

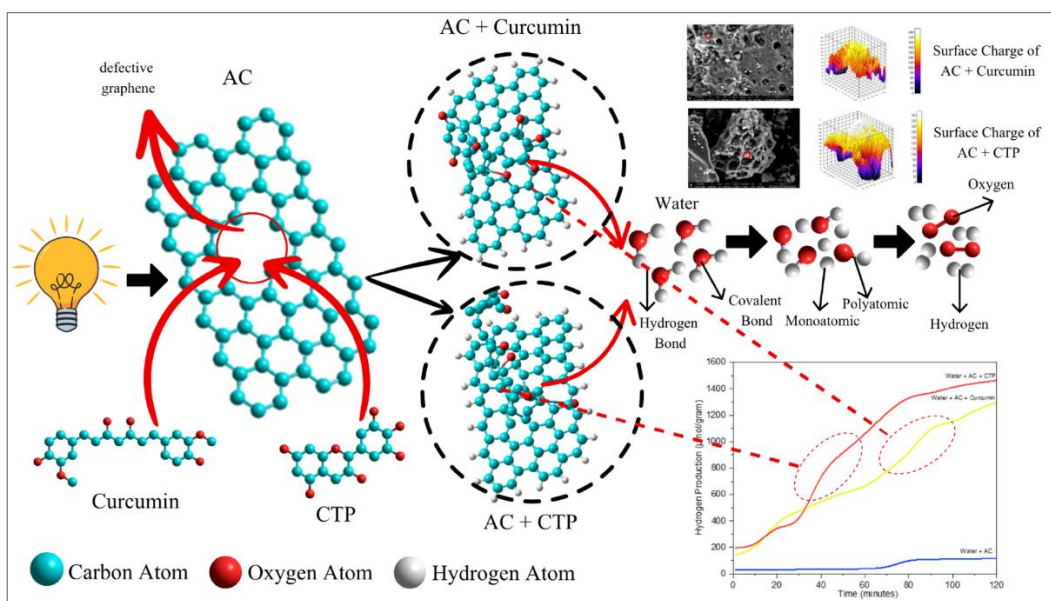
The role of aromatic rings, heterocyclic rings, and hydroxyl groups in increasing hydrogen production using activated carbon-based photocatalysts

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Highlights:

- Activated carbon combined with curcumin and Clitoria Ternatea Powder exhibits enhanced photocatalytic hydrogen production
- The AC + CTP systems shows superior hydrogen production performance compared to AC + Curcumin, indicating a more effective role of heterocyclic oxygen containing structures in charge transfer processes
- The presense of pyran based heterocyclic configurations promotes improved light absorption and charge carrier dynamics in the carbon-based photocatalyst
- These findings highlight the importance of molecular structure driven surface modification in designing efficient carbon-based photocatalysts for hydrogen production

Abstract

Hydrogen production using photocatalysis with activated carbon (AC) combined with curcumin and CTP has been investigated. Curcumin contains two aromatic rings and two –OH groups, while CTP contains two aromatic rings, one pyran heterocyclic ring, and six –OH groups at specific positions. However, the combined performance of these materials with AC has not been fully optimized, highlighting the need for further research to understand their chemical interactions in photocatalytic processes and their potential for renewable energy applications. This study aimed to determine the role of pyran heterocyclic rings and –OH groups in hydrogen production. The results showed that hydrogen production using pure AC was 115.75 μmol/g, while AC + curcumin and AC + CTP produced 1297.8 μmol/g and 1462.6 μmol/g, respectively. The higher hydrogen production in AC + CTP compared to AC + curcumin is attributed to the presence of pyran heterocyclic rings, which enhance photocatalyst stability and efficiency by reducing electron-hole

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recombination and expanding the light absorption spectrum, thereby increasing hydrogen evolution. Although the stacking interactions and active sites in the form of –OH, C–H, and C–O groups in AC + CTP are fewer than in AC + curcumin, the presence of oxygen atoms in the pyran heterocyclic ring contributes to greater hydrogen production. This study contributes to the selection of effective photocatalyst materials based on compound composition to support clean and sustainable hydrogen energy as an alternative to fossil fuels.

Keywords: Activated carbon; Clitoria ternatea powder; Curcumin; Hydrogen production; Defective graphene; Heterocyclic rings

1. Introduction

Hydrogen production through photocatalysis using active materials such as activated carbon (AC) has emerged as a promising method for generating environmentally friendly renewable energy. Activated carbon as a photocatalyst material offers significant advantages related to its high adsorption properties and good electronic conductivity [1], [2], [3]. To further enhance its photocatalytic performance, AC has been combined with organic compounds such as curcumin and CTP (Clitoria Ternatea Powder), which possess conjugated molecular frameworks and heteroatom-rich functional groups capable of modifying the surface electronic structure of carbon materials. Such modifications are expected to influence light absorption behavior and charge carrier dynamics, which are critical factors governing photocatalytic hydrogen production. Recent research shows that these extra elements have the potential to increase photocatalytic activity. However, the interaction between these materials and AC in the photocatalysis system requires further study to ensure its effectiveness in hydrogen production [4], [5]. However, the main challenge in using activated carbon for photocatalysis lies in its limited efficiency, especially in optimising photocatalytic reactions, which often depend on specific conditions, including sufficient ultraviolet light intensity [6]. Further development is needed to improve the efficiency and stability of the photocatalytic system and to understand the specific interactions that occur between activated carbon and the additives used [7], [8]. In this case, applying a more holistic approach to developing photocatalytic materials with better characteristics could help overcome these obstacles, making it a subject that continues to receive attention in renewable energy research [9].

Although activated carbon is a material widely used in hydrogen production by photocatalysis, the use of curcumin and CTP as additives to improve its performance has disadvantages that need to be considered. A lack of in-depth understanding of how curcumin and CTP play a role in improving the efficiency of photocatalytic reactions makes it difficult to achieve consistent results in various studies [10], [11]. Curcumin has a chemical structure consisting of two aromatic rings and two -OH groups [12]. The main compound in CTP is the anthocyanin type ternatin, which is a polyacylation derivative of delphinidin 3,3',5'-triglycoside that has two aromatic rings, one heterocyclic ring (pyran), and several -OH groups in certain positions [13]. However, the combined performance of these two materials with activated carbon has not yet been maximized, indicating the need for further research to understand the chemical interactions of each compound in the context of photocatalysis and the potential for renewable energy development [14]. The specific role of each compound in the photocatalysis process needs to be further investigated [8].

The problem in this research is that there is no clear understanding of the effect of the structure of curcumin and CTP compounds on hydrogen production, especially in relation to their structural differences. Curcumin and CTP have different chemical structures, where CTP contains one pyran heterocyclic ring and six -OH groups, the impact of which has not been widely studied in photocatalysis systems for hydrogen production [13]. The pyran heterocyclic ring in CTP serves to expand the π -conjugated system, which can reduce the energy gap between the HOMO and LUMO orbitals, thereby increasing the material's ability to absorb photons, facilitate charge transfer, and accelerate electron-hole pair separation. The oxygen in the pyran ring also acts as a nucleophilic center that facilitates adsorption and electron transfer on the semiconductor surface [15], [16]. The -OH group increases local charge separation and accelerates electron and hole migration, thereby reducing electron-hole pair recombination [17], [18]. The -OH group also polarizes the catalyst surface and enhances the adsorption and activation of H^+ protons [19]. In addition, the -OH group can lower the work function and create a local electric field that supports charge transfer and redox reactions [19], [20]. The hypothesis of this study is that combining CTP with AC will produce more hydrogen than adding curcumin due to the presence of pyran heterocyclic rings and more -OH groups in CTP. To achieve this goal, this study will compare the hydrogen production results between AC combined with curcumin and AC combined with CTP. The

difference in hydrogen production results is expected to be attributed to the influence of the pyran heterocyclic ring and the greater number of -OH groups in CTP. The contribution of this research is to provide a new understanding that, in addition to aromatic rings, the presence of pyran heterocyclic rings and -OH groups also has a significant influence on increasing hydrogen production in photocatalysis.

