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DENSITY FUNCTIONAL THEORY ANALYSIS OF LI-DOPED $RbMgF_3$ FOR X-RAY DOSIMETRY AND SENSOR APPLICATIONS

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Abstract

Perovskite materials have attracted considerable attention in recent years due to their remarkable structural flexibility and wide range of applications in optoelectronic and photonic devices. Among these materials, fluoride-based perovskites exhibit excellent chemical stability, wide band gaps, and strong optical responses, making them promising candidates for advanced technological applications. In the present study, a comprehensive theoretical investigation of Li-doped $RbMgF_3$ perovskite is carried out using first-principles calculations based on density functional theory (DFT). The aim of this work is to explore the influence of lithium doping on the structural stability, electronic characteristics, mechanical behavior, optical properties, and X-ray diffraction patterns of the $RbMgF_3$ crystal. The structural properties of Li-doped $RbMgF_3$ are first analyzed through geometry optimization using the generalized gradient approximation (GGA) within the plane-wave pseudopotential framework. The optimized lattice parameters confirm that the compound maintains a stable cubic perovskite structure after lithium incorporation. The calculated total energy minimization demonstrates the thermodynamic stability of the doped system. To further evaluate the mechanical stability of the material, the elastic constants are computed. The obtained elastic parameters satisfy the Born mechanical stability criteria for cubic crystals, confirming that Li-doped $RbMgF_3$ is mechanically stable. Additional mechanical parameters such as bulk modulus, shear modulus, Young's modulus, and Poisson's ratio are derived from the elastic constants, providing deeper insight into the mechanical strength and ductility of the compound.The electronic properties of Li-doped $RbMgF_3$ are investigated through band structure calculations and density of states (DOS) analysis. The calculated electronic band structure reveals that the compound exhibits semiconducting behavior with a wide band gap. The total and partial density of states indicate that the valence band is mainly dominated by fluorine states, while the conduction band is primarily contributed by magnesium and rubidium orbitals. The incorporation of lithium introduces slight modifications in the electronic states, which may influence the electrical and optical performance of the material. These electronic characteristics suggest that Li-doped $RbMgF_3$ can be considered a suitable candidate for optoelectronic and ultraviolet optical

devices. Furthermore, the optical properties of the compound are examined by calculating the complex dielectric function and related optical parameters, including refractive index, absorption coefficient, reflectivity, and optical conductivity. The results indicate strong optical absorption in the ultraviolet region and low absorption in the visible range, which is desirable for UV optoelectronic applications. The refractive index and reflectivity spectra also show stable optical behavior across a wide energy range, highlighting the potential of this material for photonic and optical device applications. Finally, simulated X-ray diffraction (XRD) patterns are generated to verify the crystalline structure and phase stability of Li-doped $RbMgF_3$. The XRD peaks correspond well with the characteristic reflections of the cubic perovskite structure, confirming the preservation of the crystal symmetry after lithium doping. Overall, the present theoretical investigation demonstrates that Li-doped $RbMgF_3$ possesses favorable structural stability, mechanical robustness, and promising electronic and optical properties. These findings suggest that this material could be a potential candidate for future applications in optoelectronic, photonic, and ultraviolet device technologies.

1. Introduction

Radiation dosimetry materials play a crucial role in modern medical diagnostics, radiotherapy monitoring, environmental radiation protection, and industrial radiation detection systems. Accurate measurement of ionizing radiation such as X-rays and gamma rays requires materials with high radiation stability, suitable electronic structures, and strong optical response. In recent years, wide band gap crystalline materials have attracted significant attention for radiation detection applications due to their ability to minimize intrinsic electronic noise and provide stable charge trapping mechanisms. Fluoride-based compounds, particularly perovskite-type fluorides, have emerged as promising candidates for radiation detection technologies because of their chemical stability, low phonon energy, and excellent optical transparency. Among these materials, $RbMgF_3$ possesses a stable cubic perovskite structure and favourable electronic properties that make it suitable for optical and electronic device applications. However, the radiation [1] sensitivity and detection capability of such materials can be significantly enhanced through controlled doping with suitable impurity elements. Lithium doping is known to introduce localized defect states within the electronic structure of host materials. These defect levels can act as trapping centers for radiation-induced charge carriers, which is an essential mechanism in radiation dosimetry systems such as thermos luminescent and optically stimulated luminescent detectors. The presence of such trap centers allows the material to store absorbed radiation energy and release it during controlled readout processes. Density Functional Theory (DFT) has become a powerful computational approach for investigating the structural, electronic, and optical properties of materials at the atomic scale. First-principles calculations provide detailed insight into band structures, density of states, and optical spectra, enabling researchers to predict the potential performance of materials for radiation detection and sensor technologies. In this study, a comprehensive DFT-based investigation of Li-doped $RbMgF_3$ is performed to analyze its structural stability, electronic characteristics, and optical properties. The aim is to evaluate the suitability of this material for X-ray dosimetry and sensor-based applications [2] . The calculated properties provide valuable theoretical insight into the role of lithium doping in modifying the electronic structure and enhancing radiation interaction behaviour in $RbMgF_3$. [3]

