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RESEARCH ARTICLE

Investigating the Optical, Magnetic, and Mechanical Properties of La_2NiMnO_6 via Sr-Eu Co-Doping

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ABSTRACT: The study investigates the effect on properties of La_2NiMn0_6 (LNMO) by doping with Co-dopants, Sr-Eu at A-site respectively. The exploration is done by using Density Functional Theory (DFT) in combination with LDA (Local Density Approximation) and Hubbard's Correction (LDA+U). On comprehensive analysis we show how these dopants influence the properties like optical, magnetic, mechanical, electrical and spintronic characteristics of LNMO. The research reveals the use of dopants modifies the electronic structure of LNMO and the alterations improved the materials dielectric properties which are important for the applications requiring high dielectric constant. Additionally, the doping resulted an improvement in the optical conductivity, improving the features of light absorption and photoconductivity efficiently highly suitable for optoelectronics devices, where light management is essentially in operational process. With related to magnetic properties the doping by Sr-Eu showed an enhancement in properties regarding to spintronics where control of spin is mandatory. The improvement in both the properties (electrical & magnetic) are considerable parameters in energy storage devices in determining its efficiency and effectivity. In addition to it the mechanical properties show resilience and stability while doping by Sr-Eu notable in determining the longevity and durability of devices respectively. On estimation this paper focus on potentiality in technology with wider applications in spintronics, optoelectronics and energy storage devices respectively. The current study and findings provide new ways of synthesizing the materials, providing new alternative paths for the development of exotic materials of tailored functionalities with future prospects in consideration

Keywords: Perovskites, Double perovskites, LNMO, Co-Doping.

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1. INTRODUCTION

During the inception of research studies in material science [1]. The oxides have gained familiarity in minds of researchers due to its vast and varied potentiality in the device making process [2]. Oxides being Acidic, Basic, Amphoteric etc. in nature reflects the broader categories of the substance [3]. Thus, a sample for wider applications and technologies as reported earlier by different researchers [4]. While analyzing, the oxides have resorted to outstanding phenomena which include magnetism, superconductivity with key openings for new avenues in the field of exploration and innovation, respectively [5, 6]. These materials have been proved efficient in terms of cost effectiveness, low in power consumption and also resorted to flaws [7, 8]. The synthesis is achievable by incorporating appropriate dopants, resulting in remarkable outcomes. This efficiency makes it highly suitable for future technological applications [9]. With broader range of availability of oxides like thin film, bulk crystalline or polycrystalline powders, these are used in the synthesis or development of sensors, electro-optic devices, actuators, memory devices, and so on [10-12].

Among different types of oxides, one respectable category of oxides are perovskites with general formula

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$AB0_3$ where A & B are cations in origin and O represents the oxygen [11-13]. The flexibility at A and B site in perovskites has resorted to wider chemical compositions considerably achieving varied physical and tailored functionality in devices [14]. The perovskites are rich in properties, as such one of notable property is of colossal magneto-resistance (adjacent change in electrical resistance with altering change in magnetic field), the potential property of considering the needs of modern society in terms of power Consumption and electronic appliances [15]. The double perovskites were synthesized with a hope of catering the needs of modern-day population [16]. The general formula of double perovskites is $A_2BB'0_6$, where A is divalent cation in origin specifically from group II of periodic-table (Alkaline Earth Metals) or f - block elements (Rare-earth metals). B & B' can be a metal from group I (Alkali Metals), group II (Alkaline Earth Metals) or Transition / d block elements, respectively [17, 18]. Due to continuous repetition of perovskite cells enormous properties ranging from half-metallicity, magneto-capacitance, ferromagnetism is obtained [5, 6]. Multiple approaches can be used to tune up the properties to tailored functionalities, among them one of the most cost-effective and reportable method is of doping [13]. For example, the doping can modify the electronic and magnetic properties to a newer state and thus the interactions can be utilized in betterment of specific applications [14]. In addition to it, the wider diffusion lengths along with high light absorption and lower temperature processing capacities gives them the dominance than conventional solar cells notable silicon based [13, 14]. With related to efficiency and toxicity the perovskites show leverage against the conventional based solar-cells, as per reports the efficiency of around 22.7% is generated against the 3.8% in conventional based solar cells [15, 16]. Hence fueled research further paved the way to double perovskites. One of most cited and extensively studied compound of double perovskites is La_2NiMn0_6 (LNMO). Due to its uniqueness in transition state around room temperature and magneto-dielectric behavior [17]. It has generated huge interest in the field of applications and technology in the minds of researchers with consideration of physical properties. The LNMO exists in two solid-phases monoclinic and rhombohedral. One phase is observed around room temperature and is most studied one. The other phase i.e. rhombohedral structure, the phase is observed when temperature is kept high [12].

