

NATURE'S SYMPHONY

ISSN-E: 3007-2034

ISSN-P: 3007-2026

Website link: www.tsfn.com

First Principles Simulation of Ferromagnetic A_2MnCl_6 ($A = K, Rb, Cs$) Double Perovskites for Energy Efficient Spintronic Applications

Ghulam M. Mustafa, N. A. Noor, Arman Zamir, Adnan Mustafa, Abrar Ashraf

To cite: Mustafa, GM., Noor, NA., Zamir, A., Mustafa, A., Ashraf, A. First Principles Simulation of Ferromagnetic A_2MnCl_6 ($A = K, Rb, Cs$) Double Perovskites for Energy Efficient Spintronic Applications. *Nature's Symphony*, 2(1):09-27.

DOI: <https://doi.org/10.69547/NS.21.02>

Article QR



Published online: 25 March 2024

Submit your article to this journal: <https://tsfjb.com/ojs/index.php/tsfn/about/submissions>

View archive: <https://tsfjb.com/ojs/index.php/tsfn/issue/archive/>



NATURE'S SYMPHONY
Volume 2 Issue 1, Spring 2024

First Principles Simulation of Ferromagnetic A₂MnCl₆ (A = K, Rb, Cs) Double Perovskites for Energy Efficient Spintronic Applications

Ghulam M. Mustafa^{1*} | N.A. Noor² | Arman Zamir³ | Adnan Mustafa⁴ | Abrar Ahraf⁵

¹Department of Physics, Division of Science and Technology, University of Education, Lahore, Pakistan

²Department of Physics, University of Sargodha, Sargodha, Pakistan

³Department of Physics, University of Agriculture Faisalabad, Faisalabad, Pakistan.

⁴National Textile University Faisalabad

⁵Departamento de Engenharia de Materiais, Escola de Engenharia de Lorena (EEL), Universidade de São Paulo (USP), Lorena, São Paulo, Brazil

*Correspondence

Ghulam M. Mustafa

Email:

gmmustafa25@gmail.com

Keywords: Ferromagnetic semiconductors; DFT analysis; Magnetic moments; Figure of merit

ABSTRACT

Double perovskites are emerging due to their eco-friendly, and spin-polarized characteristics, and present an appealing option for applications in spintronics. In current investigation, we delve into the effect of Mn d-electrons on the magnetic response of A₂MnCl₆ (A = K, Rb, Cs) through theoretical analysis using the WIEN2k code. The value of lattice constant increased from 9.61 to 9.69 and 9.82 Å when K is replaced with Rb and Cs respectively which caused a reduction in Bulk modulus from 39.91 to 39.29 and 38.71 GPa. The calculated formation energy values (-1.64, -1.82, and -1.96 eV) affirm the thermodynamic stability of the system. Examination of band structure and density of states divulges a half-metallic ferromagnetic character, elucidated through exchange energies and exchange constants. Our calculations indicate that the interplay of basic hybridization processes, exchange energies and crystal field effects play a pivotal role in the development of ferromagnetism driven by the spin of electrons. Finally, an assessment of electrical (0.2-1.02x10¹⁹/Ωms) and thermal conductivity (0-4.8x10¹⁴ W/mKs), Seebeck coefficient (>200 μV/K), power factor (0-4.5x10¹¹ W/mK²s), magnetic susceptibility (0-1.6x10⁻⁹ m³/mol), and figure of merit (up to 0.97) is performed to evaluate the prospective of the inspected compounds for potential applications in energy harvesting technologies.

1. INTRODUCTION

Spintronics, abbreviated for spin transport electronics, marks a revolutionary shift in the realm of electronics by capitalizing on the inherent spin of electrons alongside their fundamental charge. Different from conventional electronics, the functioning of spintronics is based on both the charge and the spin states, which is a new approach that not only enhances the possibility of using electronics but is also related to creating brand-new possibilities to develop energy-saving and faster components of electronics (Mustafa *et al.*, 2022; Tang and Zhu, 2022; Ramawat *et al.*,

2023). Half Metallicity is one of the most appealing aspects of spintronics and remarkably contributes to the development of spintronics applications. Half metals can be described as materials with opposite electronic types of properties; one spin channel acts like metal while the other resembles an insulator or a semiconductor. This distinct feature possesses deep implications for spintronics, especially with regard to the field of magnetic materials (Mir and Gupta, 2020). The relationship between spintronics and half-metallicity entails the enhancement of the spin-polarized material that can efficiently support

half-metallicity. Spin polarization is the process whereby the spin of the electron will be oriented in a given direction. When it comes to half metallicity, increasing the spin polarization to a higher level is inevitable for applications in spin valves, magnetic tunnel junctions, and spin filters (Abdullah and Gupta, 2023). Half metallic (HM) materials are also proven ideal for spintronics devices because they allow the transport of spins of one polarity while blocking those of the other polarity (Souidi *et al.*, 2016). Such skin-specific spin transport turns out to be highly advantageous in the generation of spin-polarized currents which further enhances the prospect of spin-based memory as well as logic components. Since the spin elements of a half metal possess different electronic characteristics, engineers working in the spintronics area consider it possible to design improved and more versatile components for the next generation of electronic equipment (Khandy and Gupta, 2021). Double perovskites appear as a separate class of crystalline materials that are described by a complex and, at that, nontrivial structure, the study of which has attracted researcher's attention given the heightened importance of the corresponding materials in the fields of spintronics and half metallicity. These materials belong to the group of perovskites, which are characterized by the crystal structure formula $A_2BB'O_6$, where A and B are cations and B' is a different cation. The unique feature of double perovskites is the presence of two dissimilar B -site cations, which make these materials outstanding in terms of electronic and magnetic properties (Leng *et al.*, 2020). The relevance of double perovskites in relation to spintronics is obvious, providing a highly versatile system of controlling electron spin, which is one of the most important prerequisites for the development of spin-based electronics (Lamrani *et al.*, 2013). The modifiability of their electronic characteristics enables the researcher to shape these materials for the characteristics that are required, making