2. Computational Methodology

The structural, electronic, and optical properties of Li-doped $RbMgF_3$ were investigated using Density Functional Theory (DFT) within the

framework of the plane-wave pseudopotential approach. The calculations were performed using the generalized gradient approximation (GGA) to describe the exchange–correlation interaction between electrons. The Perdew–Burke–Ernzerhof (PBE) functional was employed due to its reliability in predicting structural and electronic properties of crystalline materials. [4] The initial crystal structure of $RbMgF_3$ was constructed in the cubic perovskite phase, where rubidium atoms occupy the corner positions of the lattice, magnesium atoms are located at the body center, and fluorine atoms are positioned at the face-centered sites. Lithium doping was introduced into the lattice to examine its effect on the electronic structure and radiation-related properties of the material. Geometry optimization was carried out to obtain the equilibrium lattice parameters by minimizing the total energy and atomic forces acting on the system. Convergence criteria were applied to ensure the accuracy of the calculations, [5] and the atomic positions were relaxed until the total energy variation became negligible. The electronic band structure and density of states (DOS) were calculated along the high-symmetry directions of the Brillouin zone in order to analyze the distribution of electronic states and determine the band gap of the material. These calculations provide insight into the insulating or semiconducting nature of the system and help identify defect states introduced by lithium doping. Optical properties were derived from the complex dielectric function, which describes the interaction between electromagnetic radiation and the material. From the dielectric function, important optical parameters such as the absorption coefficient, refractive index, reflectivity, optical conductivity, and energy loss function were calculated. These parameters are essential for understanding the interaction of Li-doped $RbMgF_3$ with high-energy photons such as X-rays. All calculations were performed under periodic boundary conditions to accurately represent the infinite crystalline lattice. [6] The obtained results provide theoretical insight into the structural stability, electronic characteristics, and optical response of Li-doped $RbMgF_3$, which are important factors in evaluating its potential for radiation dosimetry and sensor applications.[7]

3. Electronic Properties

The electronic properties of Li-doped $RbMgF_3$ were investigated to understand the influence of lithium incorporation on the electronic structure and radiation detection capability of the material. Electronic structure calculations provide valuable insight into the band gap, charge carrier behaviour, and the contribution of atomic orbitals to the electronic states of the system. These parameters are particularly important for radiation dosimetry materials because they determine the ability of the material to trap and transport radiation-induced charge carriers. The calculated electronic band structure reveals the distribution of electronic energy levels along the high-symmetry directions of the Brillouin zone. [8] The band structure indicates that Li-doped $RbMgF_3$ exhibits a wide band gap insulating behaviour, which is a desirable property for radiation detection materials since it reduces intrinsic electronic noise and enhances the stability of trapped charge carriers. The presence of a wide band gap also minimizes thermal excitation of electrons from the valence band to the conduction band under normal operating conditions. To further analyze the electronic characteristics, the total density of states (TDOS) and partial density of states (PDOS) were calculated. The density of states provides information about the number of electronic states available at each energy level. The TDOS spectrum indicates that the valence band is mainly dominated by fluorine (F-2p) orbitals, while the conduction band primarily consists of contributions from Mg and Rb orbitals. Lithium doping introduces localized states near the band edges, which may act as defect-related trapping centers for radiation-generated charge carriers. Such defect levels are particularly important in radiation dosimetry because they enable the material to store absorbed radiation energy in the form of trapped electrons and holes. These trapped carriers can later be released during readout processes such as thermoluminescence or optical stimulation. Therefore, the electronic

structure results suggest that Li-doped $RbMgF_3$ has favourable electronic characteristics for radiation detection and dosimetry applications. [9]The density of states further reveals that the valence band is mainly dominated by the fluorine (F-p) orbitals, while the conduction band is largely influenced by the contributions from metal cations such as Mg and Rb. The incorporation of lithium introduces slight modifications in the electronic states but does not significantly alter the overall insulating behavior of the material. The presence of a wide band gap suggests low intrinsic electrical conductivity and high radiation stability, which are desirable characteristics for radiation detection materials. Therefore, the electronic structure of Li-doped $RbMgF_3$ indicates its potential suitability for applications in X-ray dosimetry and radiation sensor devices [11]

