energy gap that hinders the application of technologies in the renewable energy domain [7].

Nonetheless, the limitation of activated carbon in light absorption capacity is still one of the main challenges [8]. The energy gap in activated carbon is still relatively wide, while its thermal stability is also not optimal [9]. In response to these issues, the development of blends between activated carbon and natural fibers has been identified as a promising solution [10]. These composites can improve the adsorption properties and thermal stability of activated carbon, providing more durability in applications at high temperatures and extreme conditions. However, research on the integration of phenolic compounds in the structure of activated carbon is still limited, even though these compounds can improve the properties of activated carbon-based semiconductors.

Research on activated carbon modification shows that phenolics can affect material characteristics and increase adsorption capacity [11]. Previous studies have also shown that changes to the surface of activated carbon can improve its adsorption properties, as seen in research on activated carbon from various raw materials [12]. This opens up the possibility of designing higher-performance materials that can be applied in areas such as gas filtration, energy storage, and water purification. Although the positive effects of modifying activated carbon using phenolic compounds have been discussed, their application on a practical scale is still very much under-explored [13], [14]. Therefore, further research needs to be conducted to explore various modification methods that can improve the overall capabilities of activated carbon.

Recent research has also emphasized the importance of optimizing activated carbon treatment methods to improve its performance in more efficient technological applications [15]. One promising approach is to use thermal or hydrothermal treatment techniques that can significantly alter the microstructure of activated carbon, thereby increasing its adsorption capacity. In addition, the development of more environmentally friendly processing techniques is also a major concern to reduce the negative impact on the environment.

Phenolic compounds, with chemical structures consisting of aromatic carbon rings and hydroxyl groups, have been identified as having potential as semiconductor materials [16]. The aromatic ring allows delocalization of electrons, while the hydroxyl group plays a role in attracting those electrons, which can increase light absorption [17]. The addition of phenolic compounds is expected to contribute significantly to increasing the adsorption efficiency [18]. In addition, phenolic compounds can also affect the mechanical and thermal properties of carbon-based materials, which are crucial in improving the durability and stability of activated carbon composites. With potential new applications for carbon-based materials, the collaboration between activated carbon and phenolic compounds is expected to be further explored to find better solutions in material and energy technology applications [19].

The novelty of this study lies in the use of a unique low-temperature modification method with a ratio of AC 70 + F 30, as well as integrated UV-Vis-Tauc plot and SEM-EDS analysis to link electronic structure changes with morphological transformations, which has not been reported in previous studies. The combination of activated carbon and phenolic compounds has the potential to open new opportunities in the development of more sustainable and efficient materials for various applications in renewable energy. This research aims to reduce the energy gap in activated carbon by modifying its electronic properties. A smaller energy gap in activated carbon can increase its conductivity and potentially improve the performance of this material in various applications, such as energy storage, sensors, and catalysis. With the addition of an organic compound, phenolic, which is believed to affect its electronic structure, this research hopes to make an important contribution to the development of new technologies that are more efficient and sustainable.

2 Methode

Coconut shell activated carbon uses the HayCarb brand, which uses a mortar and blander, then sieved to obtain a uniform particle size of 200 mesh. Phenolic using Hylocereus spp Hotto brand. Ethanol 96% as a solvent in the mixing process. The phenolic addition process is shown in Fig. 1.

