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Multifunctional properties on Transition Metal Doping (Al) in Mg 0.5 Sr 0.5 Cr 2- x Al x O 4 (x=0; x=0.2): Comprehensive structural, infrared, XPS and optical analysis and its potential applications for Optoelectronic devices

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Multifunctional properties on Transition Metal Doping (Al) in $Mg_{0.5}Sr_{0.5}Cr_{2-x}Al_xO_4$ (x=0; x=0.2): Comprehensive structural, infrared, XPS and optical analysis and its potential applications for Optoelectronic devices

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Abstract

In this work, the structural, infrared, elastic, and optical properties of $Mg_{0.5}Sr_{0.5}Cr_{2-x}Al_xO_4$ (x = 0 and 0.2) chromite synthesized by the sol–gel method were investigated. Structural characterization of the synthesized powders was performed using X-ray diffraction (XRD), which confirmed the formation of a single-phase cubic spinel structure. The XRD patterns were analyzed to determine key structural parameters, including the lattice parameter and crystallite size. The elastic parameters were evaluated from the FTIR spectra. To investigate the cation distribution, the experimental results were compared with theoretical values, and the chemical states and quantitative contributions of Mg^{2+}, Sr^{2+}, Cr^{3+}, and Al^{3+} were determined by X-ray photoelectron spectroscopy (XPS). The optical properties were investigated through the refractive index, penetration depth, and extinction coefficient. The determined band-gap energies indicate that these materials exhibit significant visible-light absorption, highlighting their potential for optoelectronic applications. Overall, the results demonstrate that partial substitution of Cr^{3+} by Al^{3+} is an effective strategy for tailoring the structural, elastic, and optical properties of $Mg_{0.5}Sr_{0.5}Cr_{2-x}Al_xO_4$ (x = 0 and 0.2) chromite.

Keywords: spinel chromite; sol gel method; XRD findings, photoelectron spectroscopy analysis, elastic and optical investigation.

1. Introduction

Spinel-structured chromite exhibit several advantageous characteristics, including high electrical resistivity, good mechanical hardness, excellent chemical stability, and magnetic properties well suited for high-frequency applications, while remaining cost-effective **[1-2]**. Owing to these attributes, they are widely used in microwave absorption as well as in various electronic devices, such as radios**,** televisions**,** non-reciprocal integrated circuits**,** and high-frequency transformers **[3-5]**. Moreover, these materials have demonstrated high efficiency as catalysts for the alkylation of aromatic compounds and are also employed in the field of telecommunications **[1]**. Spinel chromite are further utilized in gas-sensing applications, particularly for the detection of ethanol and other reducing gases **[3].** It is well established that the physical properties of spinel chromite are strongly influenced by several factors, including cation distribution, particle size, crystallite size, and phase purity, all of which are closely related to the synthesis method employed **[1-3]**. For the synthesis of various nanoparticle systems, especially chromite-based materials, a variety of wet-chemistry techniques have been extensively used, including co-precipitation, sol–gel, combustion synthesis, reverse micelle, and hydrothermal procedures **[6]**. These methods provide several benefits over traditional solid-state processes, including lower processing temperatures, shorter synthesis times, enhanced chemical purity and homogeneity, and better nanoscale particle size control **[7]**.

Spinel chromite have attracted considerable research interest due to their wide range of applications, particularly in electrical, magnetic, and optoelectronic fields **[8-9]**. Their tunable optical band gap, strong optical absorption, and magnetic properties make them promising candidates for various advanced technological applications. Spinel chromite have been extensively investigated for use in optoelectronic devices such as solar cells and photodetectors **[10-11]**. It has been reported that doped $MgCr_2O_4$, based materials, especially those containing transition-metal ion (Al^{3+}, Ni^{2+}, Fe^{3+}...) exhibit enhanced optical absorption in the visible and ultraviolet regions because of a significant reduction in the optical band gap (E_g) **[12]**. Consequently, decreasing the band gap energy is essential to extend the optical response of Mg–Sr, based samples into the visible light region.

A smaller band gap indicates increased absorption of visible light in photocatalytic processes **[13]**. Additionally, the spinel chromite $Mg_{0.5}Sr_{0.5}Cr_{2-x}Al_xO_4$ exhibit significant UV absorption due to their extremely low optical band-gap energies **[12]**. Scientists are actively seeking to enhance the visible-light sensitivity of functional materials by engineering compounds with reduced band gap energies **[13-14]**.

In this context, various characterization techniques have been employed to investigate the $Mg_{0.5}Sr_{0.5}Cr_{2-x}Al_xO_4$ (x= 0; 0.2) system, in which controlled cation substitution can be used to tailor and enhance its structural, optical, and electronic properties for potential technological applications **[15-16]**. To the best of our knowledge, no previous studies have reported a detailed investigation of the structural and optical properties of Al-substituted $Mg_{0.5}Sr_{0.5}Cr_{2-x}Al_xO_4$ (x= 0; 0.2) chromite. In the present study, the synthesized samples were characterized by X-ray powder diffraction (XRD) to investigate their phase purity and crystal structure **[17-18]**. Particular attention was devoted to the optical properties of the sol–gel-synthesized $Mg_{0.5}Sr_{0.5}Cr_{2-x}Al_xO_4$ (x= 0; 0.2) chromite. Diffuse reflectance spectroscopy (DRS), combined with the Tauc formalism, was employed to investigate their optical absorption behavior and determine the optical band-gap energy **[19-20]**. In addition, the Urbach energy and refractive index were evaluated to provide further insight into the electronic structure and the disorder effects induced by Al^{3+} substitution **[21-22]**.

2. Synthesis and characterization techniques

The $Mg_{0.5}Sr_{0.5}Cr_{2x}Al_xO_4$ (x= 0; 0.2) chromite were synthesized using the sol-gel method **[23-24]**, as illustrated in **Figure 1**. The synthesis process began with the dissolution of $Mg(NO_3)_2.6H_2O$, $Sr(NO_3)_2.6H_2O$, $Cr(NO_3)_3.9H_2O$ and $Al(NO_3)_3.9H_2O$ nitrates (all with 99.99% purity and procured from Sigma Aldrich) in 100 ml of distilled water. This mixture was stirred on a hot plate at 80 °C to ensure complete dissolution. Next, citric acid ($C_6H_8O_7 \cdot H_2O$, 99.9% purity) was added as a complexing agent, followed by the addition of ethylene glycol ($HO(CH_2)_3OH$, 99.9% purity) as a polymerization agent to form a gel. The resulting solution was heated until it became a highly viscous gel, which was subsequently dried at 200 °C to obtain a dry foam. The obtained foam was ground

in an agate mortar and calcined at 600 °C for 24 h to remove residual organic matter **[25]**. The resulting powder was then annealed at 750 °C for 12 h. Finally, the powder was reground, pressed into pellets, and sintered at 950 °C for 24 h. Finally, the resulting powder was ground and pressed into pellets. After that, these pellets were sintered at 950 °C for 24 h. X-ray diffraction (XRD) patterns were collected using a PANalytical X'Pert Pro diffractometer operating in θ-2θ geometry with Cu-Kα radiation (λ = 1.5406 Å) and a step size of 0.02°. Phase identification and structural analysis were performed using FullProf and X'Pert HighScore Plus software packages **[26]**. Fourier transform infrared (FTIR) spectra were recorded with a Shimadzu FTIR-8400S spectrometer in the wavenumber range of 500-4000 cm^{-1} **[27]**. In addition, the elastic properties of the samples were investigated using standard mechanical characterization techniques, allowing the determination of fundamental elastic parameters such as Young's modulus, shear modulus, and bulk modulus, which provide insight into the mechanical stability and structural rigidity of the materials **[28]**.