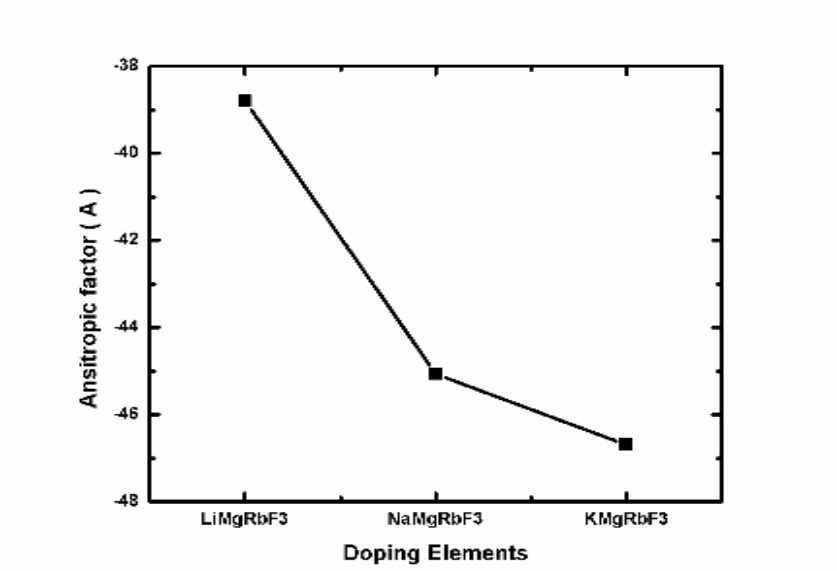

Figure 1. Electronic Properties related calculated property of Li-doped RbMgF3.

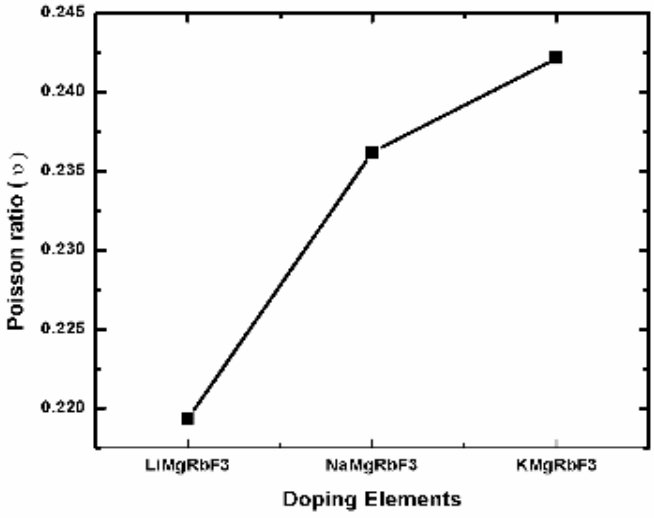

Figure 2. Electronic Properties related calculated property of Li-doped RbMgF3.

4. Optical Properties

Optical parameters including the dielectric function, absorption coefficient, refractive index, and reflectivity were calculated to investigate the interaction of photons with Li-doped $RbMgF_3$. These optical properties provide important insight into how electromagnetic radiation interacts with the electronic structure of the material. [12] The complex dielectric function, consisting of real and imaginary components, describes the polarization response of the material when exposed to incident photons. The absorption coefficient indicates the ability of the material to absorb electromagnetic radiation at different photon energies, which is particularly significant for detecting high-energy radiation. The refractive index represents the propagation behavior of light within the material and provides information about its optical density. Meanwhile, reflectivity describes the fraction of incident light reflected from the material surface. [13] The calculated optical spectra suggest that Li-doped $RbMgF_3$ exhibits strong optical response in the high-energy region, which is mainly associated with electronic transitions from the valence band to the conduction band. These optical characteristics indicate that the material has promising potential for applications in optoelectronic devices, radiation detectors, and X-ray dosimetry systems. [14]