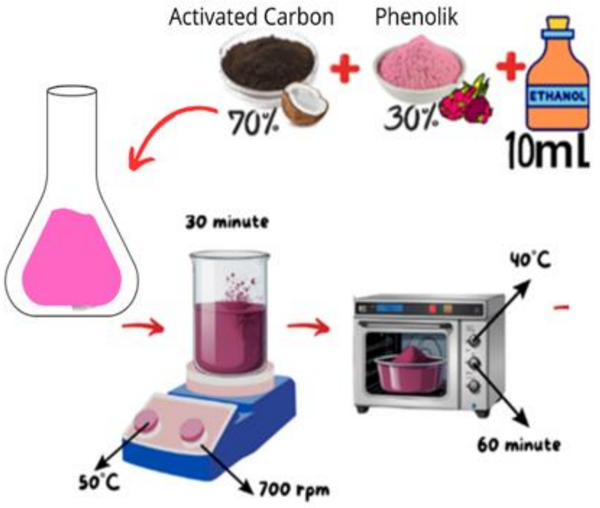

Fig.1. Phenolic addition process

In this study, the composite was prepared using a composition of 70 wt% activated carbon (AC) and 30 wt% phenolic. The mixture was combined with 10 mL of 96% ethanol, as shown in Fig. 1. The precursor mixture was then mechanically homogenized using a magnetic stirrer at a constant speed of 700 rpm for 30 minutes at a controlled temperature of 50 °C. After mixing, the slurry was subjected to a heating process in a drying oven at 110 °C for 2 hours to remove residual solvents. The dried composite was then thermally activated in a muffle furnace at 300 °C for 1 hour under atmospheric conditions to initiate structural bonding between phenolic groups and activated carbon surfaces.

For UV-Vis characterization, the samples were dispersed in ethanol at a concentration of 0.1 g per 10 mL and sonicated for 10 minutes to ensure uniform suspension before measurement. UV-Vis spectra were recorded within the wavelength range of 200–800 nm using a double-beam spectrophotometer. Band gap energy values were calculated using the Tauc plot method with equations based on indirect transitions (αhν)1/2(\alpha h\nu)^{1/2}(αhν)1/2 versus photon energy. Numerical band gap values for each sample are provided along with the corresponding UV-Vis absorbance curves.

Fourier-transform infrared (FTIR) analysis was performed in the range 400–4000 cm^{-1} to observe functional group changes due to phenolic incorporation. SEM analysis was conducted at 10 kV accelerating voltage with magnification ranging from 500× to 5000×, while EDS was used to quantify elemental composition changes before and after modification. All measurements were performed at ambient pressure and room temperature unless otherwise stated.

3 Result and discussion

The band gap is an important parameter for semiconductors, as it determines the energy required for electrons to move from the valence band to the conduction band. The smaller the band gap, the easier it is for electrons to move. Semiconductors, having a small band gap, allow the valence electrons of the material to jump to the conduction band when energized [1]. Band gaps also allow semiconductors to convert light into electricity. The process affects the energy absorbed and released by electrons that move freely between the valence band and the conduction band. When electrons are in the energy band gap area, electrons can move freely. Electron movement will produce an electric current. The band gap indicates the electrical conductivity of a material. The smaller the band gap, the more electrons will move from the valence band to the conduction band, making it easier for current to flow [20], [21].

Based on the UV-Vis results (Fig.2), the AC 70 + F 30 sample experienced a shift in the absorbance peak to the longer wavelengths. Quantitatively, the energy gap decreased from 3.60 eV (pure AC) to 2.98 eV, indicating an increase in the material's ability to absorb low-energy photons. This decrease in energy gap is associated with π-π stacking interactions between phenolic aromatic rings and amorphous carbon groups, which cause more extensive electron delocalization. This mechanism is consistent with the trend in the Tauc plot curve shifting closer to the X-axis.

Fig.2 shown sample AC 70 + F 30 wavelength shifts to the right. Where the speed of light will be inversely proportional to the wavelength [22]. Based on the Lambert-Beer law, when the wavelength is getting bigger, it produces smaller energy; on the other hand, when the wavelength is short, it produces higher energy (Eq. 1).

$$E = hc/\lambda \qquad (1)$$

This occurs because of the interaction between the anthocyanin chromophore group and AC, resulting in greater electron decolocation [23],[24]. In principle, the lower the energy gap, the lower the energy required to excite electrons from the valence band to the conduction band. This increases the material's ability to absorb light and the efficiency of the charge transfer process [25].

