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UV Studies of Nano-Crystalline Transition Metal Complexes

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Abstract

UV data analysis has been reported of complex **I** ($Ni_{0.8}Co_{0.2}Fe_2O_4$), complex **II** ($Ni_{0.6}Co_{0.4}Fe_2O_4$), complex **III** ($Ni_{0.4}Co_{0.6}Fe_2O_4$), complex **IV** ($Ni_{0.2}Co_{0.8}Fe_2O_4$) and complex **V (**$NiCoFe_2O_4$). On the basis of UV data analysis and discussion, the band gap energy values of all studies complexes have been determined by direct and indirect method are different. The order of the band gap energy shows that the band gap energy value of complex IV is maximum and of complex I is minimum. The higher value of $Ni_{0.8}$ suppresses the band gap energy and higher value of $Co_{0.8}$ enhances the value of band gap energy in this combination.

Introduction

Among the various spectroscopic techniques, UV spectroscopy emerges as a powerful analytical tool, utilizing light within the UV or visible region with wavelengths ranging from 200 to 800 nm. This technique stands versatile, capable of analyzing both colorless compounds in the UV range (400-200 nm) and colored compounds in the visible range (800-400 nm). UV spectroscopy is one of the most significant characterization methods for researching optical characteristics. In the direction of the creation of functional materials with important technological applications; it highlights the value of the UV-Vis spectroscopy technique in characterizing polymer nano composites with optically responsive nano fillers like metals, semiconductor nano crystals, and nano oxides. A derivative these days, spectrophotometers that are controlled by software may do spectrophotometry. This facilitates analysts' ability to extract meaningful information from the spectra of the corresponding chemicals. The UV spectrum derivatives provide useful information for understanding the chemicals used in pharmaceutical formulation [1-4].

Materials and Methods

Chemicals were used without additional purification after being purchased from well-known as renowned companies like E. Merck, Fluka, and Aldrich. For synthetic work, all solvents were utilised exactly as obtained, with an A.R. grade. Aldrich provided metal salt, whereas E. Merck provided Quinoline, Carbamide, Thiocarbamide, Melanic acid, and Dibenzoyl methane [5]. The Copper complex was characterized by namely UV-Visible Spectroscopy. The Copper complex was characterized by namely UV-Visible Spectroscopy. Specification 175 nm to 3300 nm, sample requirement 75mm * 5mm thin film or 100mg powder, Uv-Visible spectrophotometer in the wavelength range from 200 to 800 nm. These data were analyzed by computer software Origin.

These data were analyzed by computer software Origin. Magnetic properties of $Ni_{(1-x)}M_xFe_2O_4$ in this formula [M = Cu (II), Co, Ni], [X = 0.2, 0.4, 0.6, 0.8,….] nano-crystalline ferrites are synthesized by using chemical root method. Chemical AR grad are used 99% ranked from renowned companies like, Nano-crystalline spinel terrisen such as nickel nitrate, ferric nitrate, copper nitrate, cobalt nitrate and citric acid are used for the synthesis, it taken as 1:3 ammonia solution is added to the molar metal nitrate to maintain.

Result and Discussion

A detailed band gap analysis involves plotting and fitting the absorption data to the expected trend lines for direct and indirect band gap semiconductors. According to Beer's Lambert Law,

$A = \varepsilon cl = -\log_{10}(I_T/I_0)$ or $I_T = I_0\, e^{-\varepsilon cl}$ (1.1)

The absorbance A is first normalized to the path length *l* of the light through the material to produce the absorption coefficient, α, as per Equation 1.2

$\alpha = In(10)\varepsilon c$ (1.2)

Values of a > 10^4 cm^{-1} often obey the following relation presented by Tauc and supplied by Davis and Mott **[7-8],**

$\alpha h\nu = (h\nu - E_g)^n$ (1.3)

where n can take on values of 3, 2, 3/2, or 1/2, corresponding to indirect (forbidden), indirect (allowed), direct (forbidden), and direct (allowed) transitions, respectively **[6,9-10]**. These so-called Tauc plots **[11-13]** of $(\alpha h\nu)^n$ vs. hν yield the value of the band gap when extrapolated to the baseline are summarized as follow -

Plot	Transition
$(\alpha h\nu)^2$ vs hν	Direct (allowed)
$(\alpha h\nu)^{2/3}$ vs hν	Direct (forbidden)
$(\alpha h\nu)^{1/2}$ vs hν	Indirect (allowed)
$(\alpha h\nu)^{1/3}$ vs hν	Indirect (forbidden)

UV-Vis studies of the 5 complexes were recorded, the prominent lines were indexed. Figure 1 to 10 represents the patterns of the studied samples. The UV results of all the five samples have been shown in the following table 1 in terms of name of complexes, band gap energy using direct and indirect method.

