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RESEARCH ARTICLE

Influences of Organic Dye Molecules in Novel OLED Applications of V_2O_5 Molecules

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Abstract

Background/Objectives: The synthesis process of Vanadium Pentoxide (V_2O_5) with organic dyes like acid blue and acid yellow molecules was carried out utilizing the simple precipitation procedure with distilled water as the solvent. To understand more about the composition of the materials, the required characteristics were done on the synthesized samples. **Methods:** Initially, Powder X-ray diffraction (PXRD) investigation was done on the samples to analyze their amorphous nature. The Images from the Scanning Electron Microscope (SEM) revealed that the synthesized samples have a micro-rod-like structure. The occurrence of functional groups in both synthesized molecules was analyzed using a Fourier-Transform Infrared Spectroscopy (FTIR) study. **Findings:** The study revealed the presence of a peak at 3408 cm^{-1}, which is caused by stretching vibrations in the N-H group, a peak at 2853 cm^{-1}, which is characteristic of CH_3, a peak at 1630cm^{-1}, which relates to the presence of the group-N = N, and a peak at 1040 cm^{-1}, which is characteristic of the C-N group. Additionally, to verify the dielectric nature of the synthesized powder samples, their cut-off wavelength, 245 nm for V_2O_5 with acid blue dye, and 363 nm for V_2O_5 with acid yellow dye, can be seen in the UV-vis-NIR absorption spectra. The photoluminescence spectrum displayed red light at E_g=1.7 eV for V_2O_5 with acid blue molecule and at E_g=1.6 eV for V_2O_5 with acid yellow molecule. **Novelty:** The novelty of this study is to test the suitability of V_2O_5 molecules with acid blue and V_2O_5 molecules with acid yellow as the best materials for utilization in optoelectronic devices, which is not addressed in existing studies.

Keywords: Simple precipitation method; Powder Xray diffraction (PXRD); Scanning Electron Microscope (SEM); FourierTransform Infrared Spectroscopy (FTIR); Photoluminescence; UV visNIR

1 Introduction

Vanadium Oxides are a category of chemicals that are extremely significant for transition metals that have received a lot of attention from the technological and scientific worlds[1]. These oxides have fascinating optical, electronic, magnetic, structural properties, and electrochemical applications, including catalysis, Li+ battery cathodes, electrochromic devices, thermochromic windows, sensors, field effect transistors (FETs), and solar cells, as well as OLED applications. The most promising of the transition metal oxides is the metal oxide with the formula V_2O_5, which stands for vanadium dioxide.

As a result of its orthorhombic layered structure, it is an essential component of several types of energy storage, including lithium-ion batteries. It is a low-cost, non-toxic, and environmentally acceptable substance. It is commonly known that nanoparticles have better electrochemical performance than larger particles. An organic dye is a water-soluble organic chemical that temporarily modifies the crystal structure of colored substances when applied to a substrate[2]. A pigment is an insoluble and inorganic-colored compound. Some colored chemicals are indications, stains, or solvent dyes for coloring solvents like petrol. Rubber, Textile, cosmetics, color photography, pharmaceuticals paper printing, and other industries utilize synthetic dyes, with textile processing being the main consumer. Azo dyes are the most common and versatile synthetic dyes[3].

As the primary demonstration of efficient light emission, intensive research has been conducted to improve the functionality of the device such as driving voltage, luminous efficiency, and longevity[4]. OLEDs are dependent on electron and hole injection and recombination in the materials; therefore, improving the efficiency of carrier injection and maintaining a healthy balance between electrons and holes is vital to obtaining high efficiency and a low operating voltage[5]. In their natural state, Organic light-emitting diodes (OLEDs) are optical display devices that are flat and cover a huge surface. The numerous benefits that organic light-emitting diodes, or OLEDs, offer over semiconductor-based light-emitting diodes, such as lower cost, lower power consumption, higher brightness, more contrast, and higher internal quantum efficiency have resulted in a significant increase in their popularity. Because of the inherent properties of organic materials, fabrication of organic materials on flexible substrates is facilitated. OLEDs have received a lot of attention due to the several uses they could have, such as illumination, solid-state lighting, and flat-panel displays[6].

In this present study, examinations were carried out to observe the influences on the synthesis of V_2O_5 molecules with acid dye materials, and their characterizations were determined.