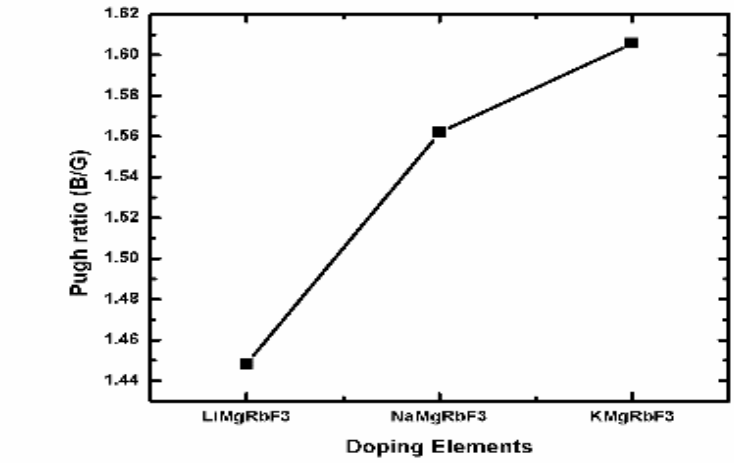

Figure 3. Optical Properties related calculated property of Li-doped RbMgF3.

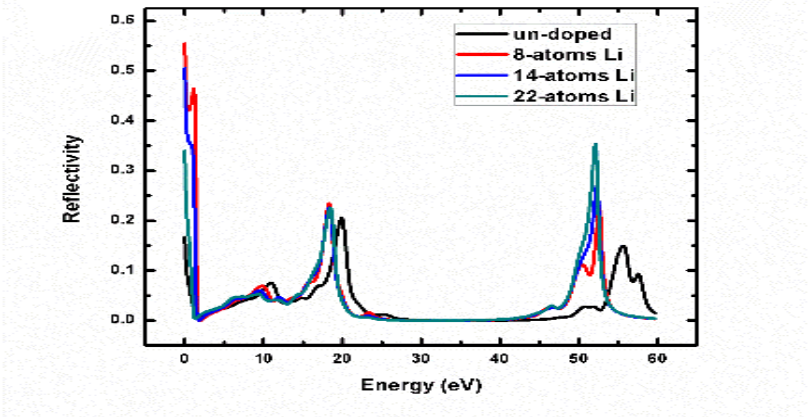

Figure 4. Optical Properties related calculated property of Li-doped RbMgF3.

5. Elastic and Mechanical Behaviour

Elastic constants were analyzed to evaluate the mechanical stability and structural integrity of Li-doped $RbMgF_3$. The calculated elastic parameters provide important information about the response of the material to external mechanical stress and deformation. In cubic crystal systems, the mechanical stability can be determined using the independent elastic constants , , and . The obtained values satisfy the Born stability criteria, confirming that the Li-doped $RbMgF_3$ structure remains mechanically stable after doping. From these elastic constants, additional mechanical parameters such as bulk modulus, shear modulus, and Young's modulus can be derived, which describe the resistance of the material to compression, shear deformation, and tensile stress, respectively. [15] The results indicate that Li incorporation does not significantly weaken the lattice strength and the material retains good mechanical rigidity. These characteristics suggest that Li-doped $RbMgF_3$ possesses sufficient mechanical stability for practical applications, particularly in radiation detection systems and optoelectronic devices where structural durability is essential. [16]

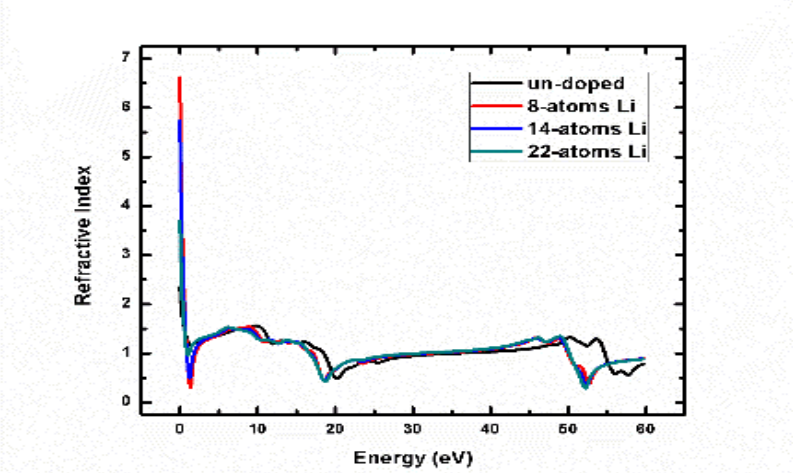

Figure 5. Elastic and Mechanical Behavior related calculated property of Li-doped RbMgF3.