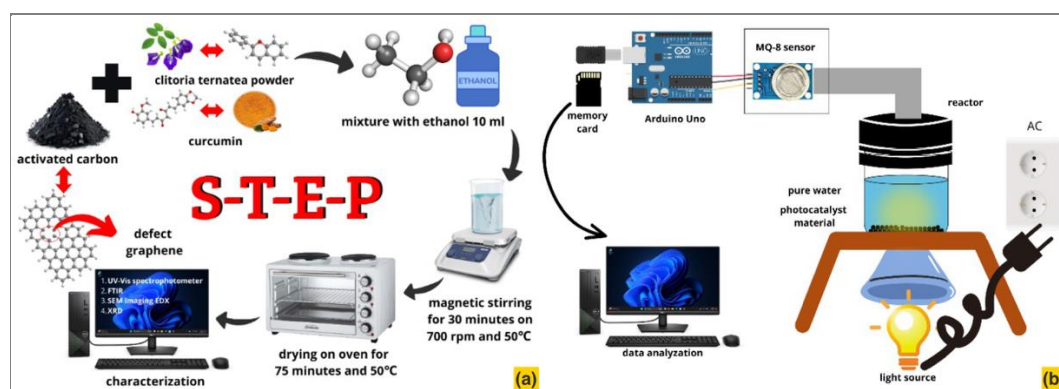
The purpose of this study was to determine the role of pyran heterocyclic rings and -OH groups in the amount of hydrogen produced. The method used in this study was to mix curcumin and CTP into AC using a magnetic stirrer heated with a hot plate with ethanol added as a solvent. This mixture was then dried and tested for photocatalysis with a yellow light. This test aims to analyze how the addition of curcumin and CTP can increase hydrogen production efficiency, with a particular focus on the role of the chemical structures that distinguish the two materials, such as the pyran heterocyclic ring and the -OH group, which is more abundant in CTP and can increase photocatalytic activity and electron transfer efficiency during the photocatalysis reaction. The pyran heterocyclic ring in the CTP structure has the potential to improve the material's ability to capture and transfer electrons, while the -OH groups in both compounds serve to strengthen the redox reactions that are crucial in photocatalysis. By linking this chemical structure to hydrogen production efficiency, this research has the potential to provide new insights into how variations in structure can affect photocatalytic performance in systems containing activated carbon. Therefore, further analysis of the interaction between these components in the context of photocatalysis is very important to maximize hydrogen production from renewable sources.

2. Methods

This study used AC, curcumin, and CTP, where AC was made from coconut shells from Haycarb™, curcumin from Desaku™, and CTP from Omah Tepung Organik™, filtered with a size of 200 mesh. The research was conducted as shown in Figure 1b sample preparation began by mixing AC with curcumin and CTP added with 10 ml of ethanol for magnetic stirring at a temperature of 50 °C at a speed of 700 rpm for 30 minutes. Then, the sample was placed in an oven to be dried at a temperature of 50 °C for 75 minutes. Subsequently, characterization of the material was performed using an Analytic Jena Specord 200 Plus UV-Vis spectrophotometer (Germany), Fourier Transform Infrared/FTIR (Shimadzu, Japan), FESEM Imaging EDS Quanta FEG 650 (America), and XRD (X-Ray Diffraction) with PXRD mode.

Hydrogen was produced in a reactor filled with pure water as shown in Figure 1b. Photocatalyst AC + curcumin and AC + CTP with a concentration of 10 mg were dissolved into 150 mL water. The lighting source for the photocatalyst reaction is a halogen lamp of 100 Watts placed under the reactor. The rate of hydrogen production was recorded with an MQ-8 hydrogen sensor stored in a memory card and then analyzed on a computer.

Figure 1.
Research steps:
(a) Material synthesis;
(b) Hydrogen
production reactor



3. Results and Discussion

3.1. UV-Vis Spectrophotometer

Absorbance analysis of AC, curcumin, and CTP using an Analytic Jena Specord 200 Plus UV-Vis Spectrophotometer with wavelengths measured in the range of 200-1100 nm. Samples consisted of AC, curcumin, CTP, AC + curcumin, and AC + CTP as shown in Figure 2. This results in an energy gap, as shown in Figure 3.

The AC energy gap is 3.911 eV, curcumin is 3.602 eV, CTP is 3.867 eV, AC + C is 3.174 eV, and AC + CTP is 3.016 eV. AC has a wide energy gap, indicating that most electrons are in localized orbitals and can only move to the conduction band with high energy. AC has many structural defects and functional groups on its surface that affect the electronic structure [21]. The addition of CTP to AC has been shown to produce a narrower energy gap. The pyran heterocyclic ring in CTP serves to expand the π -conjugated system, which can reduce the energy gap between the HOMO and LUMO orbitals [22]. This reduction in the energy gap extends light absorption to longer wavelengths, thereby increasing light absorption efficiency and charge transfer [15].

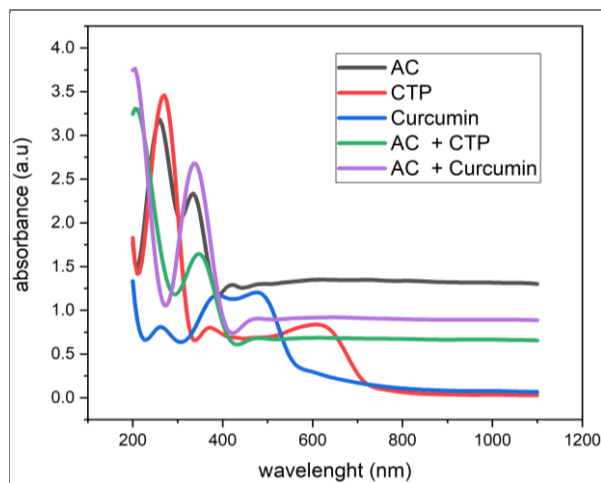


Figure 2.
Wavelengths from the UV-Vis spectrophotometer test

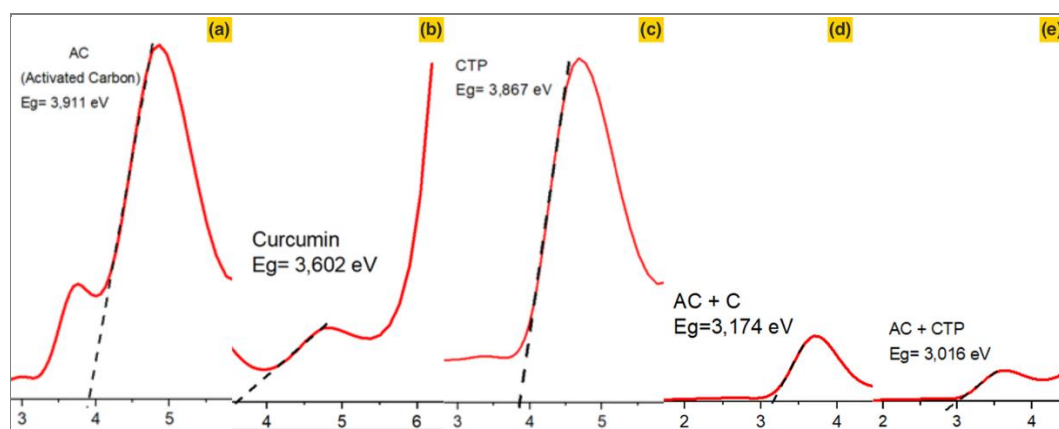


Figure 3.
Energy gap:
(a) AC;
(b) Curcumin;
(c) CTP;
(d) AC + Curcumin;
(e) AC + CTP