Tauc's method for estimating the Eg of semiconductors from optical absorption spectra by UV-Vis spectroscopy [26], [27]. Fig.3. It is assumed that the optical absorption coefficient a of the semiconductor depends on the energy (h v) [28], [29], according to the following Eq. (2-3).

$$hv = \frac{1240}{\lambda}\ (eV) \qquad (2)$$

$$(\alpha hv)^n = A\ (hv - eg) \qquad (3)$$

UV-Vis analysis using the tauc plot method, Fig. 3 lowest energy gap for AC70 +F 30 than other samples, and the tauc plot curve shifts to the left near the x-axis in accordance with Planck's law, the larger the wavelength, the smaller the energy gap [30], [31]. The shift to the left indicates that electrons can be triggered from the valence band to the conduction band with lower photon energy, and absorb light more easily. This shows that AC 70 + F 30 can absorb light with lower energy so that absorption and charge transfer increase [32].

The cause of the decrease in energy gap is due to the decrease in the content of Carbon atoms with EDS analysis (95.75% to 78.93%). This shows that the addition of anthocyanin increases the reactivity of AC by changing its electronic properties [33]. The addition of anthocyanin is able to broaden the light absorption at higher wavelengths.

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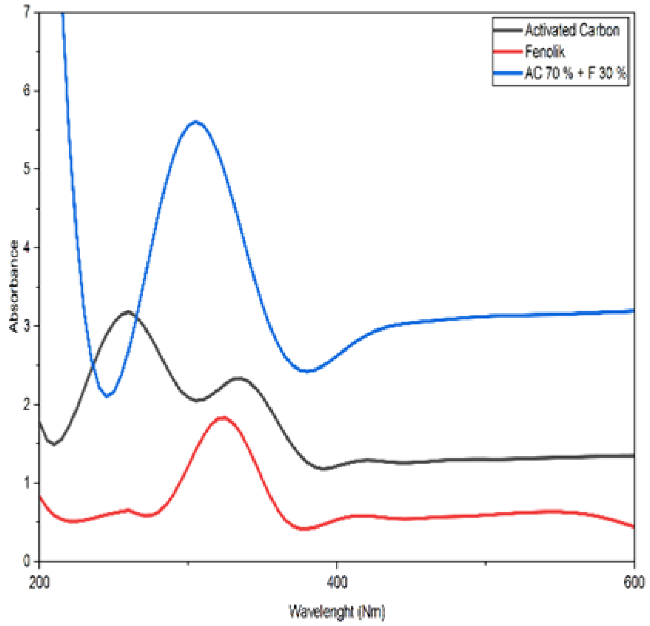

Fig.2. Uv-Vis results

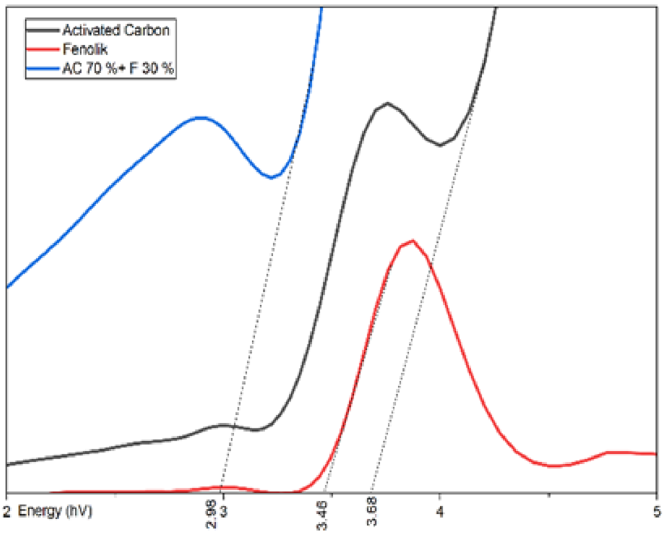

Fig.3. Uv-Vis analysis using tauc plot

SEM analysis with ImageJ software shows the porous structure of activated carbon [34]; the surface looks rough and porous, indicating a high specific surface area. And can increase the surface area due to a lot of surface area, easily accessible to molecules [35], [36], [37], [38]. The higher the level of roughness and the number of pores, the greater the uptake compared to a smooth surface [6], [39].