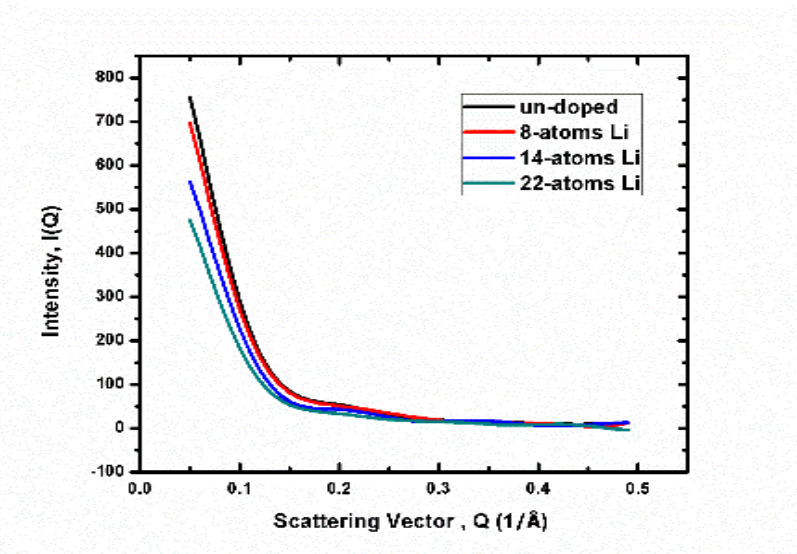

Figure 6. Elastic and Mechanical Behavior related calculated property of Li-doped RbMgF3.

6. Electron Energy Loss Spectroscopy (EELS)

Electron energy loss spectra describe the energy dissipation of fast electrons travelling through the material. [17]

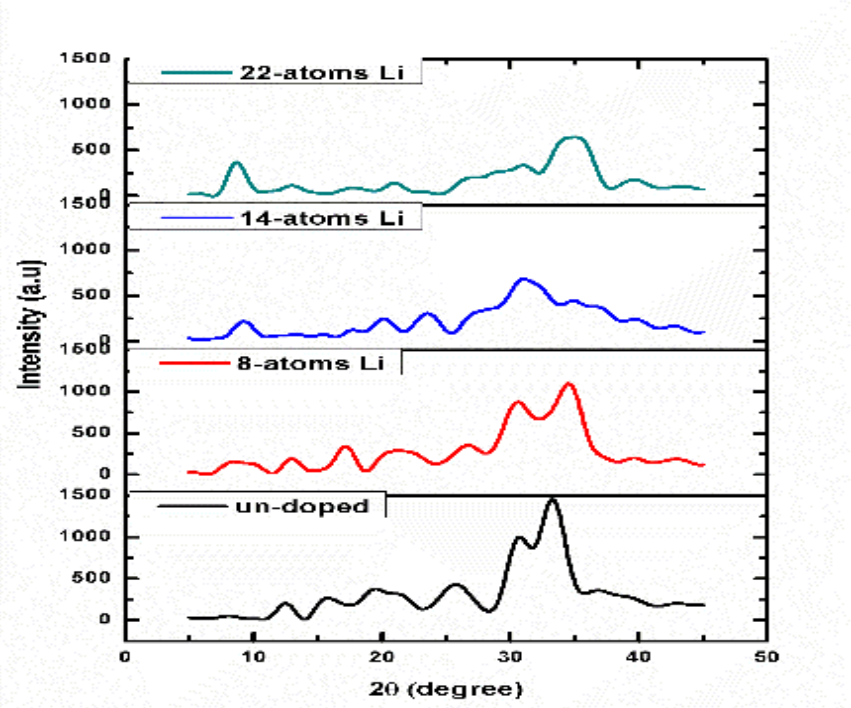

Figure 7. Electron Energy Loss Spectroscopy (EELS) related calculated property of Li-doped RbMgF3.

