Section A -Research paper
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Synthesis of V_2O_5 Molecule with Organic Dye Molecules for Opto Electronic Applications

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Abstract

Vanadium pentoxide (V_2O_5) with organic dyes such as acid orange and acid red were synthesized using Simple Precipitation method with distilled water as solvent. Powder X-ray Diffraction (PXRD) analysis was carried out to study the nature of the samples. Scanning Electron Microscopic (SEM) pictures inform the morphology of the synthesized samples which are shown as micro-rod like structures. The UV-vis-NIR absorption spectrum shows an absorption band at 231 nm for V_2O_5 with acid orange dye and 211 nm for V_2O_5 with acid red dye which are the cut off wavelength of the synthesized powder samples and hence to confirm their dielectric nature. The photoluminescence spectrum exhibits red light at E_g=1.7 eV, and E_g=1.9 eV and E_g=1.5 eV due to V_2O_5 molecule levels located inside the band gap along with acid orange molecule and acid red molecule.

Keyword: Powder XRD, SEM, FTIR, Photoluminescence, Optical materials.

1. Introduction

Organic Light Emitting Diodes (OLED) materials have wide range of applications because of the compensation of its simple developed process, lightweight, flexible substrate, energy savings, and wide viewing angle [1,2] which include solid-state light sources [3] and display devices [4,5] applications. The discovery of improved organic materials gradually improves the efficiency of organic optoelectronic devices, increasing interest in organic electronics as the next generation of electronics [6,7]. Organic light-emitting diodes have attracted the community of science interest for the very last twenty years. A small coating of an organic substance is positioned between two electrodes to form the device. Because of its lower power usage when compared to LCDs, OLED screens are particularly well suitable for such purposes [8]. OLED displays have been commercially accessible in portable small electronics applications such as smart phones, music players, automotive radios, digital cameras, and monitors (TVs) for the past nine years. [9]. Vanadium pentoxide is a latent electro active electrode for super capacitors because of its varied oxidation states, low toxicity, small cost, high capacitance, wide voltage window, and high energy density [10].V_2O_5 is a common cathode material and a catalyst [11]. Vanadium is

abundant in nonferrous metals, which are also known as ferrous metals. A crucial period of transition in the history of industrial civilization was made possible by the exceptional and distinctive qualities of the compounds and metallic vanadium and alloys it produces. Vanadium has also been helpful for the quick growth of modern industries, particularly those in steel, chemicals, petroleum, energy, and nuclear, as well as nonferrous metals, architecture, and environmental protection. Many vanadium catalysts are made up of vanadium compounds like oxides, chlorides, and complexes, as well as a range of other forms like a salt of hetero poly acids. One or more of the following additions are made to the most common active component. In the majority of oxidation catalysts, V_2O_5 is the primary active component. Catalyst made of Vanadium has been used in double catalysis for desulfurization and de-nitrification, as well as environmental purification for inorganic and organic pollutants removal. Batteries made up of Vanadium have recently piqued the curiosity of researchers working on renewable energy applications [12]. Acid dyes are categorised based on their affinity, dyeing capabilities, and chemical composition. Many acid dyes have been reported in the literature, including anthraquinone-based acid dyes, acid nitro dyes, triphenylmethane acid dyes and acid azo dyes. They're also employed in high-tech applications like lasers and non-linear optical systems, photodynamic treatment, dye-sensitive solar cells, metallochromic indicators, thermal transfer printing, and fuel cells [13]. Because of their numerous applications, acid azo dyes containing aromatic heterocyclic moiety have been studied.

2. Experimental Method

The samples were prepared using the technique of simple precipitation method. To begin the process, 3.12 g of V_2O_5 and 8.88 g of acid red dye materials were collected in one beaker, and similarly 2.72 g of V_2O_5 and 5.28 g of acid orange dye materials were combined in another beaker. Both samples were prepared in a ratio of 1:1 with distilled water as solvent. The mixtures were stirred well for ten hours while they were left at standard temperature. The powder samples were collected and filtered from the solution for further testing. Using a water bath, the filtered residues were annealed and dried for twenty-four hours at 100°C temperature. The color of the orange mixture turned to brick color during this procedure, while the color of the red mixture changed to coffee (brown) color. Figures 1a and 1b show an image of the dried and powdered samples.