Quantitative SEM analysis using ImageJ (Fig. 4) showed an increase in pore area from 12.4 µm² (pure AC) to 15.7 µm² in the AC 70 + F 30 composite. This increase in porosity indicates that phenolics not only adhere to the surface of AC but also alter the microstructure through the formation of new pores or the enlargement of existing pores. This is reinforced by the emergence of a rougher surface with a more homogeneous pore distribution, which directly affects the increase in the adsorption capacity of the material.

It also indicates a high surface area, contributing to better adsorption capacity. These surface characteristics are usually obtained through an activation process that stimulates pore formation, as illustrated by studies describing activated carbon that has pores with a specific size distribution and high specific surface area [40], [41]. The pores that are formed serve as additional areas that can be accessed by adsorbate molecules, which are very important in separation and catalysis applications [42].

The addition of pores to the activated carbon structure increases the adsorption capacity of certain materials, such as gases or ions, potentially improving performance in a variety of applications, including air and water filtration. It was found that higher porosity can increase the efficiency of activated carbon in adsorbing contaminants, as smaller molecules are more easily trapped in those voids. In addition, the rough texture of the activated carbon surface also contributes to better physical and chemical interactions with the adsorbed molecules, which strengthen the adsorption properties of the material [35].

The surface around the pores has a purple-black color [43], indicating that electrons are repelled by negatively charged electrons but attract positively charged ions [44]. The negative charge comes from the oxygen functional group on the surface of the activated carbon, so that it affects the interaction of ions around the pores [45].