them good rivals for use in applications requiring effective spin polarization and control. These characteristics form an important foundation upon which spin manipulation efficiency is enhanced and spins, generally, progress spintronics applications (Dar *et al.*, 2019). Furthermore, the arrangement of the cations in the double perovskites leads to incentivizing spin-orbit coupling, thus affecting the relation between the spin and the orbital, how electrons move in a direction perpendicular to an applied magnetic field also making them suitable for spintronic applications. The interaction they have with other spintronics materials enables their incorporation into the complex systems hence bringing closer the opportunity to create new fusions that enhance overall device performance significantly. Moreover, the variety of magnetic properties exhibited by double perovskites, which include ferromagnetic, antiferromagnetic, and ferrimagnetic behaviors provides the researcher with a versatile menu from which to design and create materials with specific spintronic applications. Some of the double perovskites also display multiferroic behavior where both, ferroelectric and magnetic ordering exist in the compound paving the way to the large category of multifunctional devices where spintronics works hand in hand with others. The study of double perovskites in the scientific literature has sparked a new wave of interest, which encouraged the probing of interesting materials, with completely new combinations of elements, and new trends in the complex world of spintronics and half-metal systems. As researchers continue developing interest in understanding the complex feature of double perovskites their promising importance cannot be overemphasized as they are pointed to changing the face of electronics, devices, and technologies in the near future (Mahmood *et al.*, 2022a).



In recent times, double perovskites have emerged as an ideal candidate for lead-based double perovskites for photovoltaic technology and others related to thermoelectric applications. Dar and Want (2023) investigated in detail the effect and understanding of structural stability, half-metallic magnetic nature, as well as the optoelectronic properties present in Cs_2KXCl_6 , where 'X' being Ti and V in the double perovskite arrangement. The study provides valuable information about the stability of the compound as well as the details of the rules that control its half-metallic magnetic properties. Moreover, the analysis of the structures and the optoelectronic behavior of Cs_2KXCl_6 education expands the overall understanding of various potential functionalities (Dar and Want, 2023). In the recent study by Radja *et al.* (2022) the authors performed a comprehensive investigation of $Cs_2AgFeCl_6$, which is a novel family of Pb-free double perovskites using predictive first-principles calculations. The paper explores a range of properties that include structural, elastic, mechanical, magnetoelectronic, and transport properties. The results provide valuable information about the material's enhanced structural organization, complex magnetic and electronic properties, as well as product opportunities for the use of thermoelectric applications (Radja *et al.*, 2022). Mahmood *et al.* (2022b) made an effort to evaluate the impacts of 5d-electrons on both thermoelectric and half-metallic ferromagnetism of $Cs_2Z(Cl/Br)_6$ (where Z stands for Os or Ir) and the results could open up application prospects of spintronics. The research reveals exciting discoveries, demonstrating that 5d-electrons significantly determine HM ferromagnetic properties present in the material. In addition, the study of various thermoelectric properties includes information concerning their suitability in spintronic applications.

Halide-based double perovskites have helped in spintronics and implied potential for spin-dependent devices like magnetic storage devices, spin valves, and spin-orbit devices due to their tunable magnetic and electrical properties. This may be indicative of the continued research investigation in this field area that holds the possible key to revolutionizing the entire information and technology for better data storage device uses. The current study aims to explore comprehensively and more scientifically the physical and mechanical characterizations of A_2MnCl_6 ($A = K, Rb, Cs$) in terms of composition, electronic, mechanical, magnetism, and transport.

2. METHODOLOGY

In this investigation, we used the WIEN2k computational tool based on the DFT-FPLAPW approach (Cai *et al.*, 2017) as our theoretical platform. The aim was to analyze in detail the potential of optimizing the structural parameters, electronic properties, and magnetic parameters of compounds K_2MnCl_6 , Rb_2MnCl_6 , and Cs_2MnCl_6 . For structural optimization, the ground state energy has been calculated for ferromagnetic (FM) and antiferromagnetic (AFM) states using the PBEsol method. In antiferromagnetic configurations, the orientation of electron spins in alternate layers was inverted. Results from our investigation disclosed that the ferromagnetic state revealed high energy release in comparison to antiferromagnetic states. Lattice constant and bulk moduli were determined by applying the Murnaghan equations of state. Recognizing the limitations inherent in the PBEsol method, especially in accurately predicting band gaps, we adopted mBJ potential (Siad *et al.*, 2021a). This particular selection of potential not only enhances computational performance but also addresses shortcomings associated with the commonly utilized HSE06 method within this



domain (Fedorovskiy *et al.*, 2020). The expressions employed for potential calculations are as follows:

$$V_{x,\sigma}^{mBJ}(r) = cV_{x,\sigma}^{BR}(r) + (3c-2)\frac{1}{x}\frac{\sqrt{5}}{12}\frac{\sqrt{2t_{\sigma}(r)}}{\rho_{\sigma}(r)} \quad (1)$$