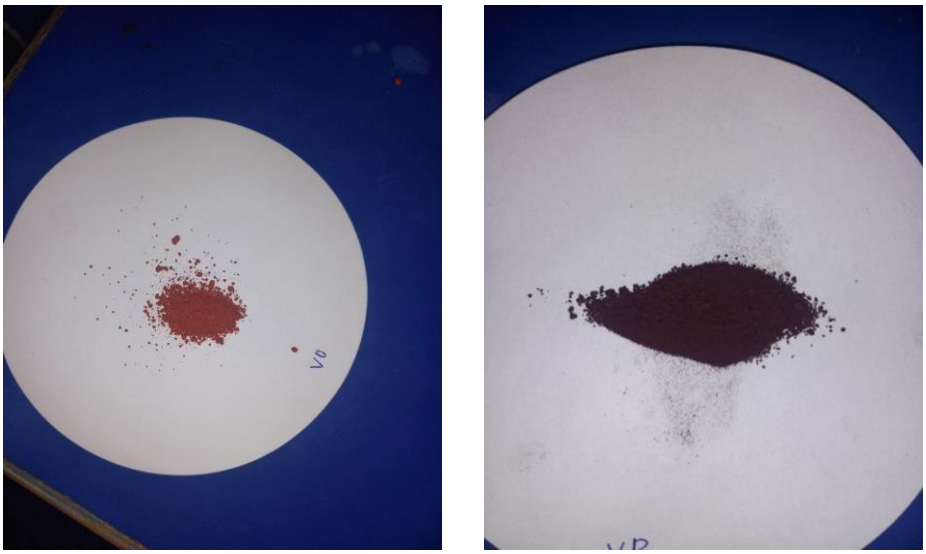


Fig 2a and 2b. Photograph of V_2O_5 with acid orange and acid red materials

3. Result and Discussion

3.1. Powder XRD Analysis

X-ray diffraction (XRD) and X-ray photoelectron spectroscopy (XPS) were employed to describe the microstructure and composition of the produced films [14]. X-ray diffraction, or XRD, is a method for determining the crystalline nature and structure of solid materials. In a nutshell, the result of a scattering process in which X-rays are scattered by electrons of atoms present in the sample is crystal X-ray diffraction , but the wavelength remains constant. The resultant diffraction pattern, which is dictated by the position and intensities of the diffraction effects, is a critical physical property of the material. This feature not only identifies the material's structure but also provides a detailed explanation of its composition [15]. Powder X-ray diffraction (PXRD) can be used to measure the diffraction pattern of crystalline material [16]. Powder XRD analysis of the manufactured sample can be performed using a CuKα radiation source with a wavelength λ= 1.5405 Å. The PXRD pattern were shown in Figure 3.1a and 3.1b for synthesized V_2O_5 with acid orange and acid red molecules which were annealed at 450°C. Scanning 2θ and intensity values were utilized to record the PXRD patterns of the powdered material. It is observed that V_2O_5 with acid red material was produced more sharp peaks than V_2O_5 with acid orange material which implies that the $V_2O_5$with acid orange material is highly amorphous than V_2O_5 with acid orange material.