2 Methodology

A Simple Precipitation method was used to get the samples ready for analysis. To get started, one beaker was given 2.1 grams of V_2O_5 and 7.9 grams of acid blue dye materials with an AR grade. Another beaker was given 2.64 grams of V_2O_5 and 3.36 grams of acid-yellow dye materials. The distilled water was used as the solvent in the production of both of the samples, and the production ratio was set at 1:1. The mixes were vigorously mixed for 10 hours for the process duration. To conduct additional tests, the powder samples were taken out of the solution and collected separately. In a water bath heated to 100°C, the filtered residues were annealed for 1 day before being dried. During this technique, the blue mixture (V_2O_5 with acid blue sample) changed to a dark green color, while the yellow mixture (V_2O_5 with acid yellow sample) likewise altered to a greenish color.

3 Results and Discussions

3.1 Powder XRD Analysis

X-ray diffraction analyses the structure and crystalline nature of solid materials. In a nutshell, crystal X-ray diffraction is brought on by a scattering mechanism in which the electrons of atoms that are present in the sample will scatter X-rays, but this will not change the wavelength. The diffraction pattern of crystalline material is measured by powder X-ray diffraction (PXRD)[7]. An analysis of the produced sample by powder XRD can be carried out with a CuKα radiation source with a wavelength of = 1.5405Å. PXRD patterns of synthesized V_2O_5 containing acid blue and acid yellow are displayed in Figure 1 a and Figure 1 b, respectively.

3.2 SEM analysis

At the micrometer to the nanometer scale, the Scanning Electron Microscope (SEM) investigates the surface structure and chemistry of materials with a beam of electrons[8]. This SEM examination can be carried out on the sample that has been prepared, and the findings can be measured with the help of the Carel Zeiss Instrument. The structural surface of V_2O_5 with acid blue and V_2O_5 with acid yellow was observed by using the SEM technique as shown in Figure 1 c and Figure 1 d.

3.3 FTIR analysis

An infrared (IR) beam is used for identifying functional groups in materials[9]. IR vibration spectroscopy is utilized to identify molecules through the examination of the bonds that keep them together. A molecule's individual chemical bonds all vibrate at slightly different frequencies. Atoms that are surrounded display various modes of oscillation due to the stretching and bending motions phenomenon. These modes exist due to the oscillations of the CH_2 group. The amount of IR light absorbed by each molecule's link was determined using infrared spectroscopy. The Fourier transform infrared (FTIR) spectrometers are third-generation infrared spectrometers. They have found widespread applications in the process of structural elucidation. It is a technique that uses time- or space-domain electromagnetic radiation technique used to acquire spectra that have been formed from coherence measurements of a radiative source. These tasks can be completed at the same time if necessary. The spectra of the Perkin Elmer instrument Recording the FTIR spectra of the produced samples, such as V_2O_5 molecules with Acid blue and V_2O_5 molecules with Acid yellow materials, required the use of an FTIR Spectrophotometer. The FTIR spectrum has a wavelength range of 4000cm^{-1} to 400cm^{-1} and is reported in Figure 1 e and Figure 1 f, respectively (Table 1).

Table 1. FTIR assessment of V_2O_5 molecules that were generated with acid blue and V_2O_5 molecules that were created with acid yellow

Wavenumber (cm^{-1})	Assessments	
	V_2O_5 with Acid blue	V_2O_5 with Acid Yellow
3452 3408	N-H -	- N-H
2992 2853	C=N -	- CH_3
1638 1630	C=O -	- -N=N
1124 1040	S=O -	- C-N
616 684	V-O -	- V-O

3.4 UV vis NIR Spectroscopy analysis

The UV-visible-NIR spectroscopy approach can be utilized for structural elucidation by evaluating the shape and position of the resultant absorption bands. UV spectroscopy is an extremely sensitive detection method of specific chemical compounds and chromophoric groups as a quantitative tool of analytical chemistry[10]. The sample is analyzed with the Varian Cary SE UV-vis-NIR Spectrophotometer in the wavelengths of 100-1000 nanometers. The cutoff wavelengths of the prepared samples are 245 nm for V_2O_5 with Acid blue and 363 nm for V_2O_5 with Acid yellow, as shown in Figure 1 g and Figure 1 h.

3.5 Photoluminescence Analysis

Because the photoluminescence (PL) signal comes from the recombination of photogenerated electron-hole pairs[11], it is possible to do a study of the separation of photogenerated charge carriers with the use of photoluminescence analysis. The study of photoluminescence, sometimes known as PL, has the potential to be used for the task of characterizing a wide variety of material properties. The investigation of discrete electronic states in photoluminescence spectroscopy requires a high level of accuracy and attention to detail. It is put to use to ascertain the interface, surface, and impurity levels, in addition to the chaotic nature of the alloy and the unevenness of the contact. The brightness of the photoluminescence signal might provide information regarding the surface and interface quality[12]. The Perkin Elmer LS 45 is a tool for recording PL spectral analyses. The measurements that were taken for the photoluminescence experiments of V_2O_5 with acid blue and acid yellow molecules are displayed in Figure 1 i and Figure 1 j respectively.