Here, $V_{x,\sigma}^{BR}(r)$ represents Becke-Roussel potential, $\rho_{\sigma}(r)$ signifies the density of states, and $t_{\sigma}(r)$ shows kinetic energy density, however, c is symbolized as;

$$c = \alpha + \left(\beta \frac{1}{V_{cell}} \int d^3r \frac{|\nabla \rho(r)|}{\rho(r)} \right)^{1/2} \quad (2)$$

In the computational software WIEN2k, we implemented specific coefficients denoted as α and β , with α set to -0.012 and β set to 1.023 bohr^{1/2}. These constants played a crucial role in our computations. To determine the solution of the wave function, we scrutinized the interstitial region and muffin tin. In the muffin tin zone, we applied a spherical harmonics-based solution, whereas for areas external to the core, plane waves approximating the solution were employed. Our computations fully incorporated effects for the core area. Various options were selected for measurements, including the radius of the muffin tin and the cutoff for plane waves,

defined as the product of R_{MT} and K_{max} , which is equal to 8. The angular momentum denoted as ℓ_{max} was set at 10, and the Gaussian factor (G_{max}) was established at 20. Achieving convergence in energy and charge measurements was dependent on the strategic placement of k-points. In our current investigation, we chose to utilize 2000 k-points, observing that the energy of the system remained consistent beyond this threshold. Through a repetitive method, the energy convergence up to a precision of 10⁻² mRy was successfully achieved. In the computation of transport response, we applied semi-classical Boltzmann expressions within the approximate relaxation time of (10⁻¹⁴) s. These calculations were performed by utilizing the Boltz-TraP package (Mahmood *et al.*, 2019).

3. RESULTS

3.1 Structural Properties

In the initial phase of examining structural characteristics of A₂MnCl₆ (A = K, Rb, Cs), we undertook optimization of lattice structure and atomic position. This involved diminishing force acting on individual atoms utilizing WC-GGA approximation (Faizan *et al.*).

Table 1. The computed values of a_0 (Å), B_0 (GPa), and ΔH (eV) calculated for A₂MnCl₆ (A = K, Rb, Cs)

DPs	a_0 (Å)	B_0 (GPa)	ΔH (eV)
K ₂ MnCl ₆	9.61	39.91	-1.64
Exp	9.64 ^a		
Rb ₂ MnCl ₆	9.69	39.29	-1.82
Exp	9.82 ^a		
Cs ₂ MnCl ₆	9.82	38.71	-1.96
Exp.	---		

^a(Moews Jr, 1966)

To determine lattice constant and bulk moduli values, meticulous analysis was conducted by fitting the information obtained from

the volume optimization plot of the Birch Murnaghan expression, as outlined by Nishio-Hamane *et al.* (2010).



$$E(V) = E_0 \frac{B_0}{B'(B'-1)} \left[V \left(\frac{V_0}{V} \right)^{B'} \right] + \frac{B_0}{B} (V - V_0) \quad (3)$$

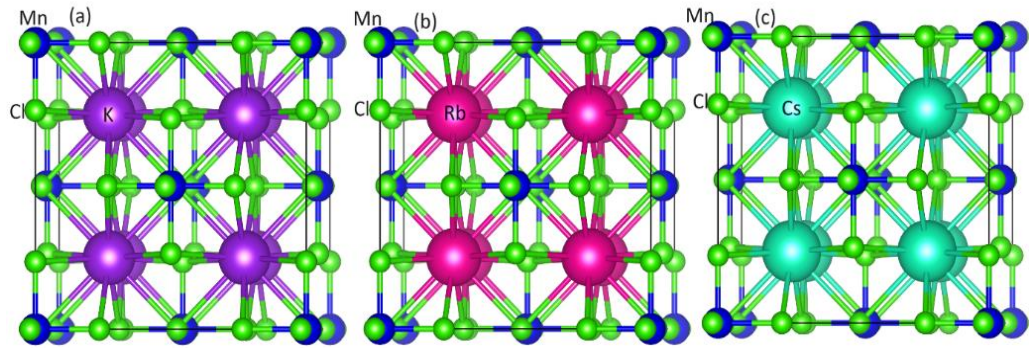


Figure 1. Crystal structure of double perovskites (a) K₂MnCl₆, (b) Rb₂MnCl₆ and (c) (a) Cs₂MnCl₆. Purple/Pink/sky blue, blue, and green spheres represent K/Rb/Cs, Mn, and Cl atoms, respectively