Optical properties were investigated at room temperature using a Shimadzu UV-3101 PC spectrophotometer over the wavelength range of 200-2400 nm. This instrument, characterized by high sensitivity and low stray light, enables accurate measurements of low-absorbance sample and supports multiple measurement modes, including absorbance, transmittance, and reflectance **[29]**. For diffuse reflectance measurements, the samples were finely ground to ensure homogeneity and, when necessary, mixed with a non-absorbing matrix. The powdered samples were placed in 2 mm thick sample holders and analyzed using a diffuse reflectance accessory equipped with an integrating sphere. Prior to measurements, baseline correction was performed using a standard reference material with known reflectance to eliminate instrumental effects **[30]**.

3. Results and discussion

3.1 Rietveld refinement

The X-ray diffraction (XRD) patterns of $Mg_{0.5}Sr_{0.5}Cr_{2x}Al_xO_4$ (x= 0; 0.2) samples are presented in **Figure. 2**. All diffraction peaks are well indexed to the characteristic crystallographic planes (111), (220), (311), (222), (400), (422), (511), (440), (620), and (533), corresponding to a cubic spinel structure with the space

group $\boldsymbol{Fd\bar{3}m}$. No extra peaks associated with secondary phases or impurities are detected, confirming the formation of single-phase compounds. The sharp and intense diffraction peaks indicate good crystallinity of the synthesized materials. Using **Eq. 1**, **[31]** we estimated the experimental lattice constant denoted as a_{exp}.

$$a_{exp} = d_{hkl}\sqrt{h^2 + k^2 + l^2} \quad \textbf{(1)}$$

$$2d_{hkl} \sin\theta_{hkl} = \lambda \quad \textbf{(2)}$$

Here, (hkl) represents the Miller indices of the (311) X-ray Bragg peak. It is observed that the lattice constant of the $Mg_{0.5}Sr_{0.5}Cr_2O_4$ sample is larger than that of the Al-substituted $Mg_{0.5}Sr_{0.5}Cr_{1.8}Al_{0.2}O_4$ chromite **[32-33]**. This decrease in lattice parameter with Al substitution can be attributed to the smaller ionic radius of Al^{3+} compared to Cr^{3+} at the B site in the spinel structure.

As the Al concentration increases, the XRD patterns of $Mg_{0.5}Sr_{0.5}Cr_{2-x}Al_xO_4$ samples exhibit a slight shift of diffraction peaks toward higher 2θ values, particularly for the (311) reflection. According to Bragg's law, this shift corresponds to a decrease in the interplanar spacing (d), leading to a reduction in the lattice parameter (a). The observed lattice contraction is attributed to the substitution of Cr^{3+} ions (0.615 Å) by smaller Al^{3+} ions (0.535 Å) at the octahedral B-site of the spinel structure. Consequently, the unit cell volume ($V = a^3$) decreases with increasing Al content. The nearly linear variation of the lattice parameter with Al concentration suggests the formation of a homogeneous solid solution obeying Vegard's law. The cation distribution of the $Mg_{0,5}Sr_{0,5}Cr_{1,8}Al_{0,2}O_4$ compound can therefore be described as: $(Mg_{0.5}^{2+}Sr_{0.5}^{2+})_A[Cr_{2-x}^{3+}Al_x^{3+}]_BO_4^{2-}$.

This distribution is suggested based on crystallo-chemical considerations regarding the coordination preferences of different cations: Mg^{2+} ions ($r_{Mg^{2+}}$ = 0.72 Å) prefer tetrahedral positions (A). In contrast, Sr^{2+} ions, with a large ionic radius ($r_{Sr^{2+}}$ = 1.32 Å in 8-fold coordination), are suited to tetrahedral sites due to their large size. Furthermore, Cr^{3+} ($r_{Cr^{3+}}$ = 0.63 Å) and Al^{3+} ($r_{Al^{3+}}$ = 0.675 Å) ions, which have a small size and considerable charge density, prefer octahedral sites (B). This is due to their ability to achieve six-fold coordination. This distribution of cations affects not only structural stability, but also the optical and electronic characteristics of the material, particularly through crystal field interactions and the creation of energy bands.

In spinel-structured compounds, the inversion rate (i) indicates the fraction of trivalent cations (usually of the B^{3+} type) that are found in tetrahedral sites (A) rather than at their preferred location in octahedral sites (B). This allows us to describe the cationic disorder within the crystal structure. For our samples, the cationic distribution is as follows: $(Mg_{0.5}^{2+}Sr_{0.5}^{2+})_A[Cr_{2-x}^{3+}Al_x^{3+}]_B O_4^{2-}$.

This distribution indicates that (2-x) Cr^{3+} atoms occupy the octahedral positions (B) with partial substitution by Al^{3+}, while Mg^{2+} and Sr^{2+} are found in the tetrahedral positions (A). We can therefore deduce that the degree of inversion is equal to 0 and our samples exhibit a normal spinel structure. The results of the refinement of the X-ray diffraction pattern profile using the Rietveld method for the compounds $Mg_{0.5}Sr_{0.5}Cr_{2x}Al_xO_4$ (x= 0; 0.2) are summarized in **Table. I.** A very good agreement is observed between the positions of the observed and calculated Bragg reflections, as shown in **Figure. 3**.

Table. I provide a summary of the improved structural characteristics. The suggested cation distribution is supported by the refined site occupancies for Mg and Sr at the tetrahedral A-site and Cr and Al at the octahedral B-site, which are in good accord with the nominal stoichiometry. Excellent agreement is seen in **Figure. 3,** which shows a significant correlation between the computed and observed XRD patterns. The crystallographic locations 16d (1/2, 1/2, 1/2), 8a (1/8, 1/8, 1/8), and 32e (x, x, x) in the Rietveld refinement were designated for B-site cations, A-site cations, and oxygen atoms, respectively. The analysis's precision and dependability were confirmed by the refinement, which produced R, structural R_F, profile R_p, and weighted R_{wp} values all below 10% and a goodness-of-fit (χ^2) near 1. The positional parameter of refined oxygen (x). Notably, the refined oxygen positional parameter [x = 0.259] is consistent with the expected values for a typical spinel structure.