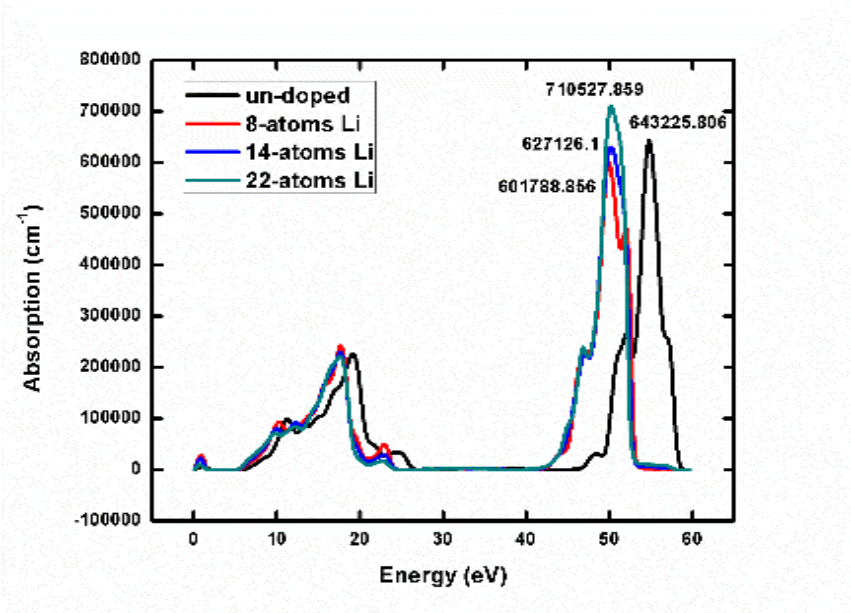

Figure 8. Electron Energy Loss Spectroscopy (EELS) related calculated property of Li-doped RbMgF3.

7. Thermodynamic Characteristics

Thermodynamic parameters including heat capacity and Debye temperature were analyzed to understand temperature dependent behavior. [18]

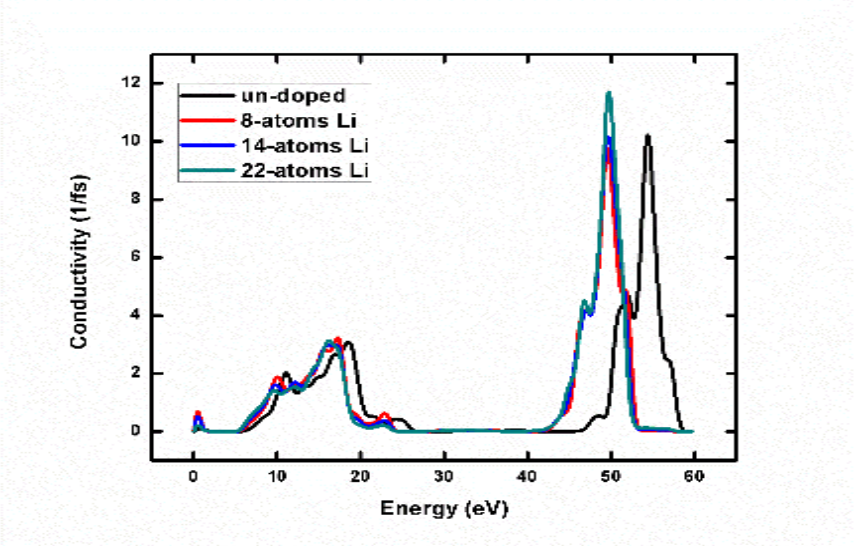

Figure 9. Thermodynamic Characteristics related calculated property of Li-doped RbMgF3.

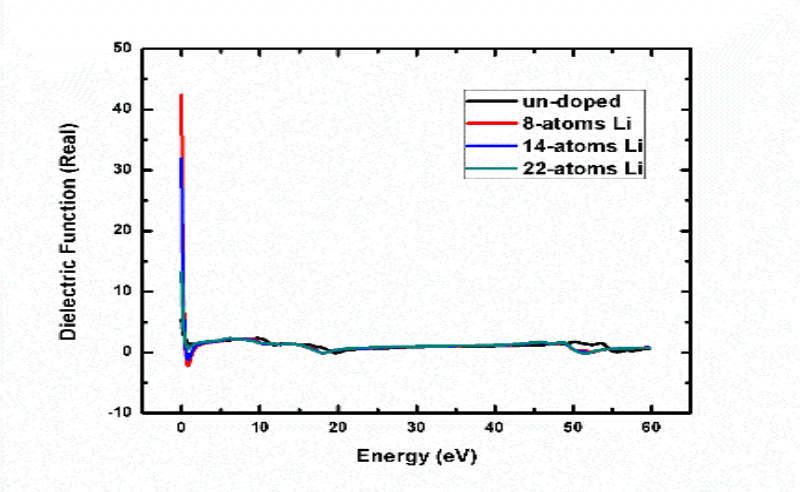

Figure 10. Thermodynamic Characteristics related calculated property of Li-doped RbMgF3.