The alteration in the physical properties through substitutional doping is a subject of study. Basically, the substitution at A- site is eventually studied maximum times [18]. The doping has affected the physical properties generally, this is due to the availability of enormous number of cations or dopants which differ in cationic state or oxidation, ionic radii and the valencies [18]. Due to these substitutions the angle of B-O-B has changed which leads to enhancing changes in the electronic, magnetic and structural properties of the materials respectively [19]. Research conducted by Guo et al. significantly reported the increase in exchange bias effect, when doped with varying concentration of Sr, along with increase in antisite disorder [19]. Zhou et al. reported the doping done by Sr induced ferromagnetic ordering with antisite defects [20]. Similarly, Ting et al. reported that doping with Ca resulted in antiphase defects, leading to a rapid increase in antiferromagnetic antiphase boundaries, along with weak ferromagnetic transition phases and long-range ferromagnetic ordering near the transition temperature [21]. For light-harvesting materials, cost-effectiveness and toxicity are primary concerns. To address these issues, researchers have developed sufficient methods. For instance, Kumar et al. achieved a power conversion efficiency of 15.42% with a bandgap variation of 1.08 to 1.19 eV in inorganic lead-free perovskite oxides by simulating the heterostructure of LNMO and TiO_2 [22].

The research work carried out will provide more insights on the monoclinic phase and its usage in solar cell. By performing substitutional doping more enhancement with respect to responses of light are observed. Our results will show the significant improvements in light absorptivity and conductivity, suggesting high viability in the devices whether it is solar or energy storage. While using Density Functional Theory (DFT), advance potential in the field of electronic industry particularly in energy storage devices, spintronics as well as photo-tonics is observed. The current research will explore the effects of Sr-Eu doping at A- site in LNMO to enlighten the advancements achieved in the optical, spintronic, electrical, mechanical and magnetic properties by using DFT in combination with (local Density Approximation) LDA + U corrections respectively. Our results will show the optical delineation by Co-doped Sr-Eu to a positive change in light absorption and conduction which are crucial parameters for the development of photovoltaic and optoelectronic devices respectively. By utilization of Co-doping by Sr-Eu, it is likely to induce the expansions with respect to lattice and modifications in the respective bond angles of B-0-B, thereby causing magnetic and electronic band interactions to a positive change with enhancement in the ferromagnetism and semiconducting behaviour of the double perovskites respectively. These are crucial parameters in spintronics. With relative to mechanical properties of doped LNMO, the mechanical stability is important in the synthesis of device-making. With the incorporation of dopants, the hardness of the material elasticity and fracture toughness are kept in mind which are key assets for device fabrication and longevity.

2. COMPUTATIONAL METHODOLOGY

2.1. Computational Details

The computations are done by using Vienna Ab Initio Simulation package (VASP), with respect to calculations pertaining to Density Function Theory. In the subject related to material science such as Solid-state Chemistry or Physics

the important assembly of density of states is crucial. The Density function theory is a strong weapon in exploring of various properties related to matter and thus can called as theoretical microscope with approach in experimental limits and abilities [23]. As such it defines the states in terms of number occupied by a statement at different levels of energy relatively. The theory describes the matter by using basic equations theoretically. The package is used to calculate the properties on Co-doping which include structural, magnetic, optical, spintronics, etc. the whole concept is based on the analogy of wave function to electron density. The following equation is utilized

$$n(r) \sim \sum_{i} \psi i * (r) \psi i (r)$$

The Density Functional Theory utilizes the exchange correlation potential to effects of Pauli principle and the potential which is coulombic beyond pure interaction. The projector- augmented wave (PAW) is utilized to describe the electron Ion interactions, as it provides utilization for using linear- Augmented plane wave method and pseudo- potential which enhances the efficiency in calculations related to DFT and the exchange co-relation potential is also adjourned to LDA + U framework to point out the strong on-site Coulombic interactions in the d-orbitals of d-block elements. It is the most commonly used Exchange Correlation approximation for computations in the Density functional theory approach. In LDA, value of exchange and correlation at any point is only dependent upon the local density [24], [25].

2.2. Structural Optimization

The initial structure of LNMO (La_2NiMn0_6) and co-doped structure ($La_{2-x}Sr_xEu_xNiMn0_6$) were analyzed and optimized till the forces on every atom were reported to 0.01 eV/Å. The process of Structural optimization (relaxation) was carried out for both (lattice constants with respect to atomic positions & fixed structure). The projector augmented wave was utilized by VASP code. The Monkhorst-pack k-point mesh of 6x6x6 and a plane-wave cutoff energy of 500ev were set in Brillouin zone integration [26].