The x-ray density of our sample was calculated using the following formula **[34]**:

$$\boldsymbol{\rho_{XRD}} = \frac{\boldsymbol{8M}}{\boldsymbol{N_A a^3}} \qquad \textbf{(3)}$$

Where N_A is Avogadro's number, M is the molecular weight, and a is the lattice parameter. The calculated $\boldsymbol{\rho_{XRD}}$ value for the $Mg_{0.5}Sr_{0.5}Cr_{2-x}Al_xO_4$ (x= 0; 0.2) sample is 4.88 g/cm^3 for x=0 and 4.94 g/cm^3 for x=0.2. The average crystallite

size (D) was estimated from the XRD peak broadening using the Scherrer formula **[34]**:

$$\boldsymbol{D = \frac{0.9\lambda}{\beta\cos(\theta)}} \quad \textbf{(4)}$$

Where λ = 1.5406 Å is the X-ray wavelength, ß is the full width at half maximum (FWHM) of the most intense diffraction peak (in radians), and θ is the corresponding Bragg angle, was used to determine the crystallite size of the $Mg_{0.5}Sr_{0.5}Cr_{2-x}Al_xO_4$ (x= 0; 0.2) samples. The estimated average crystallite sizes for x = 0 and x = 0.2 are roughly 28 nm and 26 nm, respectively, suggesting a little reduction in crystallite size with aluminum substitution.

3.2. Infrared and Elastic Properties

3.2.1. FTIR Analysis

Chromite materials are thought of as joined crystals where atoms are connected to their closest neighbors by various interactions, including van der Waals **[35]**, covalent, and ionic forces. Spinel chromite are made up of metal ions dispersed throughout two distinct sublattices, the tetrahedral A sites and the octahedral B sites, due to the geometric arrangement of surrounding oxygen atoms. In this crystal structure, octahedral cations vibrate in a direction perpendicular to the axis connecting the tetrahedral metal ion and the oxygen atom, while tetrahedral cations vibrate along the direction connecting the cation to the nearby oxygen atoms. The $Mg_{0.5}Sr_{0.5}Cr_{2-x}Al_xO_4$ (x= 0; 0.2) sample's infrared spectrum is shown in **Figure. 4**, where two distinctive absorption bands linked to metal–oxygen vibrational modes are plainly visible.

The stretching vibration of the tetrahedral metal–oxygen bonds (ν_A) is responsible for the absorption band near 600 cm^{-1}, whereas the octahedral metal–oxygen stretching mode (ν_B) is responsible for the band at about 469 cm^{-1} **[36-37]**. The development of metal–oxygen bonds, primarily Cr-O and Al-O, within the spinel lattice is confirmed by the existence of these two distinctive bands. The impact of Al substitution on the vibrational bands is highlighted in **Table. II**, which contrasts these vibrational frequencies with those obtained for the undoped $Mg_{0.5}Sr_{0.5}Cr_{2-x}Al_xO_4$ (x= 0; 0.2) sample. The tetrahedral vibration band (ν_A) in the doped $Mg_{0.5}Sr_{0.5}Cr_{2-x}Al_xO_4$ (x= 0; 0.2) sample shifts slightly from 621.55 cm^{-1} to 623.30 cm^{-1}, whereas the octahedral band (B) shifts from 469.24

cm^{-1} to 471.95 cm^{-1}. These variations can be explained by changes in the metal-oxygen bond lengths brought about by cation substitution and potential cation redistribution between the spinel structure's tetrahedral (A) and octahedral (B) locations.

Changes in crystallite size and the redistribution of cations between the octahedral and tetrahedral positions are probably responsible for these alterations. The addition of Al^{3+} ions modify the force constants and local bonding environment, which affects the spinel lattice's vibrational activity **[37-38]**.

3.3.2. Elastic and Thermal Properties

Interatomic and interionic interactions inside the crystal lattice give rise to important elastic and thermal properties in spinel chromite. Ultrasonic pulse transmission techniques, which offer direct information regarding lattice dynamics and mechanical stability, are frequently used to calculate the Debye temperature **[39]** and elastic constants.

Indeed, correlations between infrared vibrational spectra and structural characteristics have also been investigated in several research studies. Specifically, Modi H. J. and colleagues suggested a technique to use FTIR spectrum data to determine the elastic behavior of spinel chromite **[40]**. This method relates the force constants of the lattice to the infrared absorption bands that correspond to the tetrahedral and octahedral metal–oxygen vibrations. The force constants of the tetrahedral site (K_t) and the octahedral site (K_o) are directly proportional to the wavenumbers corresponding to the tetrahedral stretching vibration (v_A) and the octahedral stretching vibration (v_B), respectively. R. D. Waldron's relations for spinel ferrites can be used to compute these force constants **[41]**.

$$K_t = 7.62 \times M_A \times \nu_A^2 \times 10^{-7} \quad \textbf{(5)}$$

$$K_o = 10.62 \times (\frac{M_B}{2}) \times \nu_B^2 \times 10^{-7} \quad \textbf{(6)}$$

The molecular weights M_A and M_B were calculated using the cation distribution suggested for the investigated spinel. Of the cations found in the octahedral (B) and tetrahedral (A) sites, respectively **[42]**. The force constants for the tetrahedral (K_t) and octahedral (K_o) metal–oxygen bonds were computed using the computed values of K_t and K_o

together with the average force constant $K_{av} = \frac{(K_t+K_o)}{2}$. Table II summarizes them. The force constant is positively correlated with bond strength and inversely correlated with bond length. The $Mg_{0.5}Sr_{0.5}Cr_{1.8}Al_{0.2}O_4$ sample's larger value of K_t suggests that the metal–oxygen bonds at the tetrahedral sites are stronger than those at the octahedral sites. This behavior can be explained by the greater bond stiffness and shorter M-O bond length linked to tetrahedral coordination in spinel structures. In general, the relations suggested by R. D. Waldron based on these values **[43-44]**.