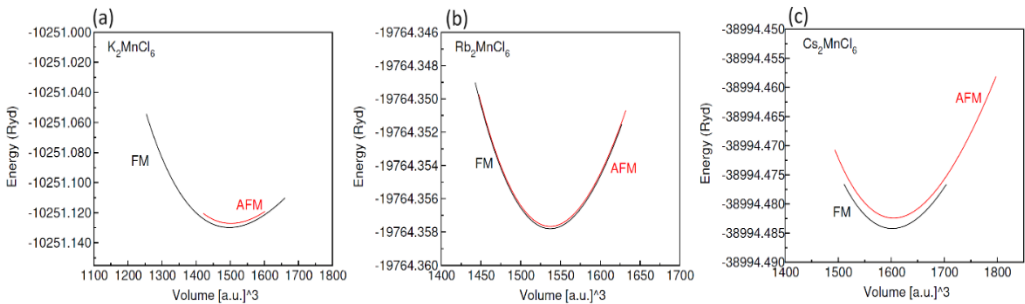


Figure 2. Energy-volume optimization of (a) K₂MnCl₆, (b) Rb₂MnCl₆ and (c) (a) Cs₂MnCl₆ in ferromagnetic (FM) and anti-ferromagnetic (AFM) phases

3.2 Electronic Properties

In the investigations of the electronic response in the A₂MnCl₆ (A = K, Rb, Cs) compound, based on the calculated geometry, we

performed computations for spin-polarized electronic band structure and density of states. The TB-mBJ was used to gather more information on the electronic nature of these compounds in detail (Mahmood *et al.*, 2019).

Table 2. The bandgap value in spin up channel, total and the local magnetic moments

DPs	↑E _g (eV)	Total (μ _B)	Int. (μ _B)	K/Rb/Cs (μ _B)	Mn (μ _B)	Cl(μ _B)
K ₂ MnCl ₆	2.20	3.0002	0.1015	0.0005	2.7281	0.0282
Rb ₂ MnCl ₆	2.25	3.0002	0.0922	0.0009	2.7777	0.0214
Cs ₂ MnCl ₆	2.30	3.0001	0.0736	0.0024	2.8222	0.0165

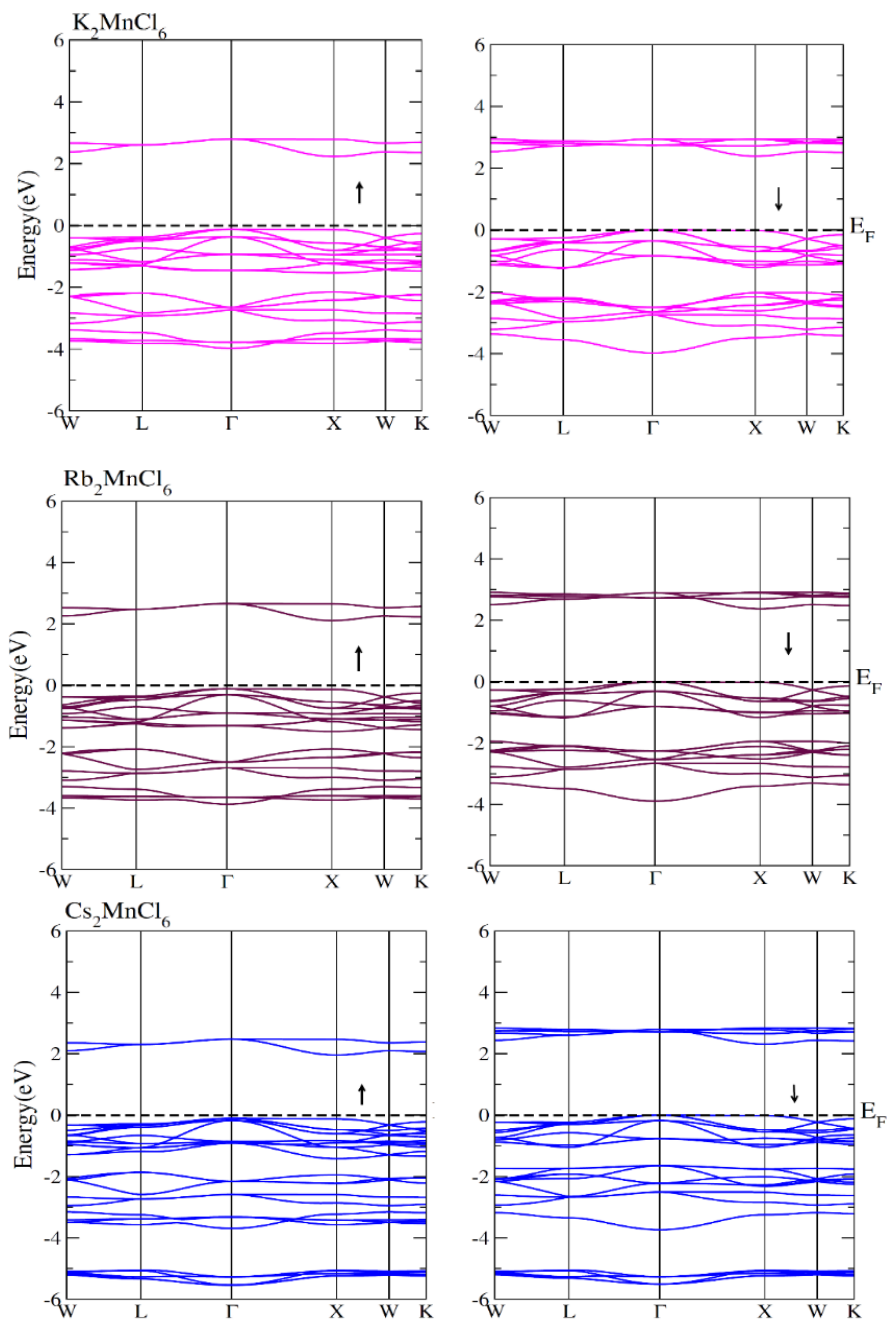


Figure 3. Computed BS for A_2MnCl_6 ($A = K, Rb, Cs$) halides for majority spin ($\uparrow$) and minority spin ($\downarrow$) channels