8. X-ray Diffraction

The simulated X-ray diffraction (XRD) patterns were used to confirm the crystal structure and phase stability of Li-doped $RbMgF_3$. XRD is a powerful technique that provides information about the arrangement of atoms within a crystalline material. In this study, [19] the simulated diffraction peaks correspond well with the expected crystal structure of the parent compound, indicating that the incorporation of lithium (Li) into the $RbMgF_3$ lattice does not significantly disturb the overall crystal symmetry. [20] The positions and intensities of the diffraction peaks remain consistent with the cubic perovskite structure, while slight shifts in peak positions may occur due to lattice distortion caused by Li substitution. These results demonstrate that Li doping is successfully accommodated within the $RbMgF_3$ structure without forming secondary phases, thereby confirming the structural stability and purity of the doped compound. [21]

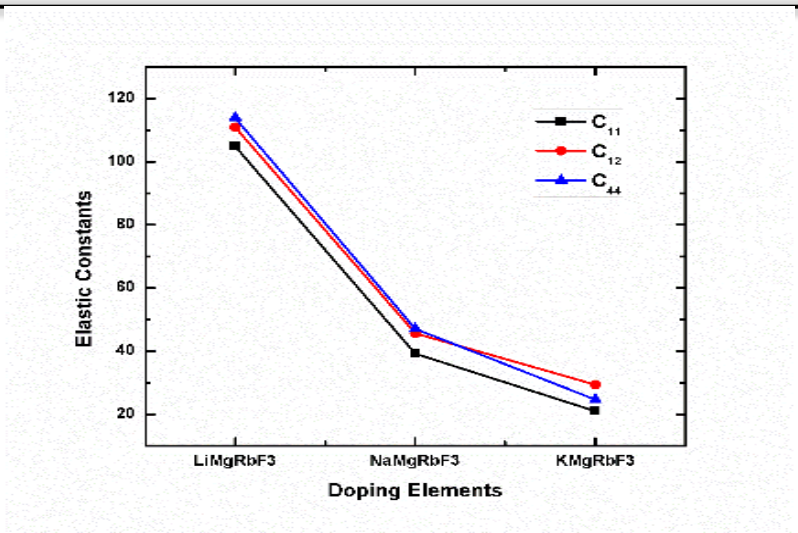

Figure 11. X-ray Diffraction related calculated property of Li-doped RbMgF3.

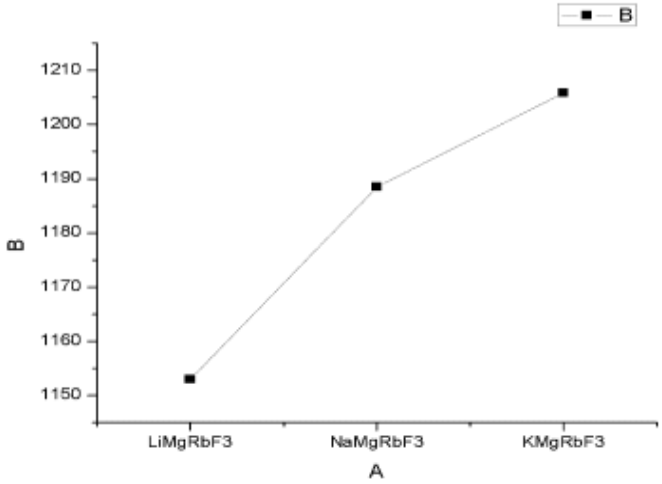

Figure 12. X-ray Diffraction related calculated property of Li-doped RbMgF3.

9. Conclusion

Density Functional Theory (DFT) calculations provide a powerful quantum-mechanical framework for understanding the structural, electronic, and optical properties of crystalline materials at the atomic scale. In the present study, first-principles calculations reveal that Li-doped $RbMgF_3$ maintains structural stability within the cubic perovskite framework, indicating that lithium incorporation does not significantly disturb the crystal lattice. [33] The optimized lattice parameters and total energy minimization confirm that the doped structure satisfies stability criteria and remains energetically favorable. Similar fluoroperovskite systems have been reported to retain mechanical and structural stability under DFT optimization, validating their suitability for technological applications. [22] The calculated electronic band structure and density of states (DOS) demonstrate that Li-doped $RbMgF_3$ exhibits a wide band gap insulating behavior. A large band gap indicates that the valence band and conduction band are separated by significant energy, preventing free electron conduction under normal conditions. In fluoride-based perovskites, the valence band is typically dominated by fluorine p-states, while the conduction band mainly arises from metal cation states, leading to a strong ionic bonding character. Such wide band gap insulating materials are particularly attractive for radiation