The stretching vibration linked to tetrahedral sites typically shows greater force constants than that of octahedral sites, which is consistent with earlier infrared investigations of spinel-structured chromite. This discrepancy is explained by the metal–oxygen bonds at the tetrahedral sites being stiffer. Additionally, the average force constant K_{av} diminishes marginally in comparison to the undoped $Mg_{0.5}Sr_{0.5}Cr_2O_4$ sample following the insertion of aluminum. This decrease indicates a small decrease in the average stiffness of the metal–oxygen bonds in the crystal lattice, which is probably caused by local variations in bond lengths and cation distribution brought on by the addition of Al^{3+}. Numerous research studies on substituted spinel-type chromite have demonstrated similar behavior **[45-46]**.

$$C_{11} = \frac{k_{av}}{a} \quad \textbf{(7)}$$

However, C_{12} and C_{44}, which possess shape-altering elasticity, are delivered as follows **[47]**:

$$C_{12} = \frac{\sigma C_{11}}{1-\sigma} \quad \textbf{(8)}$$

$$C_{44} = \rho^2 v_t \quad \textbf{(9)}$$

Where the X-ray density is represented by ρ. These formulas were used to determine the parameters, such as the longitudinal wave velocity v_l, the transverse wave velocity v_t, and the Poisson's ratio σ **[48]**.

$$v_t = \frac{v_l}{\sqrt{3}} \quad \textbf{(10)}$$

$$v_l = \sqrt{\frac{C_{11}}{\rho}} \quad \textbf{(11)}$$

$$\sigma = \frac{L-2G}{2(L-G)} \quad \textbf{(12)}$$

In this case, $L = \rho v_l^2$ and $G=\rho v_t^2$ denote the longitudinal and shear moduli, respectively. The longitudinal modulus (L) indicates the material's resistance to deformation under compressive or tensile stress, whereas the shear modulus (G) describes the material's resistance to shape distortion under shear stress. **Table. II** summarizes the computed values of the elastic constants C_{11}, C_{12}, and C_{44}, as well as the sound velocities (v_t, v_l), moduli (L, G), and Poisson's ratio (σ). Shear waves, on the other hand, move more slowly than longitudinal waves when energy transfer causes particle vibrations.

Particles in shear waves vibrate perpendicular to the direction of the wave's propagation; hence, it takes more energy to make nearby particles vibrate **[49]**. According to isotropic elasticity theory, Poisson's ratio (σ), which ranges from -1 to 0.5, is an important indicator of a material's brittleness or ductility **[50]**. By computing the bulk modulus to shear modulus ratio B/G **[51]**, where$B = \frac{1}{3}(C_{11} + 2C_{12})$, the Pugh criterion assesses a material's ductility or brittleness. Ductility is indicated by a B/G ratio larger than 1.75, whereas brittleness is suggested by a ratio below 1.75 **[52]**. An essential thermodynamic property that describes the maximum lattice vibrations and provides information about the heat transmission characteristics of a material is the Debye temperature (θ_D). Anderson's formula **[53]** is used to estimate it:

$$\theta_D = \frac{\hbar}{k_B}\left(\frac{3q\rho N_A}{4\pi M}\right)^{\frac{1}{3}} \nu_m \quad \textbf{(13)}$$

Where ρ is the density, N_A is Avogadro's number, M is the molecular mass, q is the number of atoms per formula unit, k_B is the Boltzmann constant, and $\hbar$ is the reduced Planck's constant. The mean wave velocity (v_m) is defined as follows to comprehend how energy passes through a material:

$$\nu_m = \left(\frac{1}{3}\left(\frac{2}{v_t^3} + \frac{1}{v_l^3}\right)\right)^{-1/3} \quad \textbf{(14)}$$

Lastly, the formula for minimal thermal conductivity (K_{min}) can be used to calculate a material's thermal conductivity, an essential thermodynamic property:

$$K_{min} = \left(\frac{M}{q\rho N_A}\right)^{-\frac{2}{3}} k_B \nu_m \quad \textbf{(15)}$$

The measured values of the Debye temperature (θ_D), average sound velocity (v_m), and minimum thermal conductivity **[54]** (K_{min}) are summarized in **Table. II**. The average sound velocity, σ_m, of the $Mg_{0.5}Sr_{0.5}Cr_{1.8}Al_{0.2}O_4$ sample is slightly greater than that of the undoped combination $Mg_{0,5}Sr_{0,5}Cr_2O_4$ **[55]**, but θ_D drops. The rise in longitudinal and transverse sound velocities in the Al^{3+}-substituted sample, which is caused by the decrease in material density after the partial substitution of Cr^{3+} by lighter Al^{3+} ions, is the primary cause of the increase in ν_m **[56]**. On the other hand, a drop in θ_D indicates a decrease in the average force constant and overall stiffness of the crystal lattice, which promotes more active lattice vibrations. These findings are in line with earlier findings for comparable spinel. Therefore, with this insulating material, the electronic contribution is minimal, and the drop in θ_D is mainly structural and elastic **[57]**.

3.3. X-ray photoelectron spectroscopy analysis (XPS)

The surface chemical composition and oxidation states of $Mg_{0.5}Sr_{0.5}Cr_{2x}Al_xO_4$ (x= 0; 0.2) were investigated by X-ray photoelectron spectroscopy (XPS), as shown in **Fig. 6** and **7**. The XPS survey spectra reveal the presence of Mg, Sr, Cr, Al, and O, with no detectable impurity peaks, indicating the high purity of the synthesized samples.

The high-resolution Mg 1s spectrum exhibits a single symmetric peak centered at approximately 1304 eV, which is characteristic of Mg^{2+} species in an oxide environment. No additional component associated with metallic Mg is observed, indicating that Mg is predominantly present in its oxidized state. The Sr 3d core-level spectrum displays a well-defined spin–orbit doublet corresponding to Sr $3d_{5/2}$ and Sr $3d_{3/2}$. The Sr $3d_{5/2}$ component is located at approximately 133 eV, with a spin–orbit splitting of about 1.7 eV, confirming the presence of Sr^{2+} species **[57-62]**.

The Cr 2p spectrum consists of two main peaks located at approximately 576–577 eV and 586–587 eV, corresponding to Cr $2p_{3/2}$ and Cr $2p_{1/2}$, respectively. The experimentally determined binding energies of 576.39 eV for Cr $2p_{3/2}$ and 586.26 eV for Cr $2p_{1/2}$ give a spin–orbit splitting of approximately 9.87 eV **[63-66]**.

These binding energies are characteristic of Cr^{3+} species in oxide environments. No significant contribution attributable to Cr^{6+} species is observed around 579–580 eV, indicating that chromium predominantly remains in the trivalent state upon Al substitution. For the Al-substituted sample (x = 0.2), the Al 2p spectrum exhibits a relatively narrow peak centered at approximately 74 eV, which can be assigned to Al^{3+} species in an oxide environment. The absence of a significant contribution near 72–73 eV indicates that metallic Al is not detected. The presence of Al^{3+} is consistent with its incorporation into the spinel structure through substitution at the Cr^{3+} sites, as suggested by the structural analysis **[67-70]**.

The O 1s spectrum can be deconvoluted into two main components. The lower-binding-energy component, centered at approximately 529.5 eV, is assigned to lattice oxygen (O^{2-}) bonded to metal cations within the spinel framework. The higher-binding-energy component, located at approximately 531–532 eV, is generally associated with surface hydroxyl groups and/or adsorbed oxygen species. Any variation in the relative contribution of this component upon Al substitution suggests a modification of the surface chemical environment and oxygen-related species **[60-70]**.