Fig. 1 to 10 shows the different absorption and band gap energy graphs of Complex I to V. Complex I to V are mixed ligand (cobalt + nickel) complexes as shown in table 1. On the basis of band gap energy values of these five complexes we have obtained the following order of band gap energy by direct and indirect method -

Complex IV > Complex V > Complex III > Complex II > Complex I

and the order of band gap energy from indirect band gap energy values are –

Complex IV > Complex V > Complex II > Complex III > Complex I

The above order of the band gap energy shows that the band gap energy value of complex IV is maximum and of complex I is minimum. The higher value of $Ni_{0.8}$ suppresses the band gap energy and higher value of $Co_{0.8}$ enhances the value of band gap energy in this combination.

Conclusion

On the basis of UV data analysis and discussion, the band gap energy values of all studies complexes have been determined by direct and indirect method are different. The order of the band gap energy

shows that the band gap energy value of complex IV is maximum and of complex I is minimum. Hence the higher value of $Ni_{0.8}$ suppresses the band gap energy and higher value of $Co_{0.8}$ enhances the value of band gap energy in this combination.

Table 1 - Band gap energy values of transition metal complexes

S. No.	Name of complexes	Complexes	Direct band gap energy (ev)	Indirect band gap energy (ev)
1	Complex I	$Ni_{0.8}Co_{0.2}Fe_2O_4$	3.053	3.952
2	Complex II	$Ni_{0.6}Co_{0.4}Fe_2O_4$	3.290	4.142
3	Complex III	$Ni_{0.4}Co_{0.6}Fe_2O_4$	3.441	4.038
4	Complex IV	$Ni_{0.2}Co_{0.8}Fe_2O_4$	3.753	4.246
5	Complex V	$NiCoFe_2O_4$	3.678	4.198

Fig. 1 to 10 – Direct and indirect band gap energy values of transition metal complexes

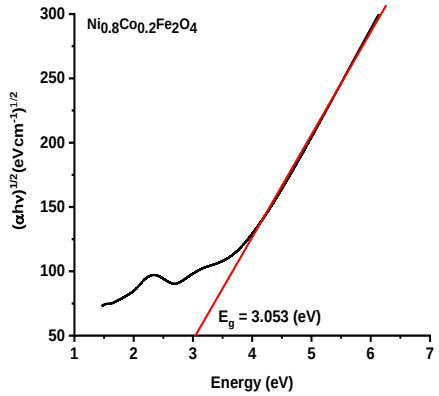

Fig. 1 – Complex I - Direct band gap (absorption factors vs. energy)

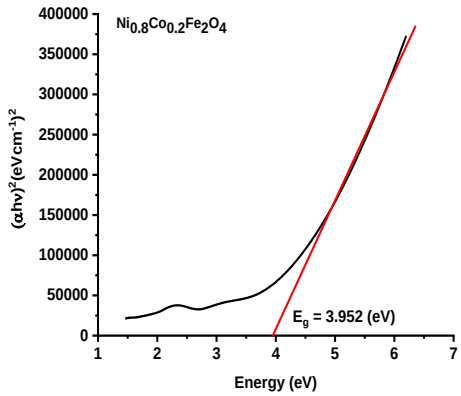

Fig. 2 – Complex I - Indirect band gap (absorption factors vs. energy)

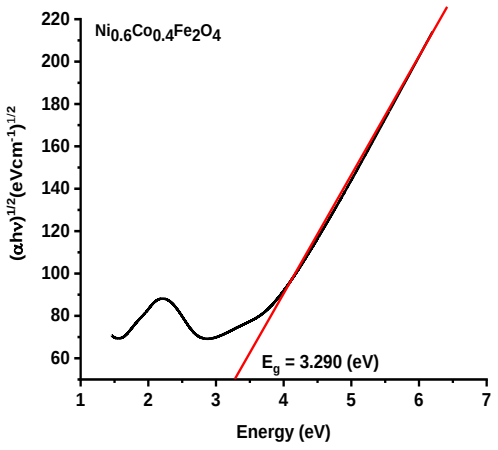

Fig. 3 – Complex II - Direct band gap (absorption factors vs. energy)

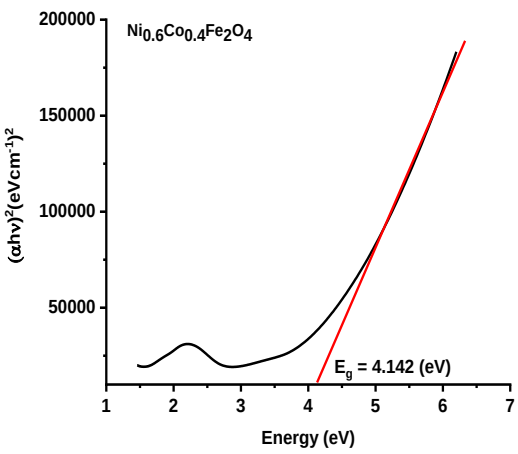

Fig. 4 – Complex II - Indirect band gap (absorption factors vs. energy)