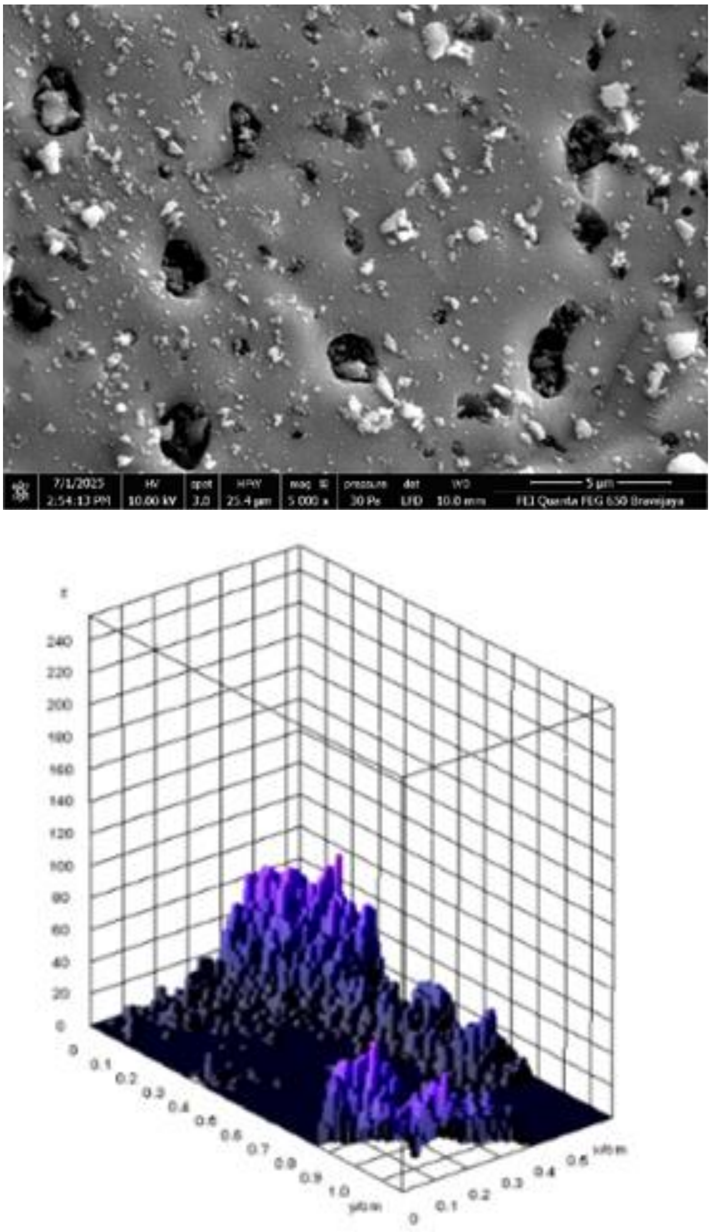

Fig.1. Result of SEM analysis and imageJ software analysis of activated carbon

The black-purple color visible around the pores in the SEM indicates the presence of negative charges on the surface of activated carbon, most likely due to the presence of oxygen functional groups (Fig.4). These groups, including carboxyl and phenol as shown in Fig. 5, serve to increase the adsorption affinity of activated carbon to other compounds, including phenolic compounds [46]. This effect occurs in the adsorption process, where strong interactions between surface charges and adsorbate molecules contribute to higher adsorption efficiency.

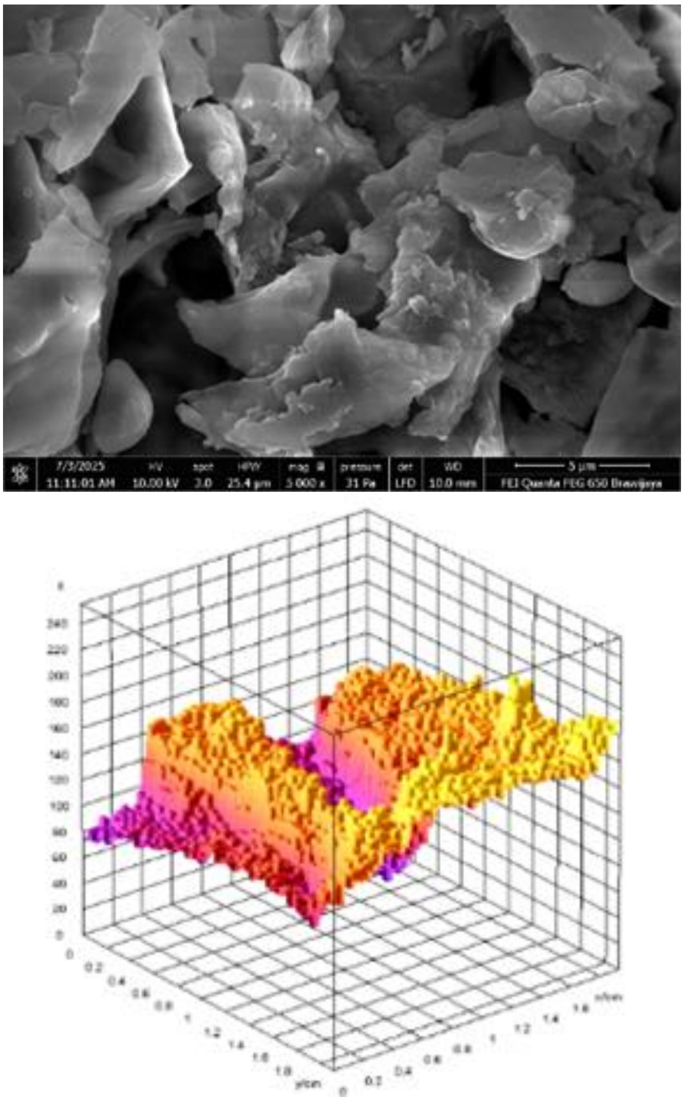

Fig.5. Result of SEM analysis and imageJ software analysis of fhenolic

The bright yellow and white colors show the electrons fired by SEM captured by the sample, the surface of phenolic and anthocinin is positively charged [47]. Partially positive H atoms in the hydroxyl group produce a brighter pattern than the results of ImageJ software analysis. Fig.6 in the AC 70 + F 30 sample, the bright yellow to white surface color shows that the specimen is positively charged because it attracts electron scattering [48].