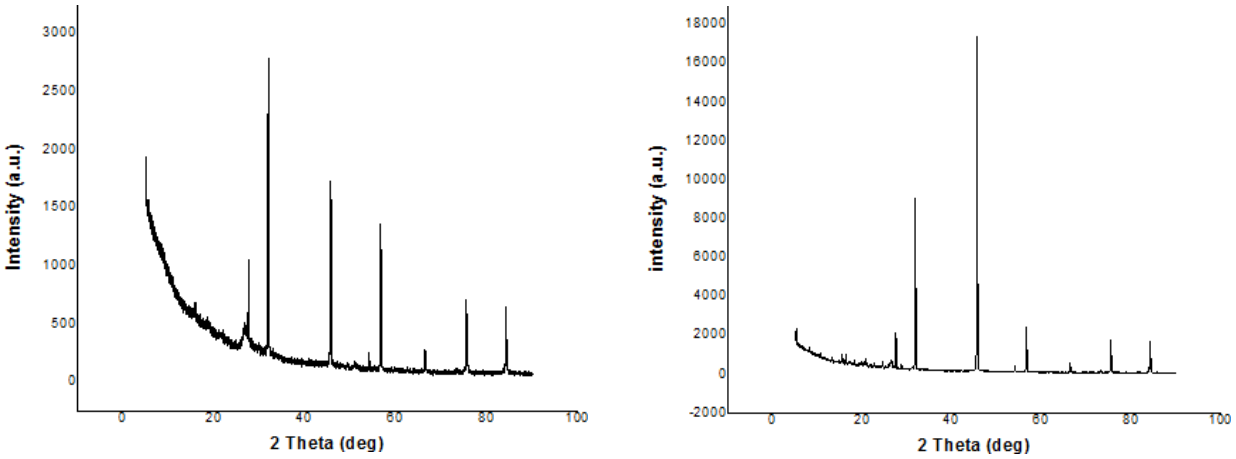


Fig 3.1a and 3.1b. PXRD spectrum of V_2O_5 with acid orange and acid red molecules

3.2. SEM analysis

By focusing a beam of high-energy electrons down onto the specimens, the scanning electron microscope (SEM) generates a variety of surface signals on solid specimens. The signals created by the electron-sample interactions offer information on the sample itself, including its exterior morphology (texture), chemical composition, crystalline structure, and orientation of the materials that comprise the sample [17]. The SEM is used regularly to investigate the micrometer- to nanometer-scale surface chemistry and structure of a wide range of synthetic and biological materials. Scanning electron microscopy is one of the most dominant and diverse characterization methods available these days [18]. Its simplicity of usage, usually straightforward sample preparation, and straightforward image interpretation, shared with its high resolution, depth of field, and ability to perform micro chemical and crystallographic analysis, have all contributed to its rise to prominence as one of the most effective and adaptable methods. The scanning

electron microscopy (SEM) technique uses a concentrated stream of high-energy electrons to make a wide range of signals on the surface of solid materials. Furthermore, the SEM can perform analysis on specific points of the sample being studied. This advance is extremely useful for qualitative or semi-quantitative chemical composition examination, as well as assessing crystalline structure and orientation [19]. The Carel Zeiss Instrument can be used to perform a SEM analysis on the prepared sample and measure the findings. Using the SEM technique, the structure surface of V_2O_5 with acid red and V_2O_5 with acid orange was observed. Figures 3.2a and 3.2b show SEM images (10.00kx and 1.96 kx) of the adsorbent, which appears to be a rod-like structure that forms microclusters. This tunability and multivalent character of vanadium pentoxide will aid in its various applications where precise rod diameters are required, such as electrochemical applications, catalysis, and so on [20].

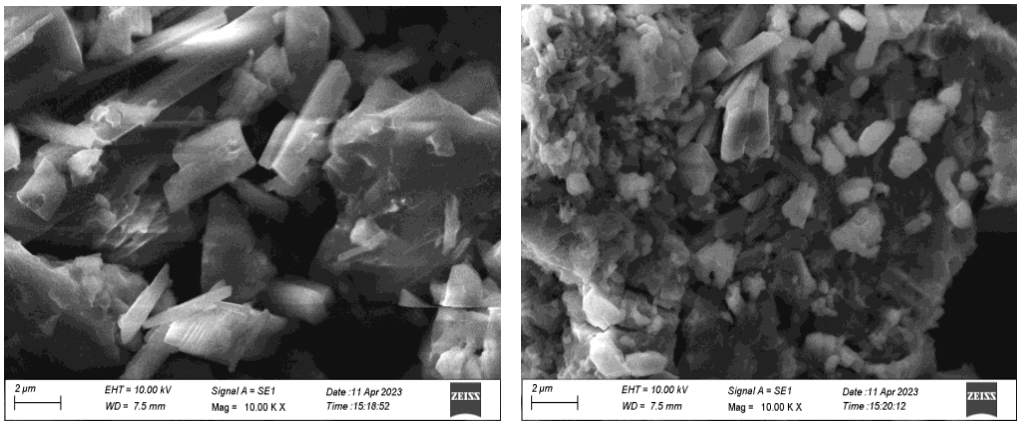


Fig 3.2a and 3.2b. SEM image of V_2O_5 with acid orange and V_2O_5 with acid red molecules