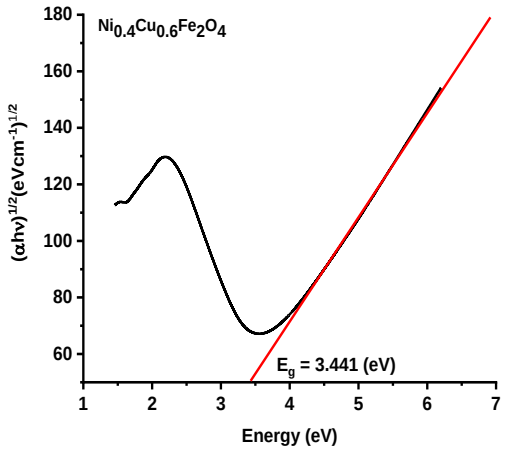

Fig. 5 – Complex III - Direct band gap (absorption factors vs. energy)

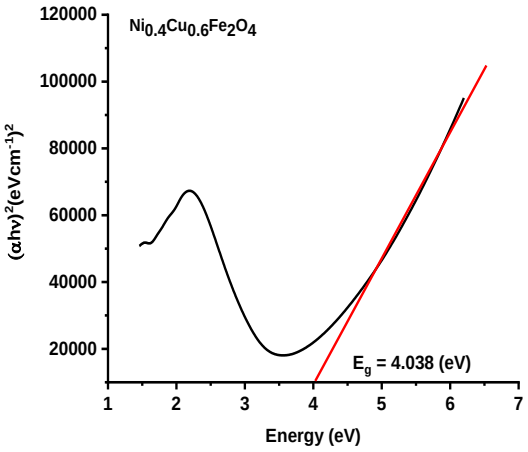

Fig. 6 – Complex III - Indirect band gap (absorption factors vs. energy)

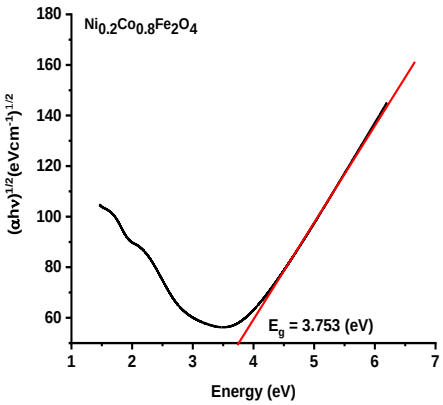

Fig. 7 – Complex IV - Direct band gap (absorption factors vs. energy)

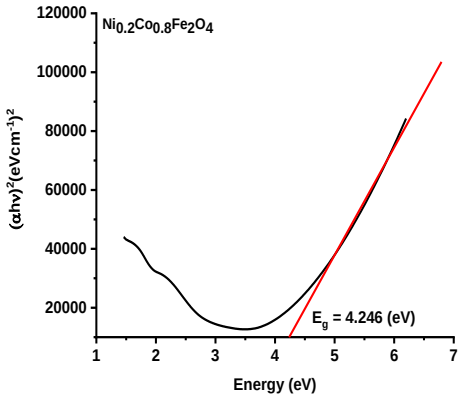

Fig. 8 – Complex IV - Indirect band gap (absorption factors vs. energy)

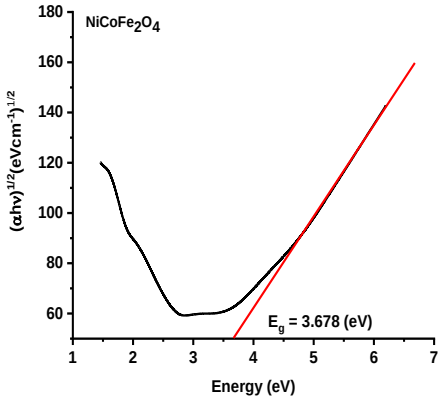

Fig. 9 – Complex V - Direct band gap (absorption factors vs. energy)

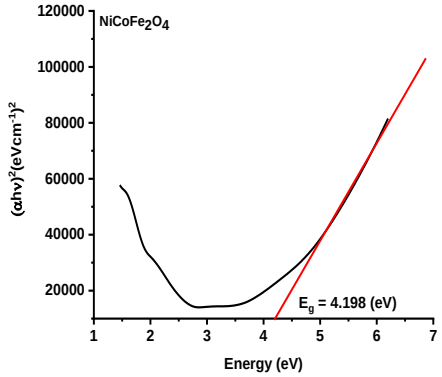

Fig. 10 – Complex VI - Indirect band gap (absorption factors vs. energy)

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