A more in-depth analysis using ImageJ software shows the distribution of charges on the surface of activated carbon. The bright colors that appear for samples mixed with phenolic compounds reflect the presence of positive charges, as a result of the interaction between the hydroxyl (-OH) groups in phenolic compounds and electrons on the surface of activated carbon [49]. With increasing concentrations of hydroxyl groups, brighter areas in the image indicate that the material surface attracts more electrons, suggesting the presence of significant positive charges. These results are consistent with studies stating that -OH groups in phenolic compounds contribute to strong interactions with activated carbon, thereby increasing surface reactivity and adsorption capacity [50].

Overall, the combination of SEM and ImageJ analysis shows that activated carbon mixed with phenolic compounds not only has a more porous and reactive surface structure but also a positive charge that strengthens electron and ion interactions. This indicates a higher potential for applications in semiconductor technology and renewable energy [51], [52]. Thus, this research contributes to the development of new materials that can be utilized in various environmental and energy applications.

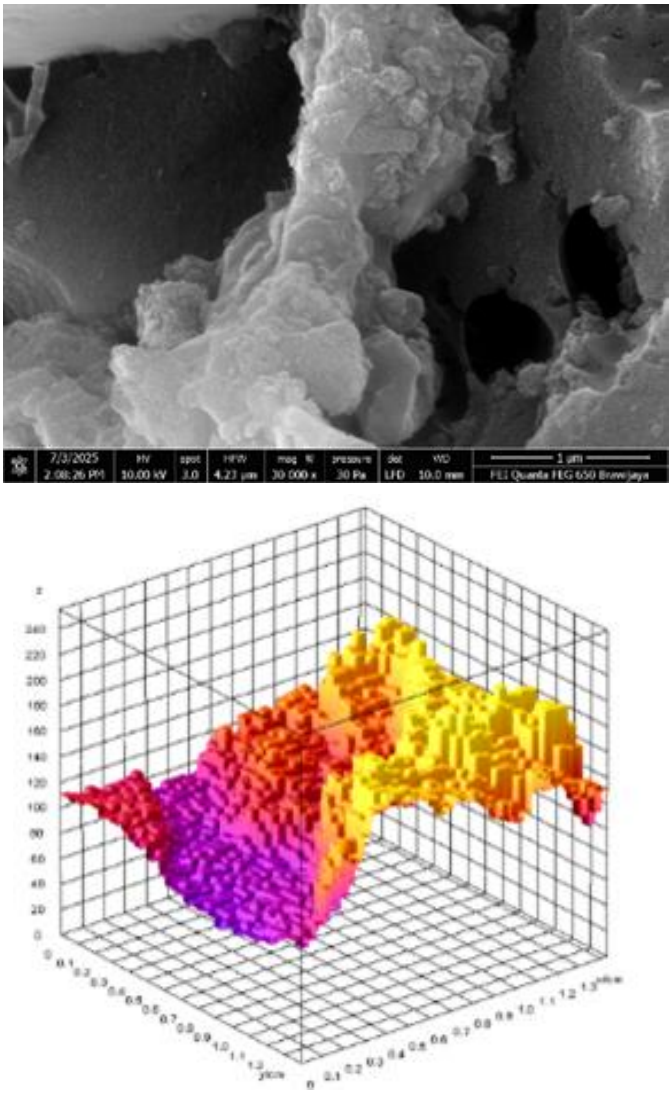

Fig.6. Result of SEM analysis and imageJ software analysis of AC 70 % + F 30%

Fig.7 EDS analysis, pure activated carbon (AC) carbon content of 95.75 proves that the material structure is still dominated by C atoms in the constituent of activated carbon [53], [54], [55], [56].