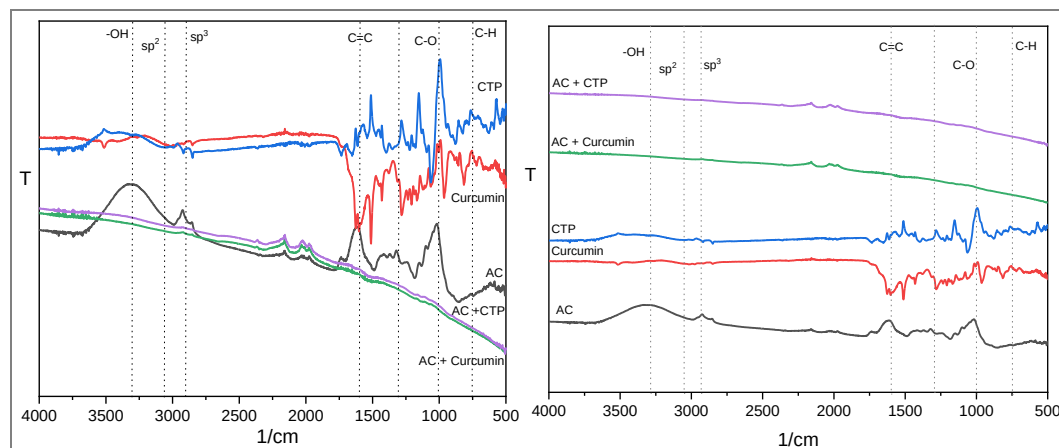
3.2. FTIR

FTIR testing detected functional groups in AC, curcumin, CTP, AC + Curcumin, and AC+CTP. The peak at 3280 cm^{-1} corresponds to the stretching vibration of the hydroxyl group (-OH), which is characteristic of phenolic compounds and is typically found in the range of 3400-3200 cm^{-1} [23]. The peak in the 1300-1000 cm^{-1} region indicates the presence of C-O stretching vibrations [24]. The peak at 3084 cm^{-1} indicates the presence of an aromatic ring, which corresponds to the C-H stretching vibration in sp^2 hybridized carbon, where the peak typically appears in the range of 3100-3000 cm^{-1} [25]. The peak at 1600 cm^{-1} indicates C=C bond absorption in the sp^2 hybridization system [26]. Peaks between 700-900 cm^{-1} , particularly at 756.10 cm^{-1} , indicate bending in C-H outside the plane in aromatic compounds [27]. Aromatic rings consisting of delocalized electrons can act as electron donors or acceptors during reactions with radicals. Then, at the peak of 2940–2850 cm^{-1} , which is usually in the range of 3000-2800 cm^{-1} , there is aliphatic C-H group stretching attached to the aromatic structure. The aromatic C-H stretching peak appears above 3000 cm^{-1} , while the aliphatic peak is below 3000 cm^{-1} [28]. AC + Curcumin and AC + CTP photocatalysts consist of more carbonyl and carboxyl functional groups compared to AC alone, as indicated by their decreasing transmittance intensity. The peak at 1740-1700 cm^{-1} indicates the stretching vibration of the C=O carbonyl group, which is usually identified in the range of 1850-1680 cm^{-1} [29]. Several C-O peaks in the range of 1300-1000 cm^{-1} [30].

FTIR analysis in Figure 4 shows significant changes in the AC + CTP photocatalyst after the doping process. When comparing AC, AC + C, and AC + CTP, it can be seen that the transmittance intensity in AC + C and AC + CTP increases its functional groups. During the doping process, it is possible that phenolic groups act as electron donors captured by defects in AC, which is supported by the increased concentration of -OH, C-O, and C-H groups. The increase in aromatic C=C is also caused by stacking in AC, which loses some C atoms through the healing mechanism of AC defects. AC + C shows the most significant increase in functional groups when compared to AC + CTP. Although FTIR analysis shows a higher density of oxygen containing functional groups, in AC + Curcumin compared to AC + CTP the hydrogen production result clearly indicate superior H_2

production over AC + CTP. This discrepancy highlights that hydrogen production cannot be directly predicted from total number of surface functional groups alone. In AC + C, the abundant phenolic -OH groups are mainly terminal in nature and tend to act as deep electron traps, which can promote charge recombination and limit effective proton reduction. In contrast, in AC + CTP oxygen atoms are predominantly incorporated within π -conjugated heterocyclic structures, such as pyran rings which preserve electron delocalization and introduce electronically active states that facilitate charge separation, proton activation, and interfacial electron transfer. Therefore, despite exhibiting fewer hydroxyl groups in FTIR spectra, AC + CTP demonstrates higher hydrogen production activity due to the more favorable electronic configuration of oxygen within conjugated heterocyclic motifs rather than the overall abundance of surface functional groups.

Figure 4.
FTIR analysis of AC,
Curcumin, CTP, AC +
Curcumin, and AC +
CTP



3.3. FESEM Imaging EDS

The characterization results of FESEM Imaging EDS can be seen in [Figure 5](#). The analysis was performed using ImageJ software with the analyzed parts highlighted in red boxes. The charge was analyzed according to the working principle of SEM, in which high energy electrons are fired at the sample. [Figure 5a](#) shows the black-purple surface of AC indicating that the fired electrons are repelled by the negatively charged surface of AC. Meanwhile, [Figure 5b](#) and [Figure 5c](#) show the red, orange, yellow, and white surfaces of curcumin and CTP indicating that the fired electrons are attracted by the positively charged surfaces of curcumin and CTP. Thus, [Figure 5d](#) and [Figure 5e](#) show that when negatively charged AC is doped with positively charged curcumin and CTP, the bottom part of the AC is dark while the top part of the curcumin and CTP is light. It can also be seen that the charge distribution in [Figure 5d](#) AC + C has a surface that tends to be orange and yellow, while in [Figure 5e](#) AC + CTP has a surface that tends to be yellow and white. FESEM images analyzed using ImageJ reveal that the AC + CTP sample exhibits a surface dominated by yellow and white contrast, indicating a more homogeneous phase distribution and stronger interfacial interaction between activated carbon and CTP. This observation suggests more effective electrostatic attraction between positively polarized sites on the activated carbon surface and negatively charged moieties within CTP. Although FTIR analysis shows that AC + Curcumin possesses a higher intensity of functional groups, the abundance of surface functionalities does not directly reflect interfacial interaction strength. In AC + Curcumin, phenolic -OH groups are largely terminal and primarily function as surface moieties, resulting in limited electronic coupling across the interface. In contrast, in AC + CTP oxygen atoms are predominantly incorporated into π conjugated heterocyclic frameworks, such as pyran rings, leading to a more delocalized charge distribution and enhanced interfacial cohesion as evidenced by the SEM morphology. This structural configuration facilitates more efficient charge separation and consequently contributes to the superior hydrogen production performance of AC + CTP, despite the lower apparent hydroxyl density observed in FTIR spectra. This is evidenced by [Figure 3](#), where the energy gap of AC + CTP is smaller than the energy gap of AC + C, indicating that the photon energy required to jump electrons from the valence band to the conduction band in AC + CTP is smaller than in AC + C. This is in accordance with the theory that the presence of a pyran heterocyclic ring plays a role in lowering the energy gap through the expansion of the π -conjugated system [22]. Conjugated and planar pyran heterocyclic rings are well known to form strong $\pi - \pi$ interactions with other aromatic systems. Importantly, such interactions are not merely structural in nature but also contribute to enhanced electronic coupling and charge delocalization at the carbon organic interface. The presence of a heteroatom (O) within