3.3. FTIR analysis

Third-generation infrared spectrometers are known as Fourier transform infrared (FTIR) spectrometers. They have been widely used in the process of structural elucidation. It is a method of gathering spectra derived from coherence measurements of a radiative source, employing measurements of electromagnetic radiation or other types of radiation in the time- or space-domain. These actions may be carried out simultaneously. When the FT function is performed, an interferogram of a sample signal is recorded and digitized using an interferometer, and the corresponding spectrum is presented. Fourier transform infrared spectroscopy (FTIR) is a process that uses an infrared light beam to determine the functional groups contained in a substance (whether it is a gas, liquid, or solid) [21]. IR vibration spectroscopy is a technique that can be used to determine in order to identify the molecules by examining the bonds that make them up. Each chemical link in a molecule has its own unique frequency at which it vibrates. Because of the stretching and bending motions of the molecules as a whole, a group of atoms within a molecule (such as CH_2) can exhibit many modes of oscillation [22]. The oscillations of the CH_2 group cause these modes to exist. Infrared spectroscopy was used to figure out how much IR light is absorbed by each molecule's connection. This process produces a spectrum, which is commonly expressed as a percentage of transmittance versus the wave number (cm^{-1}). The Perkin Elmer Spectrum FTIR Spectrophotometer is the instrument used to record the FTIR spectrum of V_2O_5 with Acid orange and V_2O_5 with Acid red. The FTIR spectrum can be acquired between 4000cm^{-1} to 400cm^{-1} in wavelength. Figure 4a and 4b depicts an FTIR spectral analysis of the prepared samples. The FT-IR spectra of V_2O_5 with Acid orange show peaks for -OH stretching vibration, C=C- stretching vibration, and -N=N- stretching vibration at 3432 cm^{-1}, 1627 cm^{-1}, 1449 cm^{-1}, and 1031'cm^{-1}, respectively. While the peak near 1031 cm^{-1} is for -S=O, indicating the dye's Sulfoxide origin [23]. The peak at 952 cm^{-1} refers to the

formation of a coordination bond with a vanadium atom and the peaks at 757 cm^{-1}, 696 cm^{-1}, and 569 cm^{-1} correspond to hydrogen bonding with an oxygen atom of the Vanadyl group (OH group) and the V-O-V vibrational mode with V-O bridges, respectively. For V_2O_5 with Acid red the band at 909 cm^{-1} is ascribed to the V-OH_2 stretching vibrational mode, which indicates the creation of coordination bonds with vanadium atoms of vanadyl groups in the interlamellar domain. The stretching vibration of the vanadyl group, the in-plane, and out-of-plane V-O-V vibrational modes associated with the V-O bridges, have been attributed to the strong and distinctive peaks of about 749 cm^{-1}, and 544 cm^{-1} belongs, respectively. The weaker band at 684 cm^{-1} could be connected to hydrogen bonding with vanadyl group oxygen atoms [24]. The band peak value at 3413 cm^{-1} for V_2O_5 with acid red dye indicates the O-H group. The stretching vibration of the S-O (SO3-H) group appears at 1196 cm^{-1} and to NO_2 from 1147 cm^{-1} to 1353 cm^{-1} [25]. Table 1 shows the FTIR assignment of the synthesized sample, which supports the chemical structure of the synthesized sample as well as V_2O_5 and organic acid orange and acid red molecules.