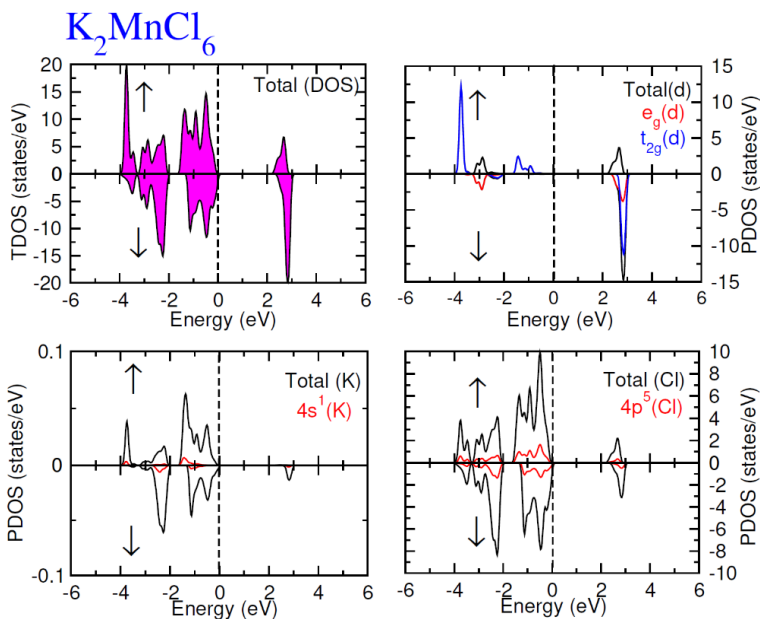


Figure 4. Computed total and partial DOS of K_2MnCl_6 in up ($\uparrow$) and down spin ($\downarrow$) channels

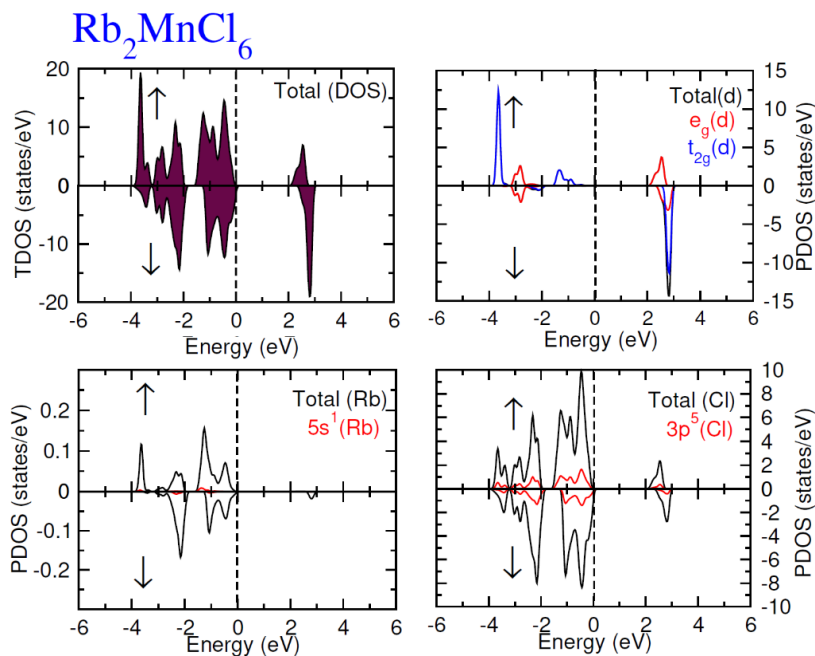


Figure 5. Computed total and partial DOS of Rb_2MnCl_6 in up ($\uparrow$) and down spin ($\downarrow$) channels



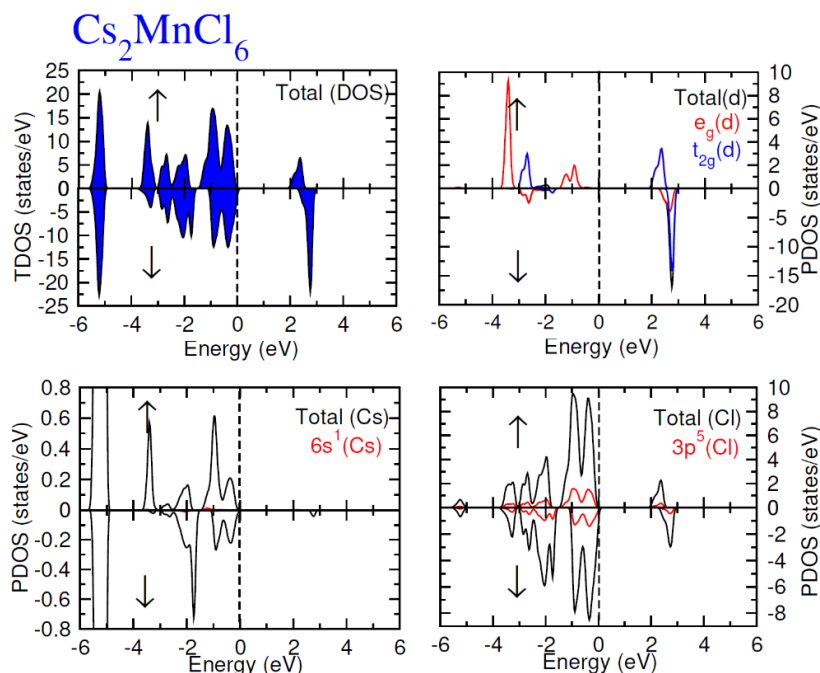


Figure 6. Computed total and partial DOS of Cs_2MnCl_6 in up ($\uparrow$) and down spin ($\downarrow$) channels