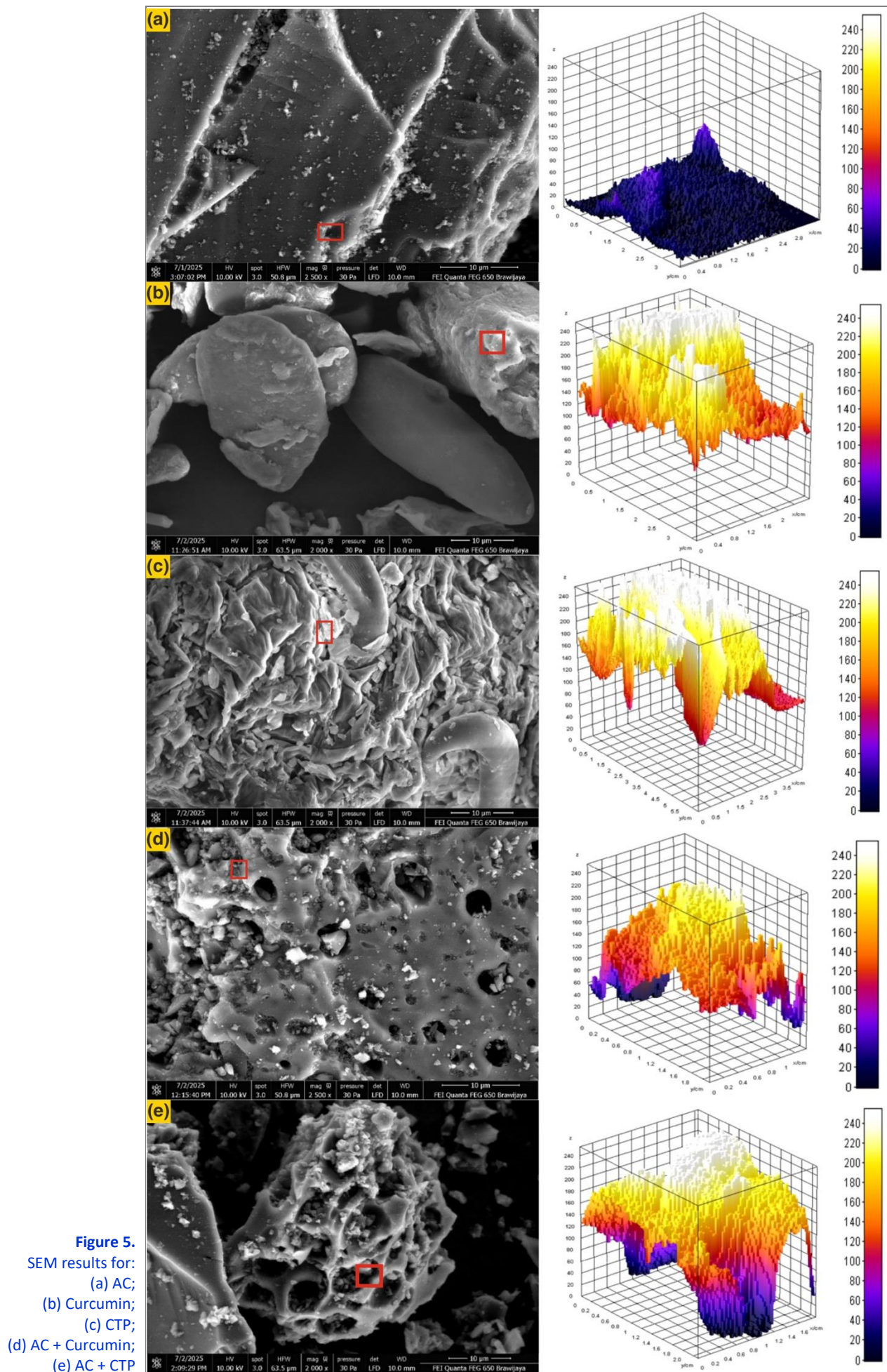


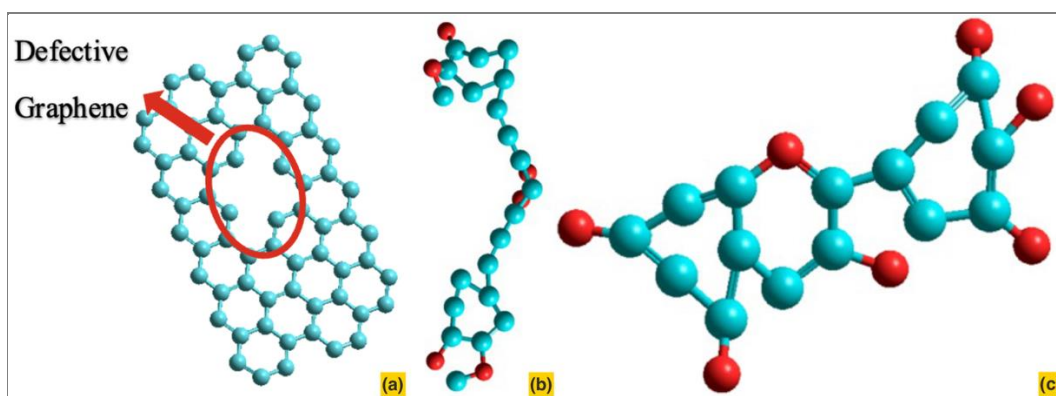
Figure 5.
SEM results for:
(a) AC;
(b) Curcumin;
(c) CTP;
(d) AC + Curcumin;
(e) AC + CTP

the pyran ring further facilitates charge redistribution, rendering the resulting $\pi - \pi$ interactions electronically active rather than passive. Phenolic compounds, such as curcumin, likewise possess aromatic moieties that enable $\pi - \pi$ interactions with the π conjugated surface of activated carbon. However, these interactions are generally more passive in terms of electronic contribution. The phenolic hydroxyl groups tend to withdraw electron density from the aromatic ring through inductive and resonance effect, promoting hydrogen bonding rather than effective charge delocalization. Consequently, although phenolic compounds may introduce a higher density of oxygen containing functional groups, their ability to enhance interfacial electronic coupling is comparatively limited. Therefore, the key distinction between pyran containing heterocycles and phenolic compounds lies not in the capability to form $\pi - \pi$ interactions, but in the effectiveness of these interactions in modifying the surface electronic structure of carbon materials. The distinction explains why CTP based materials containing pyran heterocyclic rings exhibit a more pronounced reduction in optical band gap and superior photocatalytic performance compared to curcumin, despite the higher abundance of oxygen containing functional groups observed in the latter. Crystallographic studies show the presence of offset $\pi - \pi$ interactions with a center-to-center distance of approximately 3.6 Å, indicating stable and significant attractive forces. Heterocyclic rings with electronegative atoms in the form of O atoms can interact electrostatically with other molecules, including anions, which will form additional attractive forces. Ab initio studies show that interactions between heterocyclic rings and proton acceptors can produce interaction energies of 40–80 meV, which is quite large for the category of non-covalent interactions [31], [32].

Figure 7a shows the EDX results for AC, which consists of 96.89% carbon, 0.04% potassium, 0.04% calcium, and 3.03% oxygen. The photocatalytic enhancement is not governed by a high overall oxygen concentration but by the selective incorporation of carbonyl functionalities, which effectively modulate the surface electronic structure, improve visible light absorption, and facilitate the generation and separation of reactive charge carriers. Excessive oxygen content, however disrupts π electron delocalization and hampers charge transport [33]. The O atom in AC can bond with the H atom to form a hydroxyl group -OH, where the hydroxyl group has polar properties due to the difference in electronegativity between the O and H atoms. The O atom is negatively charged while the H atom is positively charged, so between the two they produce a dipole moment that interacts with electric fields or electromagnetic waves. When the frequency of the photon matches the frequency of the dipole vibration or rotation, energy absorption occurs through vibrational transition. In the IR spectrum, the -OH group absorbs photons in the range of 3200-3600 cm^{-1} . The absorbance of AC is shown in Figure 2.

Figure 7b and Figure 7c show the EDX results for curcumin and CTP, where curcumin consists of 81.75% carbon, 16.02% oxygen, 0.24% magnesium, 1.58% potassium, 0.23% chlorine, and 0.19% phosphorus. Meanwhile, CTP consists of 76.92% carbon atoms, 19.42% oxygen, 0.65% magnesium, 1.94% potassium, 0.33% calcium, 0.40% phosphorus, 0.21% sulfur, and 0.12% chlorine. The concentration of O atoms in curcumin and CTP is much higher than in AC. The O atoms in curcumin are mostly bonded to H atoms, while the O atoms in CTP are partly bonded to H atoms and partly to pyran heterocyclic rings. Polar hydroxyl groups create a surface polarization effect that disrupts local symmetry and distorts the electrostatic field, thereby altering the distribution of electron density between the valence band and the conduction band. Hydroxyl groups enhance proton transfer and active sites [34]. Meanwhile, pyran heterocyclic rings will expand the π -conjugated system, thereby increasing the material's ability to absorb photons, facilitating charge transfer, and accelerating electron-hole pair separation [35]. Figure 6 shows the molecular structures of AC, curcumin, and CTP.