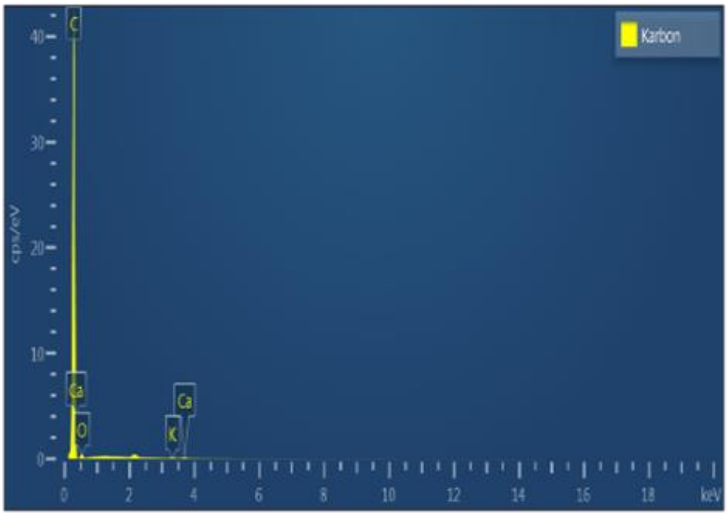

Fig.7. Results of EDS of activated carbon

After mixing with organic compounds in the form of phenolics and anthocyanins, the C content decreased significantly [57]. This happens because other elements are detected so that carbon atoms are reduced [58], [59], [60].

With the addition of relatively fewer phenolics, the distribution of non-carbon atoms from organic compounds continued to cover the AC surface. This phenomenon shows a strong interaction between the functional groups of organic compounds and the activated carbon skeleton, which then modifies the surface structure of the material.

Fig.8 shown fhenolic has many polar functional groups, which tend to bind to the AC surface through hydrogen bonds and π-π polar interactions [35], [61]. Phenolics are more effective in reducing Carbon content, indicating that phenolics tend to interact more reactively with AC. This decrease indicates that the presence of organic compounds with -OH, C=O, or C-O-C functional groups on phenolics begins to replace the dominance of carbon atoms.

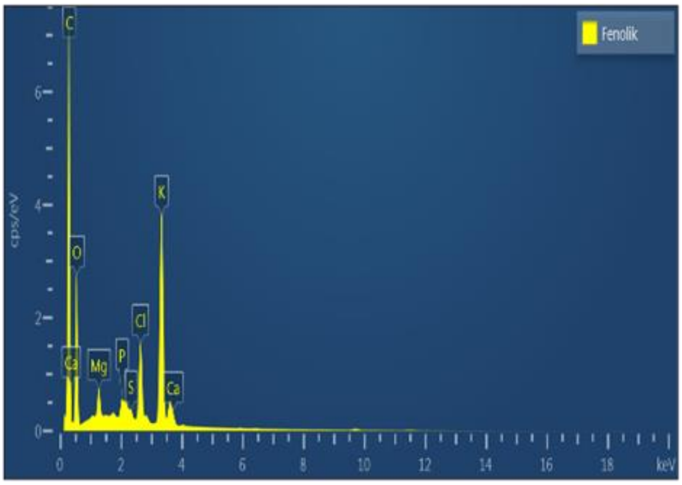

Fig.8. Results of EDS of fhenolic

EDS analysis shows that the oxygen (O) content in pure activated carbon (AC) of 3.99% has increased significantly after the mixing process (Fig.9). The oxygen content in the AC 70 + Phenolic 30 sample became 9.94 compared to pure activated carbon. Phenolic is an organic compound from the flavonoid group, rich in -OH functional groups, and has an aromatic ring structure with relatively labile π bonds. When phenolics are added to the activated carbon (AC) matrix, the oxygen groups of anthocyanins interact with the pore surface of activated carbon through hydrogen bonds and partial covalent bonds. With 30% phenolic concentration, the distribution of phenolic molecules becomes more even, so that oxygen groups can be more effectively bound. The increase in oxygen content indicates the formation of more oxygen functional groups on the surface of the material [62], potentially increasing the surface active properties and electron interaction capabilities of activated carbon-based semiconductor materials [63].