To enhance our understanding of electronic properties within the A_2MnCl_6 ($\text{A} = \text{K}, \text{Rb}, \text{Cs}$) framework, a comprehensive analysis of the total (TDOS) and partial (PDOS) density of states was conducted. Fig. (4-6) provides detailed insights into DOS calculated for all compositions.

3.3 Magnetic Properties

The interaction between electron spins is facilitated by the coupling of various states near band edges. Understanding this exchange process involves the computation of crystal field energy (ΔE_{cry}), $\Delta(\text{pd})$, and $\Delta(\text{d})$ exchange energies. The direct $\Delta(\text{d})$ is computed by the disparity in energy levels of the d state in spin- $(\uparrow)$ and spin- $(\downarrow)$ mode. On the other hand, indirect $\Delta(\text{pd})$ is calculated using contrasting electron energies in p and d orbitals within the same spin down ($\downarrow$) channel (Mahmood *et al.*, 2016b; Li *et al.*, 2019; Flemban *et al.*, 2022).

An alternative method for $\Delta(\text{pd})$ computation encompasses inspecting the location of the s state of K/Rb/Cs in the spin-down channel. This approach provides a straightforward means to exchange interaction energy calculation. A force from the crystal field, driving it to ground energies, influences the Mn t_{2g} state, also known as the bonding phase. Contrarily, the e_g state of Mn, referred to as an antibonding state, experiences an elevation in energy levels due to the crystal field. The computation of crystal field energy involves determining the energy difference between t_{2g} and e_g states. For a prevailing ferromagnetic nature, ΔE_{cry} should be less than $\Delta(\text{d})$. The exchange interface is influenced by the difference $\Delta(\text{d}) - \Delta E_{\text{cry}}$, thereby potentially altering the magnetic characteristics of various compounds. Another pivotal factor is $\Delta(\text{pd})$, arising from the interaction between the d states of Mn and the 4s/5s/6s states of K/Rb/Cs (Mahmood *et al.*, 2020).

Table 3. The computed values of $\Delta E_{\text{crystal}}$, $\Delta_x(d)$, $\Delta_x(pd)$ and $N_o\alpha$ and $N_o\beta$ in ground state of $A_2\text{MnCl}_6$ ($A = \text{K, Rb, Cs}$) halides

DPs	$(\Delta E_{\text{crystal}})$	$\Delta_x(d)$	$\Delta_x(pd)$	$N_o\alpha$	$N_o\beta$
K_2MnCl_6	3.8	6.6	-0.3	-0.24	-0.21
Rb_2MnCl_6	3.4	6.2	-0.2	-0.28	-0.14
Cs_2MnCl_6	3.0	6.0	-0.1	-0.34	-0.08

3.4 Thermoelectric Properties

The evaluation of thermoelectric performance relies on ZT , denoted by the expression $ZT = S^2\sigma k/T$. Achieving optimal ZT values necessitates low thermal conductivity (κ_e/τ) coupled with high Seebeck coefficient (S) and electrical conductivity (σ/τ) (Ashiq *et al.*, 2023). The computed transport response is visually represented in Fig. 7 (a-f). The thermal conductivity (κ_e/τ) comprises contributions

from both electrons (κ_e) and phonons (κ_p). Because Boltzmann's theory confines, our focus is solely on κ_e . To determine phonon contributions, κ_p is independently computed using the ShengBTE code. BoltzTraP code calculations address Fermi integration, presenting thermoelectric characteristics concerning carrier doping and temperature. Additionally, κ_e and σ are normalized by 10^{-14} s relaxation time, representing the average duration of collisions in the atomic system.