3.6 Discussions

Recording the PXRD patterns of the powdered material requires both scanning at 2θ and intensity measurements to be accomplished. It was discovered that V_2O_5 with acid yellow material formed extra sharp peaks than V_2O_5 with acid blue material, implying that V_2O_5 with acid blue material is more amorphous than V_2O_5 with acid yellow material.

In SEM images, the adsorbents look like rods and microclusters. Some examples of these applications include electrochemical applications and optoelectronic device applications.

Considering the FTIR Spectrum, the fact that the wave numbers add up to 3452 cm^{-1} has led researchers to conclude that the N-H group of acid blue 9 molecules must be present. The peaks at 2992 cm^{-1} and 2249 cm^{-1} relate to the presence of stretching modes of the C=N molecule. The peak at 1638 cm^{-1} belongs to the C=O stretching of the COOH molecule, while the peak at 1124 cm^{-1} corresponds to the S=O stretching of the organic acid blue 9 dye molecules. There is a possibility that hydrogen bonding with vanadyl group oxygen atoms is responsible for the weaker band at 616 cm^{-1}.

The spectrum of V_2O_5 with acid yellow dye is measured by the Fourier transform of the infrared light. The analysis reveals the existence of a peak at 3408 cm^{-1}, which is caused by stretching vibrations in the N-H group, a peak at 2853 cm^{-1}, which is