Figure 6.
Chemical structure:
(a) AC;
(b) Curcumin;
(c) CTP



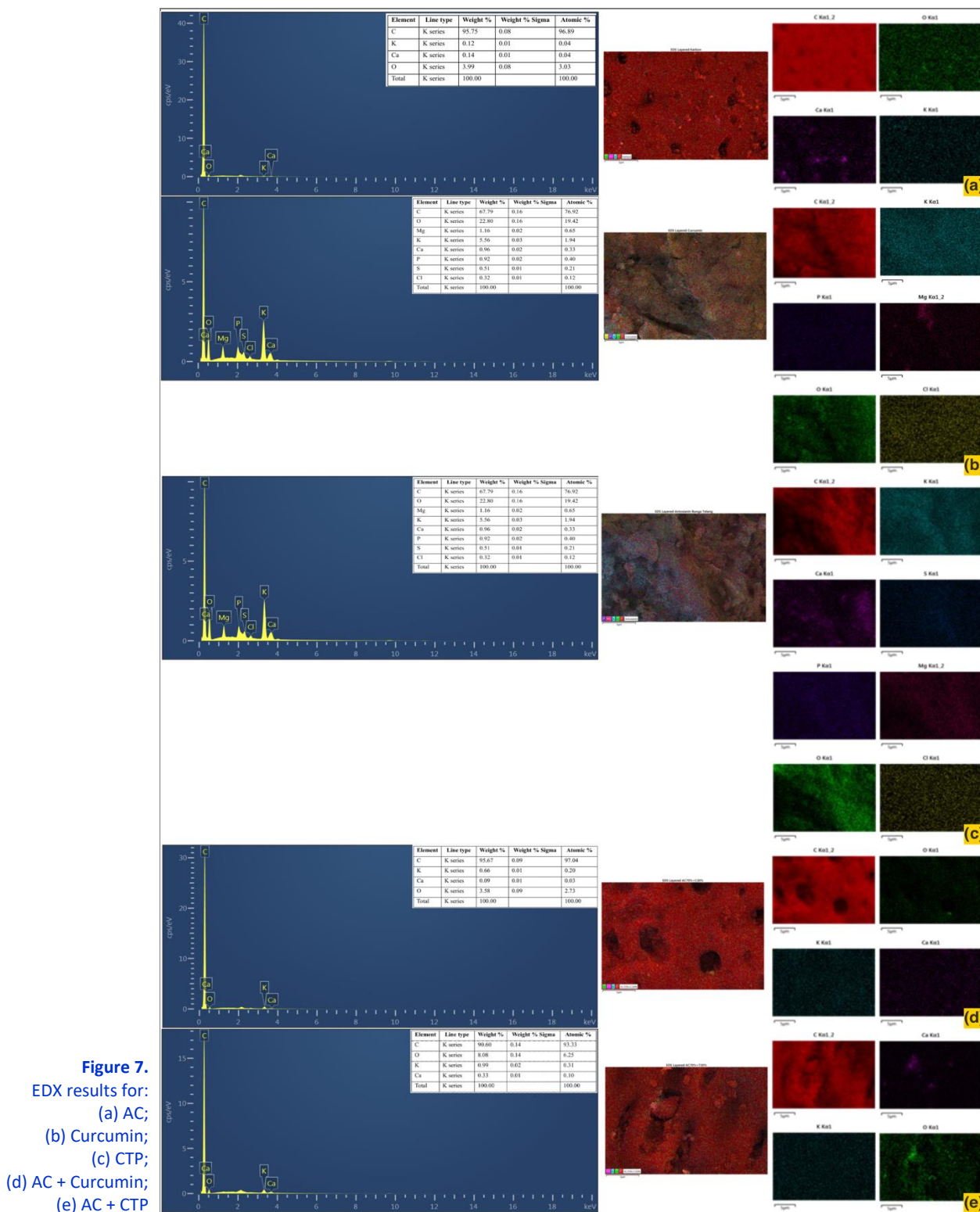


Figure 7d shows the EDX results for AC + C, which consists of 97.04% carbon, 0.20% potassium, 0.03% calcium, and 2.73% oxygen. Meanwhile, **Figure 7e** shows the EDX results for AC + CTP, which consists of 93.33% carbon, 6.25% oxygen, 0.31% potassium, and 0.10% calcium. The C atom plays a major role as the basic substrate in the photocatalytic process, especially as a charge transfer regulator [36]. In AC + C, the carbon atom content is higher, which means that there are more conjugated interactions than in AC + CTP. Curcumin C atoms bound to AC C atoms through stacking interactions act as electron transfer bridges and accelerate redox reactions on the photocatalyst surface [37]. This is confirmed by **Figure 4**, which shows that in the range of 1400-1600 cm^{-1} , the aromatic C=C stretching vibration in AC + C is greater in intensity than in AC + CTP, which is also reinforced by the C-H stretching vibration in sp^2 hybridized carbon in the range of 3000-3100 cm^{-1} , which is the region where stacking interactions occur.

In the AC + CTP system, a higher oxygen content is observed compared to AC + Curcumin. However, the enhancement in photocatalytic performance is governed by the chemical configuration of oxygen rather than its absolute concentration. Oxygen present as hydroxyl containing functional groups primarily contributes to surface polarity and adsorption capacity, but such groups tend to localize charge density and have a limited role in promoting charge delocalization within the carbon framework. In contrast, oxygen atoms incorporated into pyran heterocyclic rings play a more significant role in modulating the electronic structure of the material. Within the pyran framework, oxygen participates directly in the π conjugated system, enabling stronger $\pi - \pi$ interaction with the sp^2 carbon network of activated carbon. This conjugated heterocyclic configuration extends light absorption into the visible region and facilitates efficient electron-hole separation by enhancing charge delocalization and accelerating interfacial electron transfer, thereby suppressing charge recombination. Therefore, while hydroxyl associated oxygen mainly enhances surface reactivity, oxygen integrated within pyran heterocyclic rings exerts a more pronounced influence on the photocatalytic process through its contribution to π electron delocalization and charge transfer dynamics. The presence of hetero atoms, such as O in pyran, creates additional active sites that can interact with substrates or target molecules, accelerating the photocatalytic reaction [38].

Stacking interactions can occur due to the presence of AC defects through a healing mechanism. AC consists of defects that tend to recover their lost carbon atoms. The more defects there are, the better the active carbon is for use as a catalyst because it creates more reactive active sites that can attract surrounding carbon molecules [39]. Defects in AC, AC + C, and AC + CTP can be seen in [Figure 8](#).

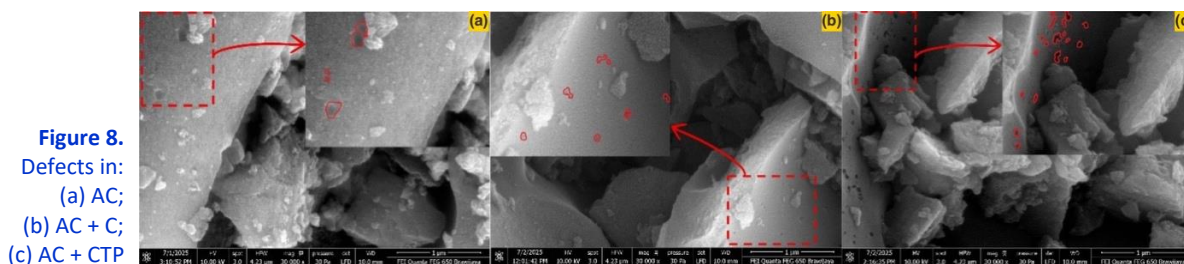


Figure 8.
Defects in:
(a) AC;
(b) AC + C;
(c) AC + CTP

3.4. XRD

Analysis of the composition, phase, and crystallinity of AC, Curcumin, CTP, AC + C, and AC + CTP using X'Pert HighScore Plus. In AC, the crystallographic spectrum shows diffraction bands observed at Bragg angles of 26.55, 27.68, 29.43, 43.44, 44.57, and 50.71, which visualize different crystallographic planes with the highest intensity at atom C at 43.44. C atoms at 002, 103, 101, and 106. Ca elements at 111, and O₂ at 210. C atoms at angles of 26.55, 43.44, 44.57, and 50.71 indicate a hexagonal crystal system. This is in accordance with [40], that AC is composed of graphene sheets in the shape of hexagonal atoms.

For curcumin, the crystallographic spectrum shows diffraction bands at Bragg angles of 17.33, 18.35, 22.11, 24.66, 25.79, 26.60, 29.0, and 32.29, indicating different crystallographic planes. P atoms are located on the 020 plane, O atoms on the 110 plane, C₇₀ atoms on the 202 and 214 planes, C₆₀ atoms on the 121 plane, C atoms on the 110 and 002 planes, and Cl₂ atoms on the 200 plane. Atoms C at an angle of 25.79 form an orthorhombic crystal system, while at 26.60 they form a hexagonal crystal system. This is consistent with [41], where the curcumin structure consists of delocalized hexagonal aromatic rings.

For the CTP crystallographic spectrum showing diffraction bands at Bragg angles 14.10, 19.11, 21.80, 24.26, 30.20, 32.25, 34.72, 36.10, 38.22, 40.08, 43.45, 44.67, 47.84, 51.5, and 82.05, which indicate different crystallographic planes. Carbon atom C₆₀ on plane 200, sulfur atom S on plane 202, carbon atom C on planes 004, 110, 002, 111, 020, 021, 112, 102, 103, 018, and 313. Chlorine atom Cl₂ on planes 202 and 221. C atoms at Bragg angles 24.26, 30.20, 32.25, 34.72, 38.22, 40.08, and 82.05 form an orthorhombic crystal system, C atoms at an angle of 21.80 form a cubic crystal system, Carbon atoms at angles of 43.45 and 44.67 in the hexagonal crystal system. Carbon atoms at an angle of 47.84 in the rhombohedral crystal system.