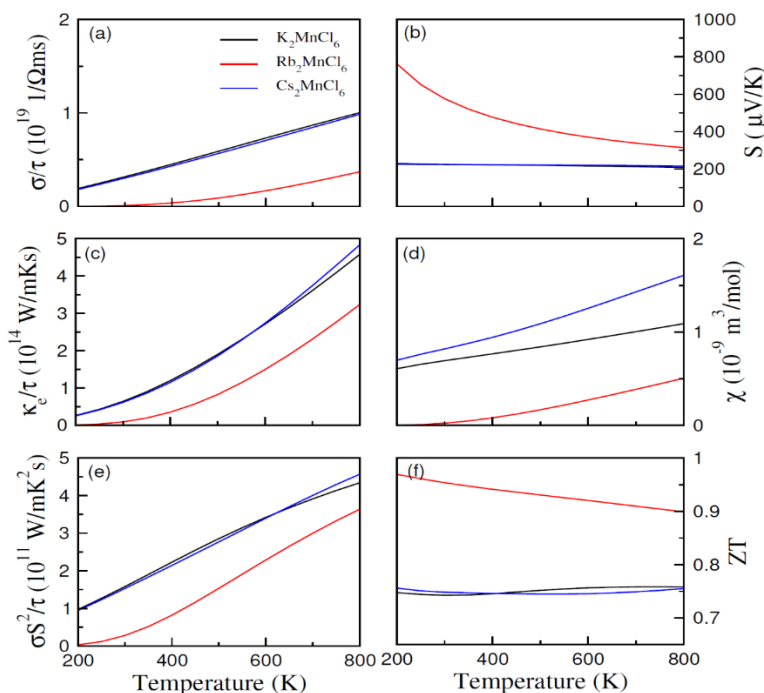


Figure 7. The computed (a) electrical conductivity (σ/τ), (b) thermal conductivity (κ_e/τ), (c) Seebeck coefficients (S), (d) Specific heat capacity (C_v), (e) power factor, and (f) figure of merit against temperature for DPs $A_2\text{MnCl}_6$ ($A = \text{K, Rb, Cs}$) halides



The Seebeck coefficient (S) plays a pivotal role in gauging the potential variation among different metal contacts, vital for optimizing the device's thermoelectric efficiency (Wang *et al.*, 2019; Mahmood *et al.*, 2021). The susceptibility of any material is indicative of its magnetic response. In the case of semiconductors, the typical value is on the order of 10^{-9} . The power factor (PF), represented as $\sigma S^2/\tau$, offers insights into the thermoelectric capabilities of materials without accounting for thermal conductivity (κ_e/τ). Moreover, the ZT is computed to assess the thermoelectric response of the investigated composition.

3.5 Elastic Properties

The investigation of elastic properties of $A_2\text{MnCl}_6$ (A = K, Rb, Cs) involves the

application of tensor examination to nonlinear differential equations utilizing the Chapin approach. The three key elastic constants (C_{11} , C_{12} , and C_{44}), are employed to convey mechanical stability and characteristics associated with cubic symmetry (Noor *et al.*, 2018b). The criteria for Born conditions, supported by stability, are articulated through the expressions $C_{44} > 0$, $C_{11} - C_{12} > 0$, $C_{12} < B_0 < C_{11}$, and $C_{11} + 2C_{12} > 0$, with their computed values detailed in Table 4. Application of stress to any material reveals important elastic constants crucial for validating a crystal structure's mechanical stability (Noor *et al.*, 2018a). Anisotropy is quantified by a relation $A = 2C_{44}/(C_{11} - C_{12})$, a pivotal factor in assessing material characteristics.

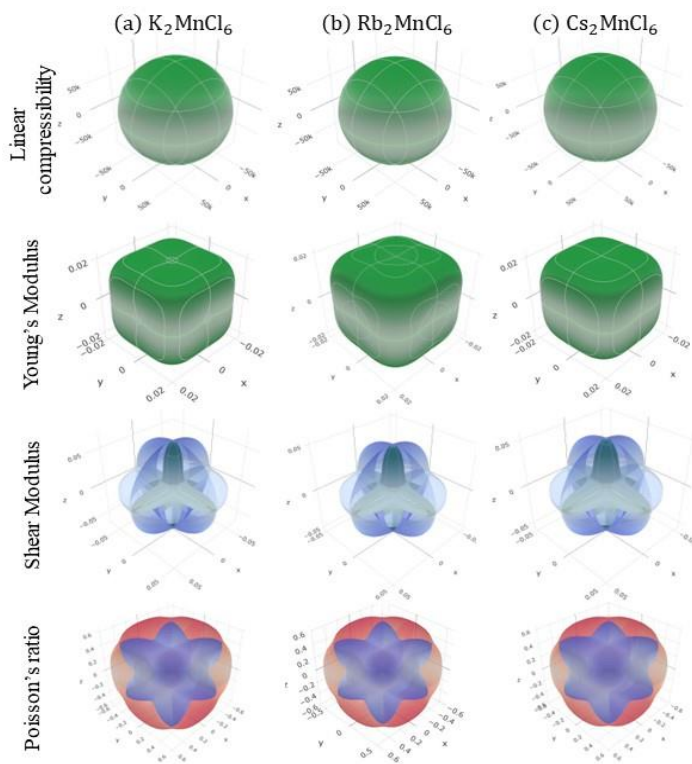


Figure 8. Representation of elastic moduli in three dimensions



Table 4. Elastic constants of A₂MnCl₆ (A= K, Rb, Cs) in GPa

Compounds	Elastic Constant		
	C ₁₁	C ₁₂	C ₄₄
K ₂ MnCl ₆	76.27	21.35	15.04
Rb ₂ MnCl ₆	74.08	20.95	13.30
Cs ₂ MnCl ₆	73.25	19.45	12.15

Table 5. Bulk modulus B(GPa), Shear modulus G(GPa), Young’s modulus E(GPa), Poisson’s ratio (ν) of A₂MnCl₆ (A= K, Rb, Cs) at 0 GPa

Compounds	Bulk modulus	Shear modulus	Young’s modulus	Poisson’s ratio
K ₂ MnCl ₆	40.23	19.07	49.35	0.301
Rb ₂ MnCl ₆	38.65	17.41	45.19	0.304
Cs ₂ MnCl ₆	37.38	16.80	43.94	0.305