2.3. Electronic and Optical Properties

The electronic properties were investigated by calculating the density of states (DOS) and band structures, which help in understanding the impact of Sr-Eu co-doping on LNMO. The DOS analysis provides insight into the distribution of electron states at different energy levels, while the band structure calculations reveal the changes in the energy bands, including any shifts in the conduction and valence bands. These calculations are crucial for identifying the potential of co-doped LNMO in electronic applications.

Additionally, the optical properties were studied by deriving the dielectric function from the frequency-dependent complex dielectric function. This function comprises both real and imaginary parts, which are essential for understanding the material's response to electromagnetic waves. By analyzing these properties, we can determine crucial parameters such as refractive index, absorption coefficient, and reflectivity, which are pivotal for evaluating the suitability of co-doped LNMO in optoelectronic devices.

2.4. Magnetic Properties

The magnetic properties were assessed by calculating both total and partial magnetic moments. These calculations help in understanding the magnetic behavior of the co-doped LNMO at the atomic level. The total magnetic moment provides an overall measure of the magnetic strength, while the partial magnetic moments offer detailed insights into the contributions from individual atoms or ions.

Furthermore, spin polarization calculations were conducted to evaluate the potential of Sr-Eu co-doped LNMO for spintronic applications. Spin polarization measures the degree of alignment of electron spins in the material, which is a critical factor for developing spintronic devices that rely on the manipulation of spin rather than charge.

2.4. Mechanical Properties

The mechanical properties were analyzed by computing the elastic constants of the co-doped LNMO structures. These constants, which include parameters such as C_{11}, C_{12}, and C_{44}, provide information about the material's response to applied stresses and its overall rigidity and mechanical strength.

From these elastic constants, further mechanical parameters were derived, including the shear modulus, bulk modulus, and Young's modulus. The shear modulus indicates the material's ability to resist shear deformation, the bulk modulus measures resistance to uniform compression, and Young's modulus quantifies the stiffness of the material. These parameters are essential for evaluating the mechanical stability and suitability of co-doped LNMO in practical applications, particularly in the fabrication and longevity of devices.

3. RESULT AND DISCUSSION

3.1. Structural Properties

The structural properties of LNMO and its co-doped compound $La_{1.9}Sr_{0.1}Eu_{0.1}NiMnO_6$ were evaluated based on lattice constants. The substitutional doping of La with Sr-Eu dopants was found to effectively alter the lattice constants, indicating successful incorporation into the LNMO structure. The results are presented in Table 1, which provides a clear comparison of the lattice constants for both the undoped and co-doped compounds. This tabular representation aids in

better understanding the structural optimization resulting from the doping process.

As shown in Table 1 and Figure 1, the lattice constants for the co-doped compound $La_{1.9}Sr_{0.1}Eu_{0.1}NiMnO_6$ are slightly larger than those of the undoped La_2NiMnO_6. Specifically, the lattice constant 'a' increased from 5.54 Å to 5.57 Å, and the lattice constant 'c' increased from 7.81 Å to 7.84 Å. This expansion in the lattice constants is indicative of the successful incorporation of Sr and Eu into the LNMO structure, resulting in lattice strain and adjustments to accommodate the dopants.

3.2. Electronic Properties and Density of States

To understand the nature of the band gap and identify the contributing factors from electrons, orbitals, and atoms, we considered the maxima and minima of the valence and conduction bands. Both the density of states (DOS) and band structure are crucial for this analysis. The band structures indicate the allowed energy states and determine the electrical and electronic properties of the material. The calculated band gaps for both the doped and undoped structures are shown in Table 2.

As presented in Table 2 and figure 2, the undoped La_2NiMnO_6 has a bandgap of 1.2 eV, while the co-doped $La_{1.9}Sr_{0.1}Eu_{0.1}NiMnO_6$ shows a reduced bandgap of 0.9 eV. This slight narrowing of the bandgap in the co-doped LNMO indicates enhanced electrical conductivity, as a smaller bandgap facilitates easier movement of electrons from the valence band to the conduction band.

The density of states (DOS) is a major consideration in solid-state or condensed matter physics as it determines the number of states a system can occupy at different energy levels. The DOS analysis for both undoped and co-doped LNMO reveals critical insights into the material's electronic structure.

Upon observation, it is noted that the co-doping introduces additional states near the Fermi level, leading to an increase in carrier density. This increase in carrier density is crucial for enhancing the material's electrical conductivity and overall performance in electronic applications. The co-doping of Sr and Eu into LNMO has a significant impact on its electronic properties, making it a more efficient material for applications that require enhanced electrical conductivity and tailored electronic characteristics.