For the AC + C crystallographic spectrum showing diffraction bands at Bragg angles 15.15, 17.08, 21.96, 24.28, 26.55, 27.97, 29.32, 35.66, 38.2, 43.54, and 68.03, indicating different crystallographic planes. C atoms are located on the 001, 002, 103, 020, 012, and 113 planes. C₆₀ atoms are located on the 222, 121, and 440 planes. Ca atoms are located on the 111 plane, and O₂

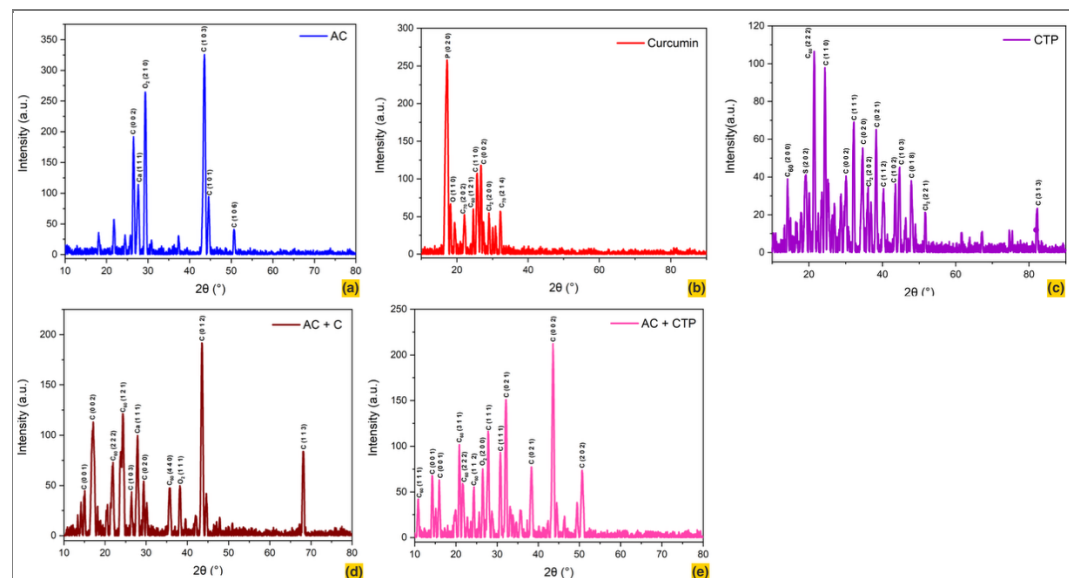
atoms are located on the 111 plane. Atoms C at angles 15.15, 29.32, and 68.03 form an orthorhombic crystal system, while atoms C at angles 17.08 and 26.55 form a hexagonal crystal system. With intensity decreasing sharply when compared to AC, it can be concluded that the crystallinity of the AC + C material has decreased or, in other words, the material has become more amorphous.

For AC + CTP, the crystallographic spectrum shows diffraction bands at Bragg angles of 10.95, 14.14, 16.01, 20.78, 21.53, 24.31, 26.59, 27.84, 30.69, 32.2, 38.4, 43.59, and 50.7, indicating different crystallographic planes. C₆₀ atoms are located on the 111, 311, 222, and 112 planes. C atoms are located on the 001, 111, 200, 021, 002, and 202 planes. Meanwhile, O₂ is on the 200 plane. C atoms are at angles of 14.14, 16.01, 30.69, 38.4, and 50.7 in the orthorhombic crystal system, while at angles of 27.84 and 32.2, they are in the cubic crystal system. For C atoms at angles of 43.59, the crystal system is hexagonal. With a sharp decrease in intensity compared to AC, it can be concluded that the crystallinity of the AC + C material has decreased or, in other words, the material has become more amorphous.

The crystal system has an influence on the catalytic process, in which the hexagonal crystal system acts as a conductive path where electron delocalization occurs [42], whereas an orthorhombic crystal system indicates the presence of defects or disorders that are favorable for charge trapping and molecular adsorption [43]. Defects also have a healing mechanism that attracts surrounding C atoms, forming a hexagonal crystal system. The cubic crystal system indicates the presence of an oxide phase that can act as a co-catalyst that can enhancing electron transfer [44].

From the Figure 9, it can be concluded that the addition of curcumin and CTP to AC increases the amorphous level in the material, which is indicated by a decrease in intensity. With an increase in the amorphous level in the material, active sites in the form of defects, functional groups, and C atoms with sp² and sp³ hybridization also increase [45]. This is consistent with FTIR data, where the -OH, C=C, C-O, and C-H groups increase, resulting in more locations where electrons can accumulate. The -OH and C-O groups can increase the number of free electron pairs on oxygen, thereby increasing electron density [46]. The C=C group has a higher electron density compared to single bonds, thereby increasing the local electron density [47]. The C-H group plays a role in providing more potential sites for functionalization that can produce new groups that are richer in electrons, such as -OH and C-O [48]. The synergy of these groups will result in an increase in local electron density because these groups attract or repel electrons through inductive effects due to differences in electronegativity, where the -OH and C-O groups attract electrons from the C atom, thereby increasing the local electron density on the C-H bond, which results in a stronger and more stable C-H covalent bond. In addition, changes in charge distribution cause polarization in the C-H bond, resulting in increased electron density [49].

Figure 9.
XRD results for:
(a) AC;
(b) Curcumin;
(c) CTP;
(d) AC + Curcumin;
(e) AC + CTP



3.5. Hydrogen Production

Figure 10 shows hydrogen production from AC photocatalysts, AC + Curcumin, and AC + CTP using yellow light irradiation with a power of 100 Watts. The blue line shows hydrogen production

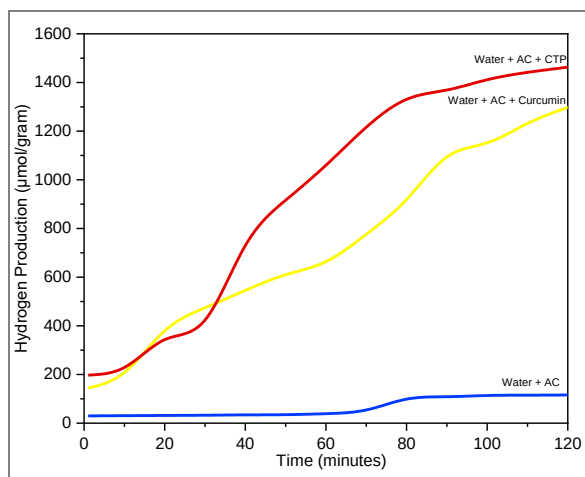


Figure 10.
Hydrogen production

played a role in increasing charge separation [50], adsorption energy adjustment [51], and increased electron transfer [52]. The weak C-H stretching vibration associated with sp^2 hybridized carbon suggests a limited contribution of exposed aromatic C-H groups, which may indicate a compact and ordered carbon framework. The small amount of oxygen groups is evidenced by the EDX test results in Figure 7a, where the oxygen group concentration is only 3.03% compared to 96.89% for C atoms. Furthermore, based on the XRD test results as shown in Figure 9a, the highest intensity of C atoms at 43.44 in the hexagonal crystal system has an intensity of 327.5 a.u., indicating that AC tends to have high crystallinity. This is directly proportional to the statement that AC with high crystallinity tends to have a lower surface -OH group content [53]. Therefore, in AC as a photocatalyst for hydrogen production, the role of active sites is very small, while delocalized electrons in aromatic rings cannot effectively decompose water into hydrogen because they are covered by graphene sheets that have very little contact. When the photocatalyst obtains photon energy, the electrons in the graphene defect will be excited towards the conduction band so that the negative charge is around the AC pores.

AC + Curcumin photocatalyst produces 1297.8 75 $\mu\text{mol/gram}$ hydrogen, which is higher than AC. Curcumin consists of two aromatic rings and two -OH groups that have a synergistic effect in increasing photocatalytic activity. The two aromatic rings in curcumin play an important role in light absorption and charge transfer. This aromatic structure forms π - π bonds with the AC surface, thereby strengthening adsorption and electron transfer. It also increases electrostatic strength, modifying the catalyst surface to be more reactive in breaking down hydrocarbon molecules and producing hydrogen [54]. Aromatic rings also extend light absorption into the visible region, thereby increasing photocatalytic efficiency [55]. Meanwhile, the polar -OH group creates a surface polarization effect that disrupts local symmetry and distorts the electrostatic field, thereby altering the distribution of electron density between the valence band and the conduction band. The hydroxyl group enhances proton transfer and active sites. Delocalized electrons in the aromatic ring of curcumin produce an electric field similar to that of AC, but in curcumin, this is supported by the presence of O atoms bonded to H atoms from water to form -OH groups, which absorb higher photon energy than AC, as shown in Figure 2. This is supported by the FTIR test results in Figure 4, which show an increase in -OH, C=C, C-O, and C-H groups that enhance photocatalytic activity. As shown in Figure 5, the surface of curcumin tends to be positively charged, attracting O atoms so that the hydrogen bonds in water are weak, while protons from H atoms are repelled. This is what can increase the amount of hydrogen production much higher than AC.