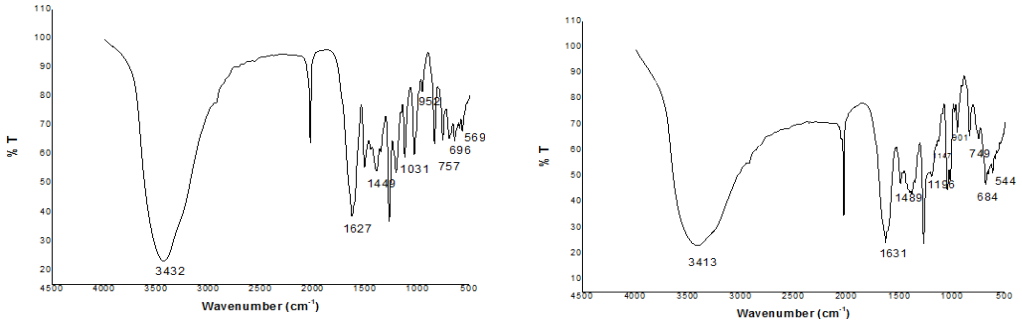


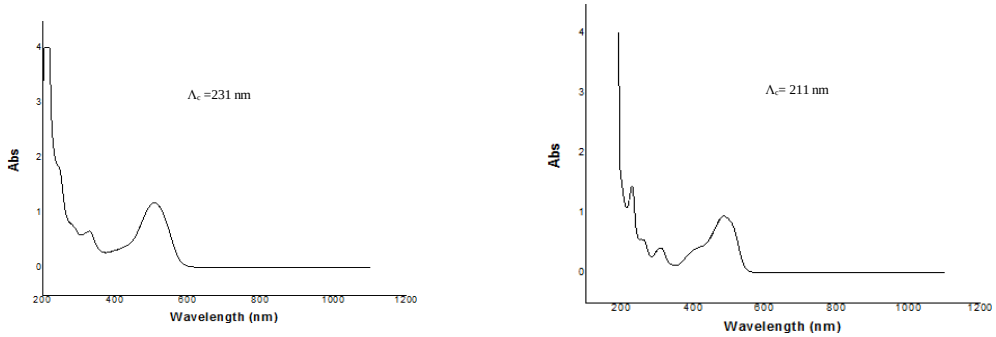
Fig 3.3a and 3.3b. FTIR spectrum of V_2O_5 with acid orange and V_2O_5 with acid red molecules

Table 1. FTIR assignment of synthesized V_2O_5 with acid orange and V_2O_5 with acid red molecules

Wavenumber (cm^{-1})	Assignments	
	Acid Orange	**Acid Red**
3432 3413	OH -	- OH
1627 1631	-C=C- -	- COOH
1449 1489	-N=N- -	- -N=N-
1031 1353 1196	-S=O - -	- NO_2 S-O (SO_3-H)
952 909	V-OH_2 -	- V-OH_2
757 749	V-O-V -	- V-O-V
696 684	O-H -	- O-H
569	V-O	-
544	-	V-O

3.4. UV vis Spectroscopy analysis

UV/VIS absorption spectroscopy is a powerful yet inexpensive tool for identifying organic compounds and measuring the quantity of principal and trace constituents in liquid, gas, and solid test samples [26]. The concentration of major and trace constituents in liquid, gas, and solid test samples can be determined using this method. The ultraviolet-visible-near-infrared spectrum is the result of electromagnetic radiation interacting with molecules, ions, or complexes in the UV-vis-NIR range. It is used to investigate a wide range of substances, together with inorganic, organic, and semi organic molecules. These determinations have applications in research, industry, clinical laboratories, and the chemical evaluation of environmental samples. The amount of visible light absorbed defines the hue of the sample and triggers electron transitions. The absorbance value is proportional to the path length "b" and sample concentration "c" [27]. The Varian Cary SE UV-vis-NIR Spectrophotometer can record the results of the sample's UV-vis-NIR spectral analysis. The UV-vis-NIR Spectrum of the both samples can be obtained by measuring the absorbance in the wavelength ranges of 100nm and 1000 nanometers. The prepared samples' cut off wavelengths are 231 nm for V_2O_5 with Acid orange and 211 nm for V_2O_5 with Acid red, as illustrated in Fig 3.4a and 3.4b. The strong absorption peaks obtained at 231 and 211 nm in both samples due to the transition holes process between V and O [28].The value of the energy gap is calculated by applying the formula $E_g = hC/\lambda_c$, where λ_c is the cut-off wavelength, h is Planck's constant, and C is the velocity of light. Based on this formula, the value of the energy gap will be calculated as 5.38 eV for V_2O_5 with acid orange and 5.89 eV for V_2O_5 with acid red. From the observed values of bandgap, it is concluded that V_2O_5 with acid red has more dielectric property as compared to V_2O_5 with acid Orange molecule. The calculated band gap values of the samples were revealed that the samples are type of insulating materials. As a result, the sample are prominent materials used in optoelectronic devices applications.