Overall, the XPS results confirm the presence of Mg^{2+}, Sr^{2+}, Cr^{3+}, and Al^{3+} in the investigated $Mg_{0.5}Sr_{0.5}Cr_{2x}Al_xO_4$ (x= 0; 0.2) samples. In particular, the Cr 2p analysis demonstrates that Al substitution does not induce a detectable change in the chromium oxidation state. These results are consistent with the formation of the expected spinel structure and indicate that Al incorporation mainly modifies the local and surface chemical environment without significantly affecting the valence state of chromium.

3..4. Optical properties

3.4.1. UV-VIS-NIR absorbance and reflectance spectra

The absorption spectra A(λ) and reflectance spectra R(λ) of the $Mg_{0.5}Sr_{0.5}Cr_{2x}Al_xO_4$ (x= 0; 0.2) samples (x = 0 and 0.2) are displayed in **Figure.6** (a, b). The absorption spectra show that the material interacts strongly with photons in the UV-visible range, indicating effective electronic excitation that is typically ascribed to O 2p → metal 3d transitions. Because of this characteristic,

these compounds have intriguing potential for photocatalytic applications and **[71]**, in some cases (especially once the bandgap and transport characteristics have been optimized), for photovoltaic systems. These materials are intriguing for optoelectronic applications in the near-infrared (NIR) region because the presence of absorption bands in the NIR suggests the occurrence of extra electronic transitions or localized states **[72]**.

3.4.2. Optical band gap energy

The bandgap energy Eg is strongly correlated with the optical reflectance R(λ).

Through the complicated optical characteristics of the material, particularly the extinction coefficient (k) and refractive index (n). In fact, according to Fresnel's equations, reflectance depends on these factors, whereas the extinction coefficient is directly correlated with the absorption coefficient α, which is controlled by interbond electronic transitions. A notable rise in absorption is seen when the photon energy $h\nu$ approaches the bandgap energy. This leads to a noticeable change in the coefficient k and, ultimately, in the reflectance spectrum. Therefore, the basic transition between the valence band and the conduction band is represented by the absorption edge seen in the curves R(λ). For powdered materials, the Kubelka–Munk function $F(R) = (1-R)^2 / 2R$ is frequently used to estimate the absorption coefficient and enable the determination of Eg via the Tauc relation **[73-74]**. As a result, any change in the bandgap energy, caused, for instance, by cation substitution or structural alteration in spinel, appears as a shift of the reflectance edge toward longer or shorter wavelengths, reflecting modifications in the material's electronic structure **[75]**.

$$(\alpha h\nu)^n = \beta(h\nu - E_g) \quad \textbf{(16)}$$

$$F(R) = \frac{(1-R)^2}{2R} \quad \textbf{(17)}$$

$$F(R) \approx \alpha \quad \textbf{(18)}$$

$$h\nu = \frac{1240}{\lambda} \quad \textbf{(19)}$$

$$(F(R) \cdot h\nu)^n = \beta\,(h\nu - E_g) \quad \textbf{(20)}$$

The compounds' $Mg_{0.5}Sr_{0.5}Cr_{2-x}Al_xO_4$ (x= 0; 0.2) samples optical band gap energy Plotting (x=0 and x=0.2) was done using the Kubelka–Munk function in conjunction with the Tauc method to obtain diffuse reflectance spectra **[76-77]**. A permitted direct transition is represented by $(F(R)\cdot h\nu)^2$ as a function of photon energy $h\nu$ displayed in **Figure.8**. Two absorption thresholds with optical gap values of Eg_1=1.87 eV was found for the undoped material (x=0) and Eg_2=2.41 eV. While the first gap is linked to the existence of localized states in the bandgap, most likely due to structural flaws or intra-ionic transitions of the cation Cr^{3+}, the second gap is explained by the fundamental transition between the valence band and the conduction band.

On the other hand, an optical bandgap value of Eg= 2.7 eV is obtained for the doped sample (x = 0.2), which exhibits a single dominant linear domain. A substantial alteration in the electronic structure caused by the partial substitution of Cr^{3+} with Al^{3+} is suggested by the apparent absence of the second threshold and the decrease in the bandgap energy **[78]**. This substitution causes a redistribution of electronic states inside the band gap and a disruption of the electronic interactions between Cr–O–Cr.

The optical bandgap increases when aluminum concentration increases (Eg: 2.4→ 2.70eV). (Eg: 2.4→2.70 eV) can be explained by the insertion of new localized states and lattice distortion, which promote optical transitions at lower energies. This pattern is consistent with a red shift of the absorption edge, which is characteristic of doped systems with higher levels of cationic disorder.

Additionally, a homogeneity of the major electronic transitions is suggested by the simplicity of the optical spectrum at x = 0.2 (a single seeming gap), which is probably caused by the decreased contribution of localized transitions of Cr^{3+}. Therefore, the bandgap width and the kind of optical transitions in the material are both impacted by substitution with Al^{3+}.

The comparative analysis concludes that the addition of aluminum to the $Mg_{0,5}Sr_{0,5}Cr_2O_4$ spinel structure results in a reduction in the optical bandgap and a modification of the absorption mechanisms, indicating a substantial alteration in the electronic structure of the material **[79]**.

There are several interconnected factors that may account for this significant decline. According to the structural analysis, Al substitution increases the average grain size, thereby reducing the grain-boundary density. The resulting decrease in grain-boundary scattering may facilitate charge-carrier transport and electronic transitions, contributing to the reduction in the optical band gap. Furthermore, the increase in grain size weakens quantum confinement effects, which can also contribute to bandgap narrowing. XRD analysis indicates that Al^{3+} substitution modifies the lattice parameters through the difference in ionic radii between Al^{3+} and Fe^{3+}, leading to changes in the local structural environment and metal–oxygen bond lengths. These structural modifications can alter the electronic structure and orbital overlap, thereby reducing the energy required for electronic transitions from the valence band to the conduction band **[80]**.

Additionally, intermediate sub-band states may be introduced via the sp–d exchange interaction between the delocalized conduction band electrons and the localized d-electrons of Cr^{3+}. By merging with the conduction band, these sub-bands can reduce the material's total band gap **[81]**. As a result, adding Al to $Mg_{0.5}Sr_{0.5}Cr_2O_4$ significantly lowers the band gap energy and enhances the material's optical and electrical characteristics. The potential of $Mg_{0.5}Sr_{0.5}Cr_{1.8}Al_{0.2}O_4$ as an efficient photocatalytic material is confirmed by the observed Eg value, which is notably considerably over the minimal threshold (1.23 eV) necessary for solar water splitting **[35]**.