The AC + CTP photocatalyst produces 1462.6 75 $\mu\text{mol/gram}$ hydrogen, which is higher than AC and AC + C. CTP consists of two aromatic rings, one pyran heterocyclic ring, and six -OH groups in specific positions. The number of aromatic rings between curcumin and CTP is the same, but what distinguishes them is the presence of a pyran heterocyclic ring and six -OH groups in CTP. The presence of π - π stacking interactions between C atoms and active sites in the form of -OH, C=C, C-O, and C-H groups is smaller in AC + CTP than in AC + C, as confirmed by Figure 4. The presence of a pyran heterocyclic ring makes hydrogen production in AC + CTP greater. The oxygen atom in the six-membered pyran ring provides electronegativity that allows photon excitation to produce an excited state that can transfer electrons and protons simultaneously. The pyran compound acts as a hydrogen donor in the visible light-induced HAT (Hydrogen Atom Transfer) reaction. Photon excitation of the pyran compound produces excited species capable of transferring hydrogen atoms to a suitable substrate. This process begins with photon excitation of the pyran compound,

producing high-energy species capable of transferring hydrogen atoms to a suitable substrate. In the context of photocatalysis, this HAT mechanism enables hydrogen production through efficient proton reduction. In addition, the heterocyclic structure of pyran can increase the stability and efficiency of photocatalysts by reducing electron-hole pair recombination [56], and broadening the light absorption spectrum, thereby increasing the rate of hydrogen evolution. Thus, the integration of pyran rings in photocatalyst design offers a promising approach for efficient and sustainable hydrogen production. The presence of this pyran heterocyclic ring is supported by the Figure 7, which shows the presence of 6.25% O atoms, and the Figure 4, which shows active sites of oxygen groups that are smaller than AC + C. As shown in Figure 5, CTP surface is more positively charged, as indicated by a lighter color tending towards white, compared to curcumin, whose surface is yellow, attracting O atoms so that the hydrogen bonds in water are weak, while protons from H atoms are repelled. This is what can increase the amount of hydrogen production much higher than AC + C.

The enhancement in photocatalytic stability and efficiency induced by pyran heterocyclic rings originates from their unique electronic configuration and conjugated structure. Within the pyran ring, the oxygen atom is an integral part of the π conjugated system, enabling effective overlap between the heterocycle and the sp^2 hybridized carbon framework. This extended π conjugation introduces additional electronic states near the fermi level, which reduce the effective excitation energy required for photoinduced charge generation and consequently expand the light absorption spectrum toward the visible region. Moreover, the delocalized π electron network associated with the pyran heterocycle facilitates rapid charge migration across the carbon matrix, thereby spatially separating photogenerated electrons and holes. This spatial separation suppresses electron-hole pair recombination by providing preferential charge transfer pathway and stabilizing charge carriers through resonance delocalization. In contrast to oxygen present as non-conjugated functional groups, which tend to localize charge density, the oxygen atom embedded in the pyran ring promotes charge delocalization and prolongs carrier lifetime. As a result, the presence of pyran heterocyclic rings enhances interfacial charge transfer and maintains electronic stability during photocatalytic operation, leading to improved photocatalytic efficiency and durability. These synergistic effects demonstrate that the role of oxygen in pyran heterocycles is predominantly electronic, governing light absorption behavior and charge dynamics rather than acting merely as a surface active functional group.

The interaction between AC + C and AC + CTP can be determined through simulation using HyperChem software. Simulation using HyperChem software was conducted at a temperature of 343.15 K, producing the results shown in Figure 11.

AC exhibits good stability with high total energy, but is less efficient in photocatalysis due to its low dipole moment and wide HOMO/LUMO gap [57]. In the characterization of photocatalytic materials, it is important to optimize the dipole moment and reduce the energy gap in order to increase reaction efficiency [58], [59]. Meanwhile, Curcumin has lower total energy, which can increase photocatalysis efficiency due to its higher dipole moment and larger surface area, thereby supporting the electron transfer process more effectively [60]. Curcumin is known to possess properties that enable more effective photocatalytic reactivity, especially under ambient conditions [57]. CTP offers better stability with lower total energy, despite having a smaller surface area than curcumin. This can contribute to high structural stability [61]. When AC is combined with Curcumin or CTP, the total energy decreases, indicating better stability, even though the adsorption capacity experiences a slight decrease due to specific interactions between materials that can modulate the adsorption effect on the surface [62]. The AC + CTP combination exhibits very low total energy, but instead shows optimal stability and facilitates more efficient photocatalytic reactions. With a very high dipole moment, large surface area, and high polarizability, this combination greatly supports photocatalytic reactions [59]. The narrow energy gap ensures efficient electron transfer, while the high binding energy supports optimal adsorption [61]. The highly negative free energy under these conditions demonstrates that highly favorable photocatalytic reactions can occur, making AC + CTP the best choice for photocatalysis in hydrogen production. The highly negative free energy under these conditions demonstrates that highly favorable photocatalytic reactions can occur, making AC + CTP the best choice for photocatalysis in hydrogen production [61].

Based on Figure 11, which shows simulations using HyperChem software on AC, C, CTP, AC + C, and AC + CTP. In the energy simulation, the green line shows the E_{HOMO} region, while the pink line shows the E_{LUMO} region. In AC, it can be seen that defects tend to recover to form hexagonal atoms from other carbon atoms. Because AC is pure, the loss of C atoms will take C atoms from