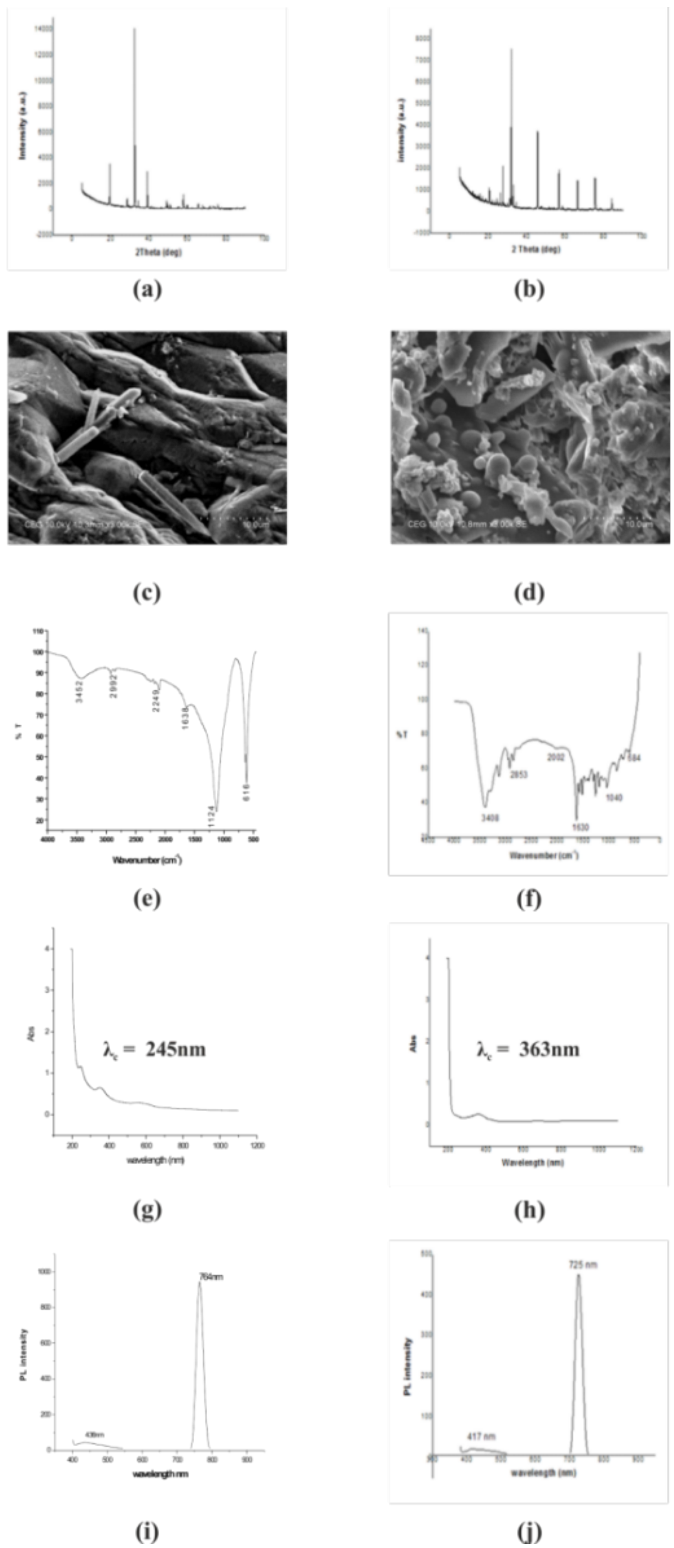

Fig 1. (a & b) PXRD spectrums of V_2O_5 with acid blue and acid yellow molecules; (c & d) SEM images of V_2O_5 with acid blue and V_2O_5 with acid yellow molecules; (e & f) FTIR spectrum of V_2O_5 with acid blue and V_2O_5 with acid yellow molecules; (g & h) UV vis NIR spectrum of V_2O_5 with molecules of acid blue and acid yellow; (i & j) Photoluminescence spectrum of V_2O_5containing molecules of acid blue and acid yellow

characteristic of CH_3, a peak at 1630cm^{-1}, which relates to the presence of the group-N = N, and a peak at 1040 cm^{-1}, which is characteristic of the C-N group. There is a chance that hydrogen interaction with the oxygen atoms in the vanadyl group is to blame for the weaker band at 616 cm^{-1} [13].

In UV vis NIR Spectroscopy analysis, both samples exhibited substantial absorption peaks at 245 and 363 nm [14]. The formula $Eg = hC/\lambda_c$, is used to calculate the energy gap, as 5.06 eV for V_2O_5 with acid blue and 3.42 eV for V_2O_5 with acid yellow, where λ_c represents the cut-off wavelength, h represents Planck's constant and C represents the speed of light. From bandgap values, it is determined that V_2O_5 with acid blue has greater dielectric properties than V_2O_5 with acid yellow molecule. According to the calculated values of the samples' band gaps, the samples belong to the category of insulating materials. As a direct consequence of this, the samples find widespread use in many applications involving optoelectronic devices.

In photoluminescence analysis, the peak of the photoluminescence emitted by pure V_2O_5 occurs at a wavelength of around λ =400 nm, which is in the blue-green region. The peak around 725-764 nm was significantly amplified when compared to other peaks, indicating the extrinsic alteration of oxygen vacancies formed in V_2O_5 as a result of the annealing process. The equivalent photon energy is Eg=1.7 eV, and Eg=1.6 eV exhibits the largest wavelength, which is red, as well as the longest absorption and emission (with tailing above 1000 nm) in the solid state. The material's potential for use in OLED applications is improved as a consequence of the incorporation of acid blue and acid yellow dye molecules into the V_2O_5 structure. This band gap energy reveals that V_2O_5 possesses acid blue and acid yellow dye molecule levels within the band gap. This finding is compatible with investigations on the optical absorption of the substance. The V_2O_5 with acid blue and acid yellow molecules generated is a potential material for optoelectronic device applications [15].

4 Conclusion

With distilled water as a solution and the simple precipitation method, molecules of V_2O_5 with acid blue and V_2O_5 with acid yellow were prepared. At T=100°C, the structure of the synthesized samples was studied by changing the sample temperature and inspecting how the structure changed. The PXRD analysis was used to figure out that the powdered samples made in the laboratory were amorphous. The SEM images showed that the addition of dye molecules to the pure V_2O_5 molecule made it more rod and micro-cluster-shaped. FTIR studies showed the presence of essential chemical bonding in the powder molecules of V_2O_5 and acid blue dye, as well as molecules of V_2O_5 and acid yellow dye. The UV-vis-NIR absorbance spectrum of both samples was measured between 100 and 1000 nm, which showed that the samples have insulating properties. The estimated energy gap value for V_2O_5 with acid blue molecules was 5.06 eV, and for V_2O_5 with acid red molecules, it was 3.42 eV. Perkin Elmer LS 45 was used to study photoluminescence peaks at 436 and 730 nm for V_2O_5 with acid blue and 417 nm and 725 nm for V_2O_5 with acid yellow molecules. Based on these optical studies, it is clear that the V_2O_5 molecules with acid blue and V_2O_5 molecules with acid yellow are excellent materials for use in optoelectronic device applications.

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