Table 1. Lattice Constants of Undoped and Co-doped LNMO.

Compound	Lattice Constant a (Å)	Lattice Constant b (Å)	Lattice Constant c (Å)
La_2NiMnO_6	5.54	5.54	7.81
$La_{1.9}Sr_{0.1}Eu_{0.1}NiMnO_6$	5.57	5.57	7.84

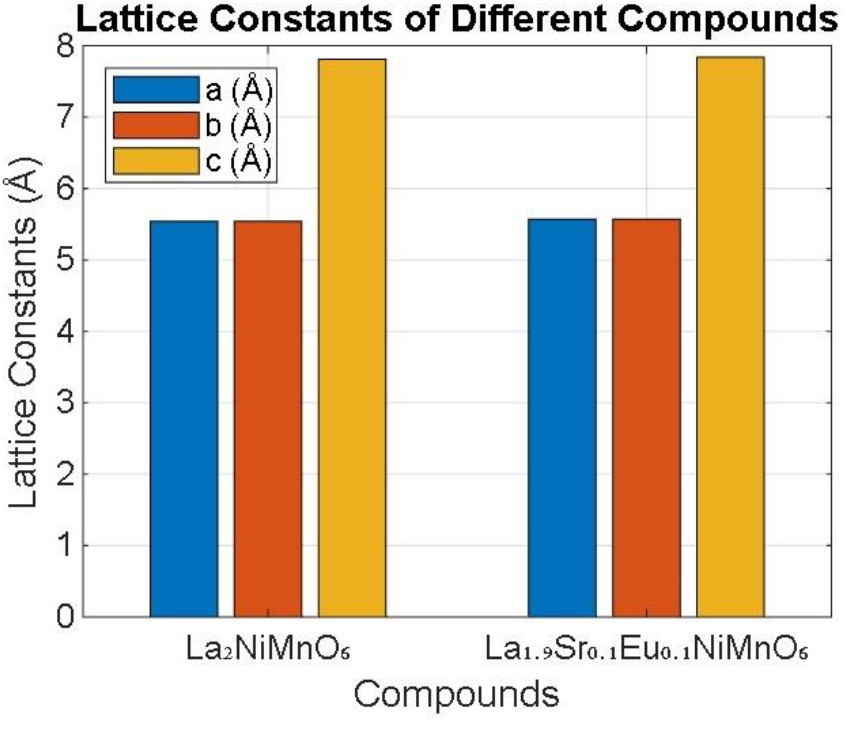

Fig. 1. Lattice constants of the undoped and co-doped LMNO.

Table 2. Bandgap of Undoped and Co-doped LNMO.

Compound	Bandgap (eV)
La_2NiMnO_6	1.2
$La_{1.9}Sr_{0.1}Eu_{0.1}NiMnO_6$	0.9

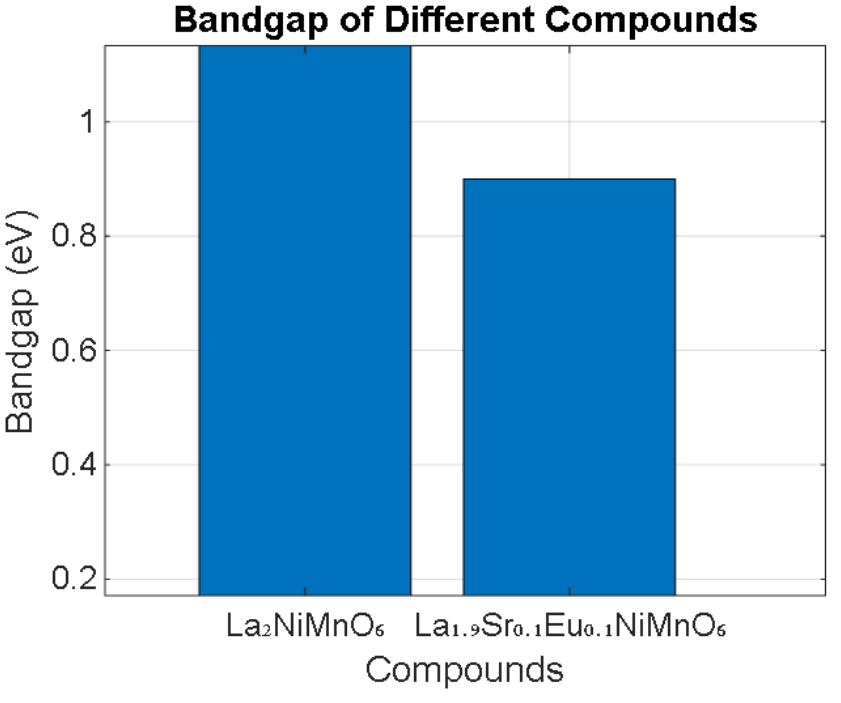

Fig. 2. Bandgap of the undoped and co-doped LMNO.