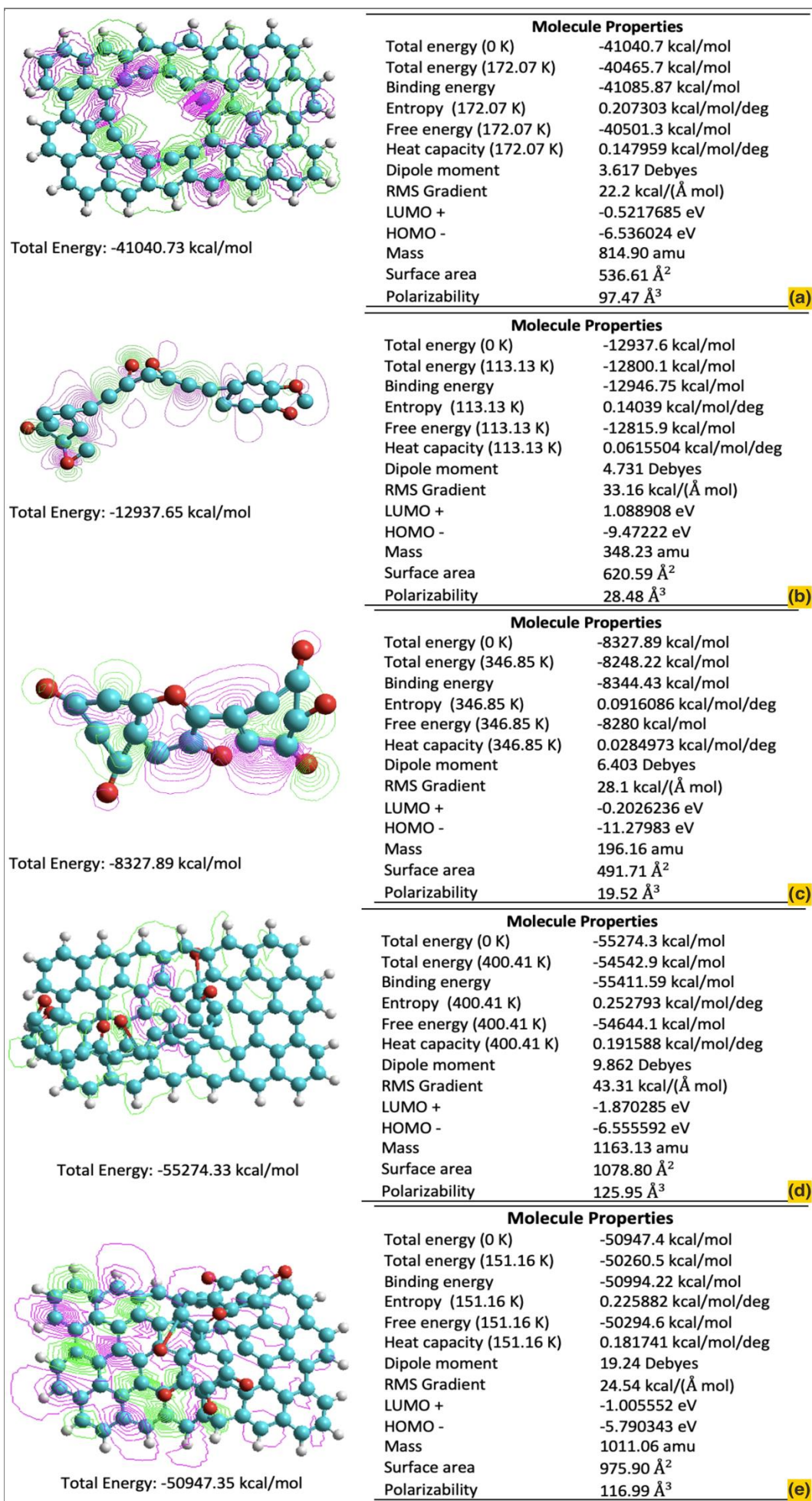
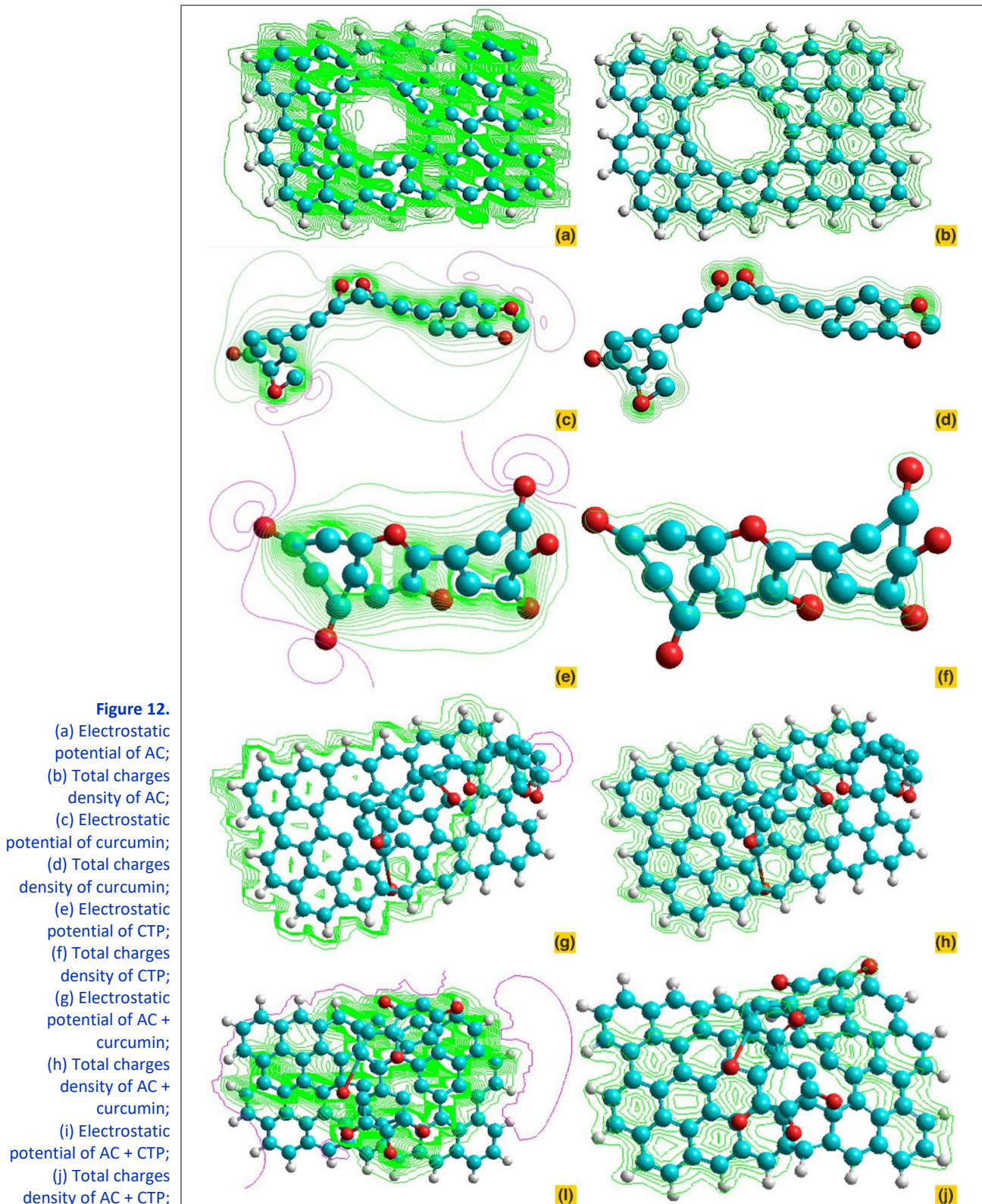


Figure 11.
Energy and properties
simulation of:
(a) AC;
(b) Curcumin;
(c) CTP;
(d) AC + Curcumin;
(e) AC + CTP

the nearest distance. It can also be seen that the energy gap in AC is 6.014 eV with a dipole moment of 3.617 Debyes. This value is obtained from $E_{\text{LUMO}} - E_{\text{HOMO}}$ to determine the energy gap value. Curcumin shows an energy gap of 10.561 eV with a dipole moment of 4.731 Debyes. CTP shows an energy gap of 11.077 eV with a dipole moment of 6.403 Debyes.

3.6. Electrostatic Potential and Total Charges Density

The assessment of electrostatic properties in various materials shows significant differences in charge distribution that affect reactivity and interaction capabilities (Figure 12.). AC exhibits prominent electrostatic potential due to a strong negative charge distribution, which effectively



attracts positive ions such as H^+ . This affinity accelerates hydrogen formation through increased reactivity toward target molecules, supported by studies showing that high total charge density on AC increases reactivity, even though electron transfer may be limited by the larger gap between the highest occupied molecular orbital (HOMO) and the lowest unoccupied molecular orbital (LUMO) [63], [64]. In contrast, curcumin exhibits a more uniform and subdued charge distribution relative to AC resulting in lower total charge density, which inhibits both adsorption capacity and electron transfer efficiency.

Further investigation into CTP reveals that its electrostatic potential is less robust compared to AC, limiting its interactions with water molecules and H^+ ions. Nevertheless, the thermal stability of CTP promotes its suitability for long-term reactions, indicating that while its charge density is lower, it can still play a functional role in specific applications [65]. When combining AC + C, the resulting charge distribution becomes more uniform, and the total charge density increases compared to curcumin alone, leading to enhanced water adsorption properties, however the capacity for electron transfer remains hampered by the significant energy gap.

In contrast, the combination of AC with CTP showcases an improved charge distribution and a markedly high total charge density, augmenting both adsorption capacity, and potentially photocatalytic efficiency. This combination is posited to benefit from a narrower energy gap, potentially facilitating more efficient electron transfer, thus positioning it as a favorable option for hydrogen photocatalysis [66], [67]. Such findings underline the importance of optimizing charge distributions in the development of materials for advanced photocatalytic applications, paving the way for innovations in sustainable energy solutions and material science.

4. Conclusion

This study aims to determine the role of pyran heterocyclic rings and -OH groups on hydrogen production rate. The results show that hydrogen production using pure AC is 115.75 $\mu\text{mol/g}$, AC + C produces 1297.8 $\mu\text{mol/g}$, and AC + CTP produces 1462.6 $\mu\text{mol/g}$, indicating a significant increase. Hydrogen production in AC + CTP is higher than in AC + C due to the presence of pyran heterocyclic rings, which can increase the stability and efficiency of photocatalysts by reducing electron-hole pair recombination and expanding the light absorption spectrum, thereby increasing the rate of hydrogen evolution. Although the stacking interactions and active sites in the form of -OH, C-H, and C-O groups are smaller than those in AC + C, the presence of O atoms, which are pyran heterocyclic rings, can produce large amounts of hydrogen. This study suggests further analysis of the role of -OH groups in certain positions so that their presence can maximize hydrogen production efficiency.

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Authors' Declaration

Authors' contributions and responsibilities - The authors made substantial contributions to the conception and design of the study. The authors took responsibility for data analysis, interpretation and discussion of results. The authors read and approved the final manuscript.

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