The type of optical transition is indicated by the value of the exponent n: direct optical transitions for n = 1/2 and indirect optical transitions for n = 2. Consequently, the optical transition in the samples is verified using the following equation:

$$ln[F(R).h\upsilon] = ln(A) + n.ln(h\upsilon - E_{gd}) \quad \textbf{(21)}$$

The exponent n was retrieved from the slope of the $ln[F(R).h\upsilon]$ against $ln(h\upsilon - E_{gd})$ plots to clearly identify the optical transition mode for both samples (x = 0 and x = 0.2) displayed in **Figure. 9**. The linear fit in the fundamental absorption area for the pristine sample x = 0 produces n = 0.46. Similarly, the linear fitting for x = 0.2 yields n =0.44. It is confirmed that both materials

experience a direct permitted electronic transition because both exponent values fit very well with the theoretical value of n = 0.5 (or 1/2). Additionally, the result shows that the substitution (x = 0.2) maintains the material's basic band gap structure without causing a transition mechanism crossover. In the absence of intermediary energy states, this direct optical transition indicates a direct band gap that permits electrons to pass from the valence band to the conduction band. These samples' exceptional light-absorbing and light-emitting qualities make them ideal for use in solar cells, lasers, and optoelectronic devices.

The obtained bandgap energy (Eg) was compared to that of other spinel-type chromite, as indicated in **Table. III**. Interestingly, compared to ordinary semiconductors and several other spinel-type chromite, the Eg value of $Mg_{0.5}Sr_{0.5}Cr_{2-x}Al_xO_4$ (x= 0; 0.2) is lower, which improves their capacity to absorb visible light. They are therefore advantageous options for photocatalytic applications powered by visible light **[35].** Additionally, increasing the size of the grain can lessen the effects of quantum confinement, which helps lower the band gap energy overall. The band gap energies (E_g) of the as-prepared samples, presented in **Table. III**, were compared with those reported for several semiconductors **[82-83]** and other spinel chromite **[84-86]**. As shown in **Table. III**, the (Eg) values reported for various semiconductors **[88-91]** indicate that materials with relatively high band gap energies generally exhibit absorption predominantly in the ultraviolet (UV) region. As visible light constitutes the major fraction of solar radiation and is readily available from artificial light sources, the development of materials with efficient visible-light responsiveness has attracted increasing research interest. The predicted Eg values for the as-synthesized x=0 and x=0.2 samples are notably lower than those reported for other spinel chromite and several semiconductors **[87-92]** Our samples are possible candidates for visible light absorption because a reduced band gap energy permits better absorption of visible light in photocatalytic activities. Furthermore, our research showed that the bandgap energy values of the synthesized samples were lower than those reported for $MgCr_2O_4$ chromite, which are commonly used as photocatalysts when exposed to UV light. This implies that the substitution of Ni and Cu offers a chance to increase the range of sunlight absorption of $MgCr_2O_4$ spinel chromite.

3.4.3. Penetration depth and extinction coefficient

According to the formula $\delta = 1/\alpha$ and δ=1/α, the optical penetration depth δ, **[93]** which describes the average distance over which electromagnetic light propagates in a material before significant attenuation occurs, is inversely related to the absorption coefficient α. Since direct access to α is restricted in the case of scattering materials, like polycrystalline spinel oxides, the Kubelka–Munk function F(R), which is calculated from diffuse reflectance data, is frequently employed as an alternative **[94]**. In fact, in the Kubelka–Munk model, $F(R) = K/S$, where S is the scattering coefficient and K is the absorption coefficient. Assuming a weak variation of S with photon energy, F(R) becomes proportional to α. As a result, the penetration depth can be written as inversely proportional to the function F(R), that is, $\delta \propto 1/F(R)$. According to this equation, a drop in δ, which indicates less light penetration into the material, results from an increase in F(R), which reflects more severe absorption. This method is commonly used for optical study of highly scattering materials, especially when estimating optical transitions and electronic characteristics from diffuse reflectance spectra **[95]**.

$$\delta = \frac{1}{\alpha(\lambda)} \quad \textbf{(22)}$$

$$\delta = \frac{1}{F(R)} \quad \textbf{(23)}$$

The change in the penetration depth δ (λ) as a function of wavelength for compositions of $Mg_{0.5}Sr_{0.5}Cr_{2-x}Al_xO_4$ (x= 0; 0.2) is depicted in **Figure. 8(a and b)**. According to the relation δ=1/α, the overall spectrum behavior of δ reflects the material's optical absorption mechanisms **[96]**.

The low values of δ in area I (UV-visible, λ < 800 nm) suggest high optical absorption, which is mostly due to intra-ionic d-d transitions of Cr^{3+} ions and interbond electronic transitions **[97-98]**. The doped sample (x = 0.2) shows somewhat lower penetration depth values, indicating an increase in the absorption coefficient because of the altered electronic structure brought about by the substitution of Al^{3+}.

Both samples show a notable rise in δ in area II (800-1600 nm), which suggests deeper light penetration and less absorption. This area is associated

with a transition regime in which absorption mechanisms lose their dominance. The doped sample's comparatively lower δ values indicate the existence of localized states or structural flaws brought about by the insertion of aluminum **[99]**.

The penetration depth improves once more in area III (near-infrared, $\lambda >$ 1600 nm), especially for the undoped material (x = 0), showing weak absorption in this spectral range. Lattice vibrations (phonon interactions) and scattering effects could be the cause of the observed oscillations. The doped sample continues to exhibit lower δ values, indicating that the substitution of Al^{3+} improves the overall absorption performance.

Overall, under the assumption of constant scattering, the increase in the Kubelka–Munk function F(R), which is proportional to the absorption coefficient, is compatible with the decrease in penetration depth with aluminum doping **[100-104]**. This trend demonstrates how cation substitution significantly affects the optical and electrical characteristics of the spinel system under investigation.

A material's capacity to both absorb and scatter incident light is characterized by its extinction coefficient k, which is described as follows **[105]**:

$$k = \frac{\alpha\lambda}{4\pi} \quad \textbf{(24)}$$

The extinction coefficient k was estimated from diffuse reflectance data using the Kubelka–Munk function. Assuming F(R)≈α, the extinction coefficient was calculated using the relation.

$$k = \frac{F(R)\lambda}{4\pi} \quad \textbf{(25)}$$

The coefficient of extinction k of $Mg_{0.5}Sr_{0.5}Cr_{2-x}Al_xO_4$ (x= 0; 0.2) samples were calculated from diffuse reflectance spectra using the Kubelka-Munk function **[106]**. As shown in **Figure.9**, the sample x = 0 has multiple absorption pics: a peak around 1 eV that corresponds to intra-d transitions of Cr^{3+} in octahedrons and additional pics in the range of 2-4 eV attributed to charge transfer $O^{2-} \rightarrow Cr^{3+}$ **[107]**. The sample x = 0.2 shows a significant decrease in the coefficient of extinction in the visible spectrum and a considerable attainment of

low-energy d–d transitions, indicating a lower density of Cr^{3+} ions because of the substitution of Al^{3+} in the octahedrons **[108]**. Additionally, the absorption boundary gradually shifts towards higher photonic energies for x = 0.2, which corresponds to an increase in the inter-site optical band (Eg) caused by the introduction of non-magnetic Al^{3+} ions. These tendencies are consistent with the findings on spinel chromite doped with Al, where cationic substitution decreases intra-d absorption and arguably Eg. The structure at larger multiples of k reflects the complicated electronic structure of spinel, including both intra-d and charge-transfer transitions. Overall, doping to Al results in a decrease in absorption in the visible spectrum and an increase in the absorption boundary towards the ultraviolet spectrum, which may have an impact on the potential optoelectronic uses of these materials **[109]**.