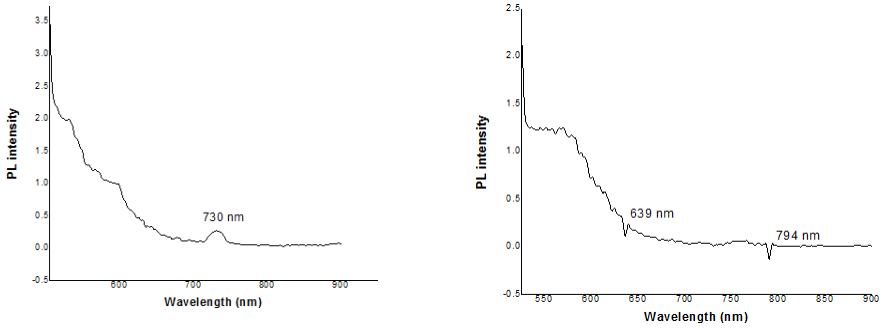
3.4a and 3.4b. UV vis NIR spectrum of V_2O_5 with acid orange and acid red molecules

3.5. Photoluminescence Analysis

Photoluminescence (PL) analysis has the potential to be used to describe a wide range of material properties. Photoluminescence spectroscopy is a discriminating and extremely careful examination of discrete electronic states.

It is used to determine surface, interface, and impurity levels, as well as alloy disorder and interface roughness. The strength of the photoluminescent signal can provide surface and interface quality data. The duration of non-equilibrium interface and the transient photoluminescence intensity under pulsed stimulation determines the bulk states.

The electric field at the surface of a sample can be mapped by watching how the photoluminescence intensity varies in response to an externally imposed bias. Thermally activated procedures, which are utilized for a wide range of evaluations, generate changes in photoluminescence intensity with temperature [29]. Compositional studies of compound semiconductor epitaxial layers and defect analyses of light-emitting materials are examples of these evaluations. Because the photoluminescence (PL) signal is formed by photo generated electron-hole pair recombination [30], photoluminescence (PL) analysis can be utilized to investigate the separation of light-generated charge carriers. The Perkin Elmer LS 45 is an instrument that can be used to record PL spectral analysis. The photoluminescence of V_2O_5 with acid orange and acid red molecules was measured, and the results are given in Fig 3.5a and 3.5b. The photoluminescence examination of pure V_2O_5 peaks at λ=400 nm, which is in the blue-green area [31]. Following the addition of acid orange and acid red dye molecules, in both samples, the peak around 639–794 nm was strongly enhanced compared with other peaks, which clearly shows that the extrinsic transition formed by oxygen vacancies of V_2O_5 due to the annealing process [32]. The equivalent photon energy will be E_g=1.7 eV, and E_g=1.9 eV and E_g=1.5 eV shows the biggest wavelength, which is red, and the most prolonged absorption and emission (with tailing above 1000 nm) in the solid state, respectively. As a result, the addition of acid orange and acid red dye molecules to V_2O_5 material improves its suitability for OLED applications. This band gap energy shows that V_2O_5 with acid orange and acid red dye molecule levels and the dye molecules are situated inside the band gap [33], which is consistent with optical absorption measurements. As a result, the produced V_2O_5 with acid orange, and acid red molecule are a promising materials for opto-electronic device applications [34].



3.5a and 3.5b. Photoluminescence spectrum of V2O5 with acid orange and acid red molecules

4. Conclusion

The synthesized V_2O_5 with acid orange and V_2O_5 with acid red molecules were successfully prepared with distilled water as solvent using simple precipitation method. By varying sample temperature on the evolution of structure (at T = 100 °C), micro rod structures of synthesized samples were investigated. The amorphous nature of the synthesized powdered samples was determined using Powder XRD analysis. The

SEM images show the rod-like shaped micro structure of the pure V_2O_5 molecule increased by adding dye molecules. The presence of V_2O_5 molecule and acid orange molecules and V_2O_5 with acid red dye molecules in the synthesized powder sample was confirmed using FTIR analysis. The UV-vis- NIR absorbance spectrum of the sample was observed within the range of 100-1000 nm which illustrates the insulating nature of the samples with the calculated energy gap value as 5.38 eV for V_2O_5 with acid orange and 5.89 eV for V_2O_5 for acid red molecules. A broad photoluminescence peak around 730 nm for V_2O_5 with acid orange and 639 nm and 794 nm for V_2O_5 with acid red were studied using Perkin Elmer LS 45. From these optical studies, it is confirmed that the synthesized V_2O_5 with acid orange and V_2O_5 with acid red molecules are a promising materials for the application of optoelectronic devices.

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