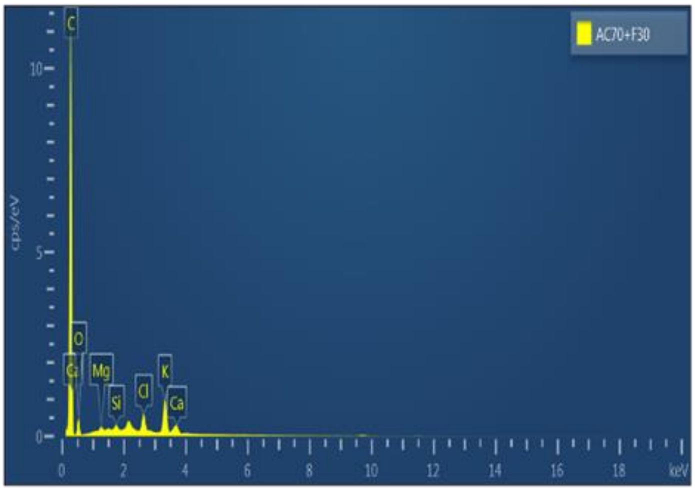

Fig.9. Results of EDS of AC 70 % + F 30%

The EDS results Fig.7.8.9. show a decrease in C content from 95.75% to 78.93% after the addition of phenolic compounds, along with a significant increase in O components from 3.99% to 9.94%. This confirms the successful attachment of –OH and C–O phenolic groups to the AC surface. This increase in oxygen content plays a role in reducing the energy gap through the formation of a new state near the valence band, thereby narrowing the distance between energy bands.

Changes in microstructure due to the addition of phenolic also have implications for the modification of the material's mechanical properties. Increased porosity and oxygen element distribution in AC–phenolic composites have the potential to reduce compressive strength but can increase energy absorption (toughness) and thermal resilience, which are important in mechanical engineering applications such as heat filtration, energy insulation, and lightweight structures. A more reactive surface and more uniform pore distribution are typically associated with lower brittleness compared to pure activated carbon, making the composite more stable against microcracks. This indicates that modification with phenolics not only alters the electronic properties but also enhances the material's potential for engineering applications with specific thermomechanical demands.

4 Conclusion

This study demonstrates that phenolic compound modification is an effective approach to improving the electronic and functional properties of activated carbon for semiconductor-related applications. The main findings are:

The addition of phenolic compounds to activated carbon can reduce the energy gap of the material. Among the tested compositions, AC 70 + F 30 sample showed the smallest energy gap shift indicates an increase in adsorption capacity and better charge transfer. These results were supported by the UV-vis test results showed the wavelength shifted to the right, indicating a smaller energy gap than pure activated carbon, and confirmed by Tauc plot method, where the curve shifted to the left, approaching the x-axis, so that the energy gap decreased from 3.60 eV to 2.98 eV.

The SEM-EDX results show a change in porous morphology and a decrease in carbon content caused by interaction with organic compounds. This increase contributes to better electronic interaction and improved thermal stability and adsorption capacity of the material, which has the potential to be more efficient in various technological applications In addition to improving semiconductor performance, the modification of activated carbon with phenolic compounds also shows potential for improving characteristics relevant to the field of mechanical engineering. Morphological and compositional analysis revealed changes in pore structure and surface bonding that could affect the mechanical properties of the material, such as thermal stability, surface roughness, and potential resistance to micro loads. This provides a scientific basis for further development of AC–phenolic composites as functional materials in engineering applications, particularly in energy systems and carbon-based devices.

Although the results show significant improvements in material performance, this study is limited to laboratory-scale testing and still requires further exploration in industrial-scale application.

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