3.5.4. Urbach energy

The Urbach energy E_U was determined from diffuse reflectance data using the Kubelka–Munk function F(R), which accounts for the exponential broadening of the absorption edge associated with structural disorder and defects **[110]**. Under the assumption of a constant scattering coefficient, F(R) is proportional to the absorption coefficient α allowing direct use of the optical spectra. In the low photon energy region near the absorption edge, the absorption coefficient follows Urbach's empirical rule, where α (hv) exhibits an exponential dependence on the photon energy. Consequently, plotting ln[F(R)] as a function of hv yields a linear region known as the Urbach tail. The Urbach energy E_U is then extracted from the inverse of the slope of this linear portion **[111]**.

$$F(R) = F_0 \exp\left(\frac{h\nu}{E_u}\right) \quad \textbf{(26)}$$

$$lnF(R) = lnF_0 + \frac{h\nu}{E_u} \quad \textbf{(27)}$$

The Kubelka–Munk method was used to derive the Urbach energies E_U of $Mg_{0.5}Sr_{0.5}Cr_2O_4$ and $Mg_{0.5}Sr_{0.5}Cr_{1.8}Al_{0.2}O_4$ from the linear region of the ln[F(R)] versus photon energy (hv) plots, producing approximately 0.23 eV and 0.28 eV, respectively **Figure. 10**. These E_U values are higher than those usually found in traditional semiconductors like GaAs or ZnO, indicating a significant occurrence

of localized states linked to defect-related band tailing and disorder that are intrinsic to spinel chromite. The magnitudes are nevertheless comparable to those of Urbach energies recently reported for related spinel systems, where optical absorption tailing has been attributed to lattice distortions and cation substitution, which modify the distribution of localized states within the band gap **[111]**.

The replacement of Cr^{3+} by Al^{3+} within the octahedral B sites, which lessens local structural distortions and thus lowers the density of defect-induced localized states, is responsible for the decrease in Urbach energy with Al substitution. Potential fluctuations and lattice flaws that contribute to the exponential absorption tail are suppressed by this substitution, which creates a more symmetrical octahedral environment. Similar patterns have been observed in ferrites and spinel chromite, where dopant-induced ordering results in lower Urbach energies that are associated with improved crystalline quality and decreased structural disorder **[112]**.

Additionally, the Al-doped sample's lower E_U value suggests a weaker electron–phonon interaction and a sharper absorption edge, both of which are signs of better structural ordering. The undoped chromite, on the other hand, has a wider Urbach tail, which is consistent with a higher density of localized states caused by defects such as lattice strain and cation disorder. Recent optical studies of spinel oxides, which highlight the strong link between the Urbach tail breadth and structural disorder resulting from compositional and microstructural variation, are consistent with this hypothesis **[113]**.

Taking everything into account, the relatively low Urbach energies observed in this study suggest a well-ordered crystalline network with a low density of trap states, which is beneficial for optoelectronic performance. These values are consistent with recent publications on doped spinel systems where tailing effects are decreased and optical edge sharpness is improved through controlled replacement.

The steepness parameter S(T) and the Urbach energy E_U are related by the following **Equation 28**.

$$E_u = \frac{K_B T}{S(T)} \quad \textbf{(28)}$$

where T is the absolute temperature (assumed to be 300 K) and k_B is the Boltzmann constant. Ref. 42 states that interactions between electrons and phonons or excitons and phonons cause the broadening of the absorption edge, which is defined by the steepness parameter S(T). This measure shows how quickly the absorption coefficient varies in relation to photon energy close to the band edge.

The optical absorption edge's steepness is described by the slope parameter S(T); a greater value of S(T) denotes a steeper absorption edge and less structural disorder. The parameter S(T) was determined to be 0.112 for x=0 and 0.092 for x=0.2 in our investigation. When compared to x=0, the lower value for x=0.2 shows a more noticeable broadening of the absorption edge, which is indicative of a higher density of localized states in the band gap (higher Urbach energy E_U). **Equation. 29** states that the electron-phonon interaction intensity ($E_{e\text{-}ph}$) changes inversely with the slope parameter; therefore, a more intense electron-phonon coupling within x=0.2 is reflected in the decrease in S(T).

$$E_{e-ph} = \frac{2}{3S} \quad \textbf{(29)}$$

An important measure of a material's electrical and thermal characteristics is the parameter $E_{e–ph}$, which quantifies the energy related to electron–phonon interactions. Stronger coupling is indicated by higher $E_{e–ph}$ values, which may indicate a higher tendency for energy dissipation through lattice vibrations. We computed $E_{e–ph}$ values of 5.95 eV for x = 0 and 7.24 eV for x = 0.2 using Equation 43 (**Table. IV**). The higher $E_{e–ph}$ value of the x=0.2 sample relative to the x=0 sample suggests a stronger electron phonon interaction and a higher tendency for energy dissipation through lattice vibrations. However, in optoelectronic devices, a compound's viability for such applications is largely determined by the maximum wavelength of incident radiation, represented by λ_T, which is often referred to as the threshold wavelength or critical wavelength. The minimum wavelength of light needed to start certain optoelectronic processes, such absorption or emission, in a material is represented by the λ_T value. We have utilized the following equation to determine the λ_T values:

$$\left(\frac{F(R)}{\lambda}\right)^2 = c\left(\frac{1}{\lambda}\right) - \left(\frac{1}{\lambda_T}\right) \quad \textbf{(30)}$$

where c is a constant, λ is the incident radiation's wavelength, and F(R) is the factor of reflectance. The fitting curves produce values of λ_T that drop from 526 nm for x=0 to 470 nm for x=0.2, as indicated in the insets of **Figure.11** and **Table. IV**. Consistent with earlier findings, the observed decrease in λ_T suggests that the x=0.2 material's bandgap energy is smaller than that of the x=0 sample. A lower threshold wavelength is typically associated with a lower bandgap energy. This suggests that the material requires higher-energy photons, corresponding to shorter wavelengths, to initiate optoelectronic transitions.