3.3. Optical Properties

Considering the needs of energy is a matter globally revolving. Hence some techniques are needed to propagate out. The most suitable and alternative choice is solar energy, since in nature it is present abundantly without the fear of loss, hence it has tremendously increased the attention of industries and researchers. Upon observation of electronic band structure, we have calculated the dielectric function by using the following equation:

$$\varepsilon(\omega) = \varepsilon_1(\omega) + i\varepsilon_2(\omega)$$

Where $\varepsilon_1(\omega)$ represents real part whereas $i\varepsilon_1(\omega)$ represents the imaginary part.
The real part of dielectric equation is given by Krammer Kronig equation [27]:

$$\varepsilon_1(\omega) = 1 + \frac{2}{\pi}\int \frac{\varepsilon_2(\omega')\omega'}{\omega'^2 - \omega^2} d\omega'$$

And imaginary part is given by

$$\varepsilon_2(\omega) = \frac{Ve^2}{2\pi\hbar m^2\omega^2}\int d^3k \sum |kn|p|kn'|^2 f(kn)[1 - f(kn')]\delta(E_{kn} - E_{kn'} - \hbar\omega)$$

E_{kn} = Eigen function, E_{kn} $f(kn)$ = Fermi distribution function, p = momentum operator

The real part determines the polarizability whereas, the absorption of the material is provided by imaginary part respectively. The following Table 3 represents the dielectric function of undoped and Table 4 represents the dielectric function of co-doped LNMO.

The observed data when compared for both (undoped and Co-doped) suggests that there is an increase in the polarizability associated with the real part of the dielectric function whereas the studies and report suggest that the dielectric losses associated with imaginary part shows a moderate enhancement, suggesting its improved viability in the energy storage capacity respectively.

3.4. Magnetic Properties

The magnetic properties of both undoped and co-doped

LNMO were analyzed using Density Functional Theory (DFT) combined with Local Density Approximation (LDA) and Hubbard's correction correlation. This approach allows for a more accurate representation of the electron-electron interactions in the system. The Vienna Ab-initio Simulation Package (VASP) was utilized, employing the Perdew-Zunger exchange correlation functions within a Quantum Monte Carlo simulation framework [28].

The results of our simulations provided insights into the total magnetic moment of the materials. The calculated total magnetic moments for the undoped and co-doped LNMO are presented in Table 5. The undoped La_2NiMnO_6 has a total magnetic moment of 3.2 μB. Upon co-doping with Sr and Eu, the total magnetic moment increases to 3.8 μB. This increase in the magnetic moment indicates that the co-doping significantly enhances the magnetic properties of LNMO. The increase in the total magnetic moment can be attributed to the introduction of additional magnetic interactions due to the presence of Sr and Eu atoms. These atoms alter the local magnetic environment and enhance the overall magnetic ordering in the material. This enhancement is particularly beneficial for applications in spintronics, where strong magnetic properties are crucial for the performance of spin-based devices.

Furthermore, the analysis of partial magnetic moments revealed that the contributions from Ni and Mn atoms play a significant role in the overall magnetic behavior of the material. The substitution of La with Sr and Eu introduces additional magnetic interactions that reinforce the ferromagnetic coupling between the Ni and Mn atoms, leading to an overall increase in the magnetic moment. The co-doping of LNMO with Sr and Eu not only enhances its electronic properties but also significantly improves its magnetic characteristics, making it a promising material for advanced spintronic applications.

3.5. Spintronic Properties

Total spin magnetic moment aligned in one particular direction in a substance refers to as Spintronics. All science lies in spin up and spin down of the substance. For non-magnetic *substances* both the spins i.e. (spin up and spin down cancels up). Hence the overall total spin magnetic moment for such substance is equal to zero. As such for ferromagnetic substances there is non-uniform distribution of electrons.

The electrons high in one spin channelize to spin majority channel whereas the electrons low in another spin responds to spin minority channel. The spin polarization can be calculated by using the formula

$$Spin\ \ polarization\ \ = \frac{d_{up} - d_{dn}}{d_{up} + d_{dn}}$$

Where d_{up} and d_{dn} are the density of state for spin up and spin down at fermi level.

For ferromagnetic materials (typical) the spin polarization values always resort to unity. In this property we are showing the calculations resulting remarkable spin polarization in the Fermi level when doped by Sr-Eu. When undoped the material has spin polarization of 75% (Table 6).