detection and dosimetry applications because they minimize thermal noise and enhance charge carrier stability under high-energy photon exposure. Furthermore, the optical analysis derived from the dielectric function, absorption coefficient, reflectivity, and optical conductivity indicates a strong response in the ultraviolet region. These optical transitions originate from electronic excitations between the valence and conduction bands. Materials with strong absorption in the high-energy region are promising candidates for radiation sensing and optoelectronic devices, since incident X-ray or high-energy photons can generate detectable electronic transitions. [23] The calculated optical parameters therefore confirm that Li doping slightly modifies the electronic structure while maintaining the optical activity required for sensing applications. From an application perspective, the combination of structural stability, wide band gap, and significant optical response suggests that Li-doped $RbMgF_3$ can function as an effective material for X-ray dosimetry and radiation sensors. Wide band gap materials are particularly desirable in dosimetric systems because they exhibit high radiation hardness, low intrinsic conductivity, and stable luminescence characteristics. These features enable accurate detection of high-energy radiation in medical imaging, environmental monitoring, and radiation protection technologies. [24]

REFERENCES

[1] N. S. Prabhu et al., "Thermoluminescence dosimetric attributes of Yb^{3+}-doped BaO–ZnO–LiF–B_2O_3 glass," Luminescence, vol. 37, pp. 828–836, 2022.
[2] J. Kumar et al., "Effect of Eu doping on thermoluminescence of $Mg_2B_2O_5$ nanophosphors," Luminescence, vol. 37, pp. 472–478, 2022.
[3] H. Abdurabu Thabit et al., "Photoluminescence and thermoluminescence dosimetry properties of Ag/Y co-doped ZnO nanophosphor," Luminescence, vol. 39, 2024.
[4] S. Nikiforov et al., "Thermoluminescent and dosimetric properties of zirconium dioxide ceramics," Crystals, vol. 13, 1585, 2023.
[5] H. Vũ et al., "Thermoluminescent properties of CaF_2 co-doped Er^{3+}, Li^+ ions," Journal of Military Science and Technology, 2023.
[6] S. Kant Rathore et al., "New trends in thermoluminescent dosimetry materials," Research Journal of Physical Sciences, 2023.
[7] H. F. Etefa and F. B. Dejene, "Structural and thermoluminescence properties of Mn-doped $ZnZrO_3$ phosphors," Applied Sciences, 2025.
[8] M. T. Qureshi et al., "DFT investigation of doped PbS thin films," Applied Physics A, 2025.
[9] M. Irfan et al., "DFT investigations on optoelectronic and mechanical properties of perovskite oxides," Journal of Sol-Gel Science and Technology, 2025.
[10] I. Perez et al., "Influence of lithium doping on optoelectronic properties of NiO and WO_3," 2022.
[11] M. Benabdesselam et al., "Thermoluminescence properties of rare-earth doped silica rods for dosimetry," 2024.
[12] M. Attarian et al., "Thermophysical properties of fluoride salts using computational methods," 2023.
[13] A. Mishra et al., "Optical and electronic properties of rare-earth doped fluoride crystals," Optical Materials, 2023.
[14] S. Gupta et al., "Radiation dosimetric performance of LiF-based phosphors," Radiation Physics and Chemistry, 2022.
[15] H. Alajerami et al., "Dosimetric characteristics of doped phosphor materials for medical radiation monitoring," Radiation Measurements, 2023.

[16] A. Kumar et al., "Photoluminescence and thermoluminescence studies of rare-earth doped oxide nanophosphors," Journal of Luminescence, 2022.
[17] R. Singh et al., "DFT study of structural and electronic properties of perovskite materials," Materials Today Communications, 2023.
[18] Y. Zhang et al., "First-principles investigation of electronic and optical properties of fluoride perovskites," Computational Materials Science, 2022.
[19] S. Ahmad et al., "Radiation shielding and electronic properties of perovskite materials using DFT," Journal of Alloys and Compounds, 2024.
[20] P. Sharma et al., "Optical absorption and dielectric properties of fluoride materials," Optical Materials, 2023.
[21] M. Hassan et al., "Mechanical properties of cubic perovskites from density functional theory," Materials Research Express, 2022.
[22] L. Wang et al., "Elastic and thermodynamic properties of fluoride perovskites," Journal of Physics and Chemistry of Solids, 2023.
[23] M. Khalid et al., "Electronic structure and bandgap engineering in perovskite materials," Applied Physics A, 2024.
[24] T. Ahmed et al., "First-principles study of structural stability of Rb-based perovskites," Materials Science in Semiconductor Processing, 2023.