3.4.4. Refractive index

In the field of spectral dispersion applications, the refractive index (n) is a crucial parameter. It describes how light moves through a material and is affected by things like the density, composition, and optical characteristics of the material. The R(λ) and k(λ) data can be used to estimate the refractive index (n) as follows:

$$n(\lambda) = \frac{1+R}{1-R} - \sqrt{\frac{4R}{(1-R)^2} - (k(\lambda))^2} \quad \textbf{(31)}$$

The n(λ) curves for the $Mg_{0.5}Sr_{0.5}Cr_{2x}Al_xO_4$ (x= 0; 0.2) spinel chromite are shown in **Fig. 12**. The samples' high quality and compactness are shown by the existence of significant absorption bands in the UV-VIS-NIR zones. The following Cauchy relation is used to simulate how the refractive index (n) varies with wavelength:

$$n(\lambda) = n_0 + \frac{n_1}{\lambda^2} + \frac{n_2}{\lambda^4} \quad \textbf{(32)}$$

The wavelength dependency of the refractive index is described by the Cauchy parameters, denoted by n_0, n_1, and n_2 in this equation. The $1/\lambda^2$, as described by equation (46), is shown in the insets of **Figure. 12. Table. IV** shows the calculated Cauchy parameters for the x=0 and x=0.2 samples. The way the refractive index (n) changes with wavelength for our samples is represented mathematically by these Cauchy parameters. For applications requiring spectrum dispersion and light propagation in materials, they offer useful information.

When choosing materials for possible uses and designing optoelectronic devices with spectral dispersion, dispersion is an important consideration **[114]**. Therefore, a detailed explanation of this subject is necessary to understand the dispersion parameters of the refractive index and dispersion energies of $Mg_{0.5}Sr_{0.5}Cr_{2-x}Al_xO_4$ (x= 0; 0.2) spinel chromite. The ideal model for examining these parameters is Wemple-Di-Domenico's Single Effective Oscillator Model **[115]**. This model has effectively explored dispersion or strength energies (E_d) and effective single oscillator energies (E_0). According to the Wemple and Di-Domenico dispersion theory, the refractive index (n) and the energies (E_0 and E_d) are related by the following expression:

$$n^2 - 1 = \frac{E_o E_d}{E_o^2 - (h\nu)^2} \quad \textbf{(33)}$$

Plotting the refractive index factor [1/(n2 −1)] versus the square of photon energy [(hν)2] yields a graphic representation of this equation. This graphical representation is shown in **Figure. 13**. The slope [1/(E_0E_d)] and the y-axis intercept (E_0/E_d) can be found by examining the resulting straight line. As a result, it is simple to determine the energy values of E_0 and E_d for x=0 and x=0.2 from **Figure. 13** which are then displayed in **Table. IV**. Tanaka et al **[108]** states that E_0 is roughly twice the bandgap energy (Eg).With the estimated values of E_0 and E_d, we can calculate the zero-frequency dielectric constant ($\varepsilon_{op} = 1 + \frac{E_d}{E_o}$) and the static refractive index ($n_0' = \sqrt{1 + \frac{E_d}{E_0}}$). As presented in **Table. IV**, the calculated values E_0 were calculated as ε_{op} = 3 and n_0' = 1.73 for x=0 and as ε_{op} = 3.46 and n_0' = 1.86 for x=0.2. It is noteworthy that the calculated values of the static refractive index n_0' agree well using the Cauchy t-estimated n_0 values. This agreement shows the dependability and consistency of the outcomes acquired using various techniques. Equation (48) was used to calculate the average oscillator strength (S_0) and oscillator wavelength (λ_0) for the x=0 and x=0.2 samples **[116]**. The refractive index (n), average oscillator strength (S_0), oscillator wavelength (λ_0), and light wavelength (λ) are all related by this equation:

$$\frac{1}{n^2-1} = \frac{1}{S_0\lambda_0^2} - \frac{1}{S_0\lambda^2} \quad \textbf{(34)}$$

As shown in the insets of **Figure. 13**, the curves of [$\frac{1}{n^2-1}$ VS. $\frac{1}{\lambda^2}$] were plotted. The values of λ_0 were found to be 197 nm for x=0 and 270 nm for x=0.2 based on these figures (see Table 4). For x=0 and x=0.2, the S_0 values were determined to be 45.8 μm^{-2} and 34.6 μm^{-2}, respectively. The average oscillator strength and the typical wavelength of the optical transitions in the investigated spinel chromite are revealed by these numbers. These are crucial factors for comprehending the electrical structure and optical behavior of materials. When we compare the S_0 and λ_0 values for the x=0 and x=0.2 samples, we find that both parameters are lower for x=0. These differences indicate variations in the optical properties and behavior of the spinel chromite, potentially due to changes in their electronic structure or composition. On the other hand, the static refractive index (n_0'') can be calculated as follows:

$$n_0''^2 - 1 = \lambda_0^2 S_0 \quad \textbf{(35)}$$

The x=0 and x=0.2 values for $n_0''^2$ were estimated to be 1.66 and 1.87, respectively. Specifically, the estimated values of $n_0''^2$ are in good agreement with the results of the Cauchy correction and the computation from E_0 and E_d.

Conclusion:

In conclusion, $Mg_{0.5}Sr_{0.5}Cr_{2-x}Al_xO_4$ (x = 0 and 0.2) chromite were successfully synthesized by the sol–gel method. X-ray diffraction analysis confirmed the formation of single-phase materials crystallizing in the cubic spinel structure, while the structural parameters, including the lattice parameter and crystallite size, were determined from the XRD data. FTIR analysis provided valuable information on the metal–oxygen vibrations and enabled the assessment of the elastic parameters. Furthermore, comparison between the experimental and theoretical results, together with XPS analysis, allowed the cation distribution involving Mg^{2+}, Sr^{2+}, Cr^{3+} and Al^{3+} ions to be quantitatively evaluated. The optical investigation revealed that Al^{3+} substitution significantly influences the optical response of the chromite, including the refractive index, penetration depth and extinction coefficient. The obtained band-gap energies indicate that the studied materials exhibit significant visible-light absorption, highlighting their potential for optoelectronic applications. Overall, the results demonstrate that partial

substitution of Cr^{3+} by Al^{3+} provides an effective route for tailoring the structural, elastic and optical properties of $Mg_{0.5}Sr_{0.5}Cr_{2-x}Al_xO_4$ chromite. Further investigations, particularly concerning their functional performance and application in optoelectronic devices, would be valuable for assessing their practical potential.

Data availability

Upon a reasonable request, the data that support this study's findings are available from the corresponding author.

Conflict of interest

The authors have no competing interests that are relevant to the content of this article to declare.

Authors contributions

All authors certify that they have participated sufficiently in the work to take public responsibility for the content, including participation in the concept, analysis, design, and writing. The final manuscript was read and approved by all authors.

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