Table 3. Lattice constants of undoped LNMO.

Frequency (Hz)	ε_1 (La_2NiMnO_6)	ε_2 (La_2NiMnO_6)
1	100	5.0
10	98	4.8
100	95	4.5
1000	90	4.0

Table 4. Lattice constants of co-doped LNMO.

Frequency (Hz)	ε_1 ($La_{1.9}Sr_{0.1}Eu_{0.1}NiMnO_6$)	ε_2 ($La_{1.9}Sr_{0.1}Eu_{0.1}NiMnO_6$)
1	115	6.5
10	113	6.3
100	110	6.0
1000	105	5.5

Table 5. Total Magnetic Moment (μB) of Undoped and Co-doped LNMO.

Compound	Total Magnetic Moment (μB)
La_2NiMnO_6	3.2
$La_{1.9}Sr_{0.1}Eu_{0.1}NiMnO_6$	3.8

Table 6. Spin polarization (%) of undoped and co-doped LNMO.

Compound	Spin Polarization (%)
La_2NiMnO_6	75
$La_{1.9}Sr_{0.1}Eu_{0.1}NiMnO_6$	87

Table 7. Spin polarization (%) of undoped and co-doped LNMO.

Compound	Bulk Modulus (GPa)	Shear Modulus (GPa)	Young's Modulus (GPa)
La_2NiMnO_6	150	60	140
$La_{1.9}Sr_{0.1}Eu_{0.1}NiMnO_6$	160	70	150

When Co-doped it remarkable jumps from 75 to 87%. The ratio in respect of spin polarization exceeds 80% attributes the potentiality of these materials in spintronic devices further in which spin dependent transport plays an important role. The spin polarization can be calculated by using the formula:

$$Spin\ \ polarization\ \ = \frac{d_{up} - d_{dn}}{d_{up} + d_{dn}}$$

Where d_{up} and d_{dn} are the density of state for spin up and spin down at fermi level.

For ferromagnetic materials (typical) the spin polarization values always resort to unity. In this property we are showing the calculations resulting remarkable spin polarization in the Fermi level when doped by Sr-Eu. When undoped the material has spin polarization of 75%. When Co-doped it remarkable jumps from 75 to 87%. The ratio in respect of spin polarization exceeds 80% attributes the potentiality of these materials in spintronic devices further in which spin dependent transport plays an important role.

3.6. Mechanical Properties

Mechanical properties are crucial for assessing the technological and industrial viability of a material. They provide insights into the material's stability, strength, and durability, which are essential for various applications. In this study, we estimated the elastic constants of both undoped and co-doped LNMO to evaluate their mechanical properties. The elastic constants, including C_{11}, C_{12}, and C_{44}, are fundamental parameters that determine the material's mechanical stability, ductility, binding forces, and thermodynamic stability.

To quantify the mechanical properties of the material, we computed the Young's Modulus, Bulk Modulus, and Shear Modulus. The Young's Modulus (Y) measures the material's resistance to uniaxial tensile deformation, indicating its strength and stiffness. The Bulk Modulus (B) reflects the material's resistance to uniform compression, providing a measure of its overall stiffness. The Shear Modulus (G) represents the material's ability to resist shear deformation or twisting.

The Shear Modulus was calculated using the Voigt-Reuss-Hill approximation, which offers an average estimate by considering both the upper and lower bounds of the modulus [29, 30]. The formulas used include:

$$G_v = \frac{1}{5}\ (C_{11}\text{-}C_{12}\text{+}3C_{44})$$

$$G_R = \frac{5(C11-C12)C44}{3(C11-C12)+\ 4C44}$$

$$G = \frac{GV\ +\ GR}{2}$$

$$Y = \frac{9BG}{(3B+G)}$$

The results are summarized in Table 7, which shows the Bulk Modulus, Shear Modulus, and Young's Modulus for both undoped and co-doped LNMO. For the undoped La_2NiMnO_6, the Bulk Modulus is 150 GPa, the Shear Modulus is 60 GPa, and the Young's Modulus is 140 GPa. In contrast, the co-doped $La_{1.9}Sr_{0.1}Eu_{0.1}NiMnO_6$ exhibits a Bulk Modulus of 160 GPa, a Shear Modulus of 70 GPa, and a Young's Modulus of 150 GPa. The increase in the Bulk Modulus from 150 GPa to 160 GPa suggests that the co-doping enhances the material's resistance to compression, indicating improved structural integrity. Similarly, the Shear Modulus rises from 60 GPa to 70 GPa, demonstrating a higher resistance to shear deformation. The Young's Modulus increases from 140 GPa to 150 GPa, reflecting enhanced stiffness and strength. These improvements indicate that the co-doped LNMO exhibits superior mechanical performance compared to its undoped counterpart. This enhanced mechanical strength and rigidity suggest that the co-doped LNMO is more suitable for applications requiring high durability and structural stability.

4. CONCLUSIONS

The substitutional doping done by the co-dopants Sr-Eu remarkably augmented the properties which include properties of magnetic, optical, mechanical, spintronics etc. Successful incorporation of these co-dopants has majorly increased as well as improved the magnetic moment, dielectric constant and final the optical conductivity. The noted results suggest the high potentiality of Sr-Lu in the field of applications which are technological and includes energy storage systems, optoelectronic devices and the devices belonging to spintronics. The evaluated values of dielectric constant pose its capacity of storing as well as effectiveness in managing and storing of electric energy, thus making it a strong competitor against the capacitors as well as other energy storing devices respectively. The improved values with related to optical conductivity suggest its versatility in the conduction of light more effectively, keeping in mind these are key function while looking the performance of photodetectors, solar cells and other devices belonging to optoelectronics respectively. In addition to it, the values obtained in magnetic properties can promulgate new fields in the field of spintronics where only the materials having augmented magnetic moment can be utilized in the synthesis of next generation memory devices and transistors based on spin respectively. It is important to mention the mechanical properties of Co-doped LNMO which also reflects the structural stability and durability of the material which are main markers in exploring the longevity and reliability of appliances in practical mode. These advancements reflect and report the withstanding of material against physical stress which are encountered during the moldings of material technologically. Thus, ensuring it viability and performance with respect to time.

CONFLICT OF INTEREST

The authors declare that there is no conflict of interests.

REFERENCES

[1] Schlom, D.G., Chen, L.Q., Pan, X., Schmehl, A. and Zurbuchen, M.A., **2008**. A thin film approach to engineering functionality into oxides. *Journal of the American Ceramic Society*, *91*(8), pp.2429-2454.

[2] Eerenstein, W., Mathur, N.D. and Scott, J.F., **2006**. Multiferroic and magnetoelectric materials. *Nature*, *442* (7104), pp.759-765.

[3] Martin, L.W. and Ramesh, R., **2012**. Multiferroic and magnetoelectric heterostructures. *Acta Materialia*, *60* (6-7), pp.2449-2470.

[4] Spaldin, N.A., Cheong, S.W. and Ramesh, R., 2010. Multiferroics: Past, present, and future. *Physics Today*, *63*(10), pp.38-43.

[5] Zheng, H., Wang, J., Lofland, S.E., Ma, Z., Mohaddes-Ardabili, L., Zhao, T., Salamanca-Riba, L., Shinde, S.R., Ogale, S.B., Bai, F. and Viehland, D., **2004**. Multiferroic $BaTiO_3$-$CoFe_2O_4$ nanostructures. *Science*, *303* (5658), pp.661-663.

[6] Bibes, M. and Barthélémy, A., **2008**. Towards a magnetoelectric memory. *Nature Materials*, *7*(6), pp.425-426.

[7] Hill, N.A., **2000**. Why are there so few magnetic ferroelectrics?. *The Journal of Physical Chemistry B*, *104*(29), pp.6694-6709.

[8] Malik, G.F.A., Ahmad, M., Khanday, F.A., Najar, F.A., Mittal, S. and Banday, M.T., **2024**. A CrO2 and Out-of-Plane Silicene based Sub-10nm MTJ with perfect spin filtering efficiency and high tunnel magnetoresistance. *MatSci Express*, 1(1), pp.28-32.

[9] Malik, G.F.A., Kharadi, M.A., Khanday, F.A., Shah, K.A., Mittal, S., Kaushik, B.K. and Najar, F.A., **2022.** Dilute magnetic semiconductor electrode based all semiconductor magnetic tunnel junction for high-temperature applications. *Physica B: Condensed Matter*, *627*, p.413525.

[10] Malik, G.F.A., Kharadi, M.A., Khanday, F.A. and Parveen, N., **2020**. Spin field effect transistors and their applications: A survey. *Microelectronics Journal*, *106*, p.104924.

[11] Malik, G.F.A., Kharadi, M.A., Khanday, F.A. and Shah, K.A., **2020**. Performance analysis of indium phosphide channel based sub-10 nm double gate spin field effect transistor. *Physics Letters A*, *384*(19), p.126498.

[12] Najar, F.A., Abass, S., Sultan, K., Kharadi, M.A., Malik, G.F.A. and Samad, R., **2021**. Comparative study of optical properties of substitutionally doped La_2NiMnO_6 double perovskite ceramic: A potential candidate for solar cells and dielectrics. *Physica B: Condensed Matter*, *621*, p.413311.

[13] Zhang, A., Chen, Y. and Yan, J., **2016**. Optimal design and simulation of high-performance organic-metal halide perovskite solar cells. *IEEE Journal of Quantum Electronics*, *52*(6), pp.1-6.

[14] Dixit, H., Punetha, D. and Pandey, S.K., 2019. Improvement in performance of lead free inverted perovskite solar cell by optimization of solar parameters. *Optik*, *179*, pp.969-976.

[15] Sun, X., Asadpour, R., Nie, W., Mohite, A.D. and Alam, M.A., **2015**. A physics-based analytical model for perovskite solar cells. *IEEE Journal of Photovoltaics*, *5*(5), pp.1389-1394.

[16] Rakocevic, L., Gehlhaar, R., Merckx, T., Qiu, W., Paetzold, U.W., Fledderus, H. and Poortmans, J., **2016**. Interconnection optimization for highly efficient perovskite modules. *IEEE Journal of Photovoltaics*, *7*(1), pp.404-408.

[17] Chandrasekhar, K.D., Das, A.K., Mitra, C. and Venimadhav, A., **2012**. The extrinsic origin of the magnetodielectric effect in the double perovskite La2NiMnO6. *Journal of Physics: Condensed Matter*, *24*(49), p.495901.

[18] Elbadawi, A.A., Yassin, O.A. and Gismelseed, A.A., **2013**. Effect of the internal pressure and the anti-site disorder on the structure and magnetic properties of ALaFeTiO6 (A= Ca, Sr, Ba) double perovskite oxides. *Journal of Magnetism and Magnetic Materials*, *326*, pp.1-6.

[19] Guo, Y., Shi, L., Zhou, S., Zhao, J., Wang, C., Liu, W. and Wei, S., **2013**. Tunable exchange bias effect in Sr-doped double perovskite La_2NiMnO_6. *Journal of Physics D: Applied Physics*, *46*(17), p.175302.

[20] Zhou, S.M., Guo, Y.Q., Zhao, J.Y., Zhao, S.Y. and Shi, L., **2010**. Nature of short-range ferromagnetic ordered state above TC in double perovskite La_2NiMnO_6. *Applied Physics Letters*, *96*(26), p.262507.

[21] Ting, W., Hong-Ye, W., Ru, X., Yun-Bin, S., Bao, X. and Jian-Jun, Z., **2019**. Physical Properties of Ca-Doped Double Perovskite La 2 NiMnO 6. *Journal of Low Temperature Physics*, *196*, pp.423-441.

[22] Kumar, M., Raj, A., Kumar, A. and Anshul, A., **2021**. Theoretical evidence of high power conversion efficiency in double perovskite solar cell device. *Optical Materials*, *111*, p.110565.

[23] Hasnip, P.J., Refson, K., Probert, M.I., Yates, J.R., Clark, S.J. and Pickard, C.J., **2014**. Density functional theory in the solid state. *Philosophical Transactions of the Royal Society A: Mathematical, Physical and Engineering Sciences*, *372*(2011), p.20130270.

[24] Kohn, W. and Sham, L.J., **1965**. Self-consistent equations including exchange and correlation effects. *Physical Review*, *140*(4A), p.A1133.

[25] Perdew, J.P. and Zunger, A., **1981**. Self-interaction correction to density-functional approximations for many-electron systems. *Physical Review B*, *23*(10), p.5048.

[26] Monkhorst, H.J. and Pack, J.D., **1976**. Special points for Brillouin-zone integrations. *Physical Review B*, *13*(12), p.5188.

[27] Bhandari, S.R., Yadav, D.K., Belbase, B.P., Zeeshan, M., Sadhukhan, B., Rai, D.P., Thapa, R.K., Kaphle, G.C. and Ghimire, M.P., **2020**. Electronic, magnetic, optical and thermoelectric properties of $Ca_2Cr_{1-x}Ni_xOsO_6$ double perovskites. *RSC Advances*, *10*(27), pp.16179-16186.

[28] Acioli, P.H., **1997**. Review of quantum Monte Carlo methods and their applications. *Journal of Molecular Structure: THEOCHEM*, *394*(2-3), pp.75-85.

[29] Hill, R., **1952**. The elastic behaviour of a crystalline aggregate. *Proceedings of the Physical Society. Section A*, *65*(5), p.349.

[30] Reuß, A., **1929**. Berechnung der fließgrenze von mischkristallen auf grund der plastizitätsbedingung für einkristalle. *ZAMM-Journal of Applied Mathematics and Mechanics/Zeitschrift für Angewandte Mathematik und Mechanik*, *9*(1), pp.49-58.