Table 6. The maximum and minimum values of elastic moduli and their anisotropy

Parameters	Linear compressibility (β) (TPa ⁻¹)			Young’s Modulus (Y) (GPa)			Shear modulus (G) (GPa)			Poisson’s ratio (ν)		
	β _{min}	β _{max}	A	Y _{min}	Y _{max}	A	G _{min}	G _{max}	A	ν _{min}	ν _{max}	A
K ₂ MnCl ₆	88990	88990	1	0.019	0.028	1.4	0.016	0.06	4.1	-0.8	-0.4	0.5
Rb ₂ MnCl ₆	89860	89860	1	0.019	0.027	1.4	0.015	0.05	3.4	-0.7	-0.3	0.5
Cs ₂ MnCl ₆	87507	87507	1	0.020	0.028	1.3	0.017	0.05	3.1	-0.7	-0.4	0.5

4. DISCUSSION

The resulting optimized structures of the unit cell are depicted in Fig. 1. As we observed, the monovalent cation (K, Rb, Cs) is surrounded by twelve halogen ions, while every tetravalent cation (Mn) exhibits coordination with 6 halogen ions, making octahedron (Amin *et al.*, 2022). The anion (Cl) is coordinated 6-fold. Each compound scrutinized in this report crystallizes in a cubic double perovskite structure having *Fm* $\bar{3}$ *m* (# 225) space group. In this arrangement, the K, Rb, and Cs atoms occupy the Wyckoff position 8c, specifically at coordinates (1/4, 1/4, 1/4), while the MnCl₆ octahedra are centered on manganese (Mn) at the 4a-position with coordinates (0, 0, 0). The

neighboring chlorine (Cl) atoms are located at the 24e position with coordinates (x, 0, 0), where the approximate value of x is around 0.2 for each compound. Our determined structural parameters, encompassing lattice constant (*a*_o), bulk moduli (*B*_o), and enthalpy of formation, are compiled in Table 1.

A brief analysis of the table reveals an apparent increase in lattice constant by changing monovalent cation in sequence *K* → *Rb* → *Cs*. Specifically, it measures 9.61 Å for K₂MnCl₆, 9.69 Å for Rb₂MnCl₆, and 9.82 Å for Cs₂MnCl₆. Moreover, it is noteworthy that the lattice constant for each compound marginally exceeds experimentally calculated data as cited in Table 1 (Moews Jr, 1966), a deviation likely

attributable to utilizing the GGA function, known to somewhat inflate lattice constants. The computation of ground state energy for each composition was carried out through the FP-LAPW method in DFT (Mera *et al.*, 2023).

In Fig. 2(a-c), a plot depicting the volume against energy is presented and calculated using GGA. The analysis reveals that each compound exhibits higher stability in the ferromagnetic (FM) phase in comparison to the antiferromagnetic (AFM) phase (Manzoor *et al.*, 2023). The rationale for this lies in the realization that energy output in the ferromagnetic phase is higher than that which is in the AFM phase. This implies that the considered FM may represent stable ferromagnetic states and have practical use, as indicated in the work (Ali *et al.*, 2021). In addition, the determination of the energy of formation ΔH_f was done to establish the thermodynamic stability of the compounds. The sign of the obtained ΔH_f values indicates the possibility of energy release during the formation of compounds, indicating the thermodynamic possibility of the compositions described. However, a higher ΔH_f has been observed in Cs_2MnCl_6 than in K_2MnCl_6 and Rb_2MnCl_6 , as indicated in Table 1. According to this examination, it can be deduced that the stability of Cs-based formation is comparatively better than that of K and Rb-based composition (Alnujaim *et al.*, 2022).

The calculated band structures for A_2MnCl_6 (K, Rb, Cs) are shown in the Fig. 3. Notably, for K_2MnCl_6 , the valence band (VBM) maxima and conduction band (CBM) minima were positioned such that their energy difference is 2.20 eV, in the 1st Brillouin zone. For Rb_2MnCl_6 valence band maxima at Γ symmetry point and conduction band minimum were located at X position with the bandgap value of 2.25 eV and for Cs_2MnCl_6 , this bandgap is further increased to 2.30 eV in spin up ($\uparrow$) configuration (Siad *et al.*, 2021b). The computations indicated that composition

exhibits a direct band gap and computed values are enlisted in Table 2.

Additionally, we present spin-polarized projected density of states plots for K, Rb, Cs, Mn, and Cl atoms to discern the individual contributions of each atom to TDOS. In Fig. 4, the edge of the VB (approximately at -4 eV) of K_2MnCl_6 is primarily composed of the d -state of Mn, the $4s$ -state of K, and the $4p$ -state of Cl. An overlay across the Fermi level is observed among the de-localized d -state of Mn and the $4p$ -state of Cl. The conduction band is made up of d -states of Mn, $4s$ -states of, and $4p$ -states of Cl. A similar scenario is observed in Rb_2MnCl_6 as presented in Fig. 5. Additionally, a sharp peak in the valence band section is attributed to the d -state of Mn, whereas the $5s$ and $3p$ states of Rb and Cl, respectively. Similarly, the same states of individual atoms are noticed to contribute to the formation of valence and conduction bands for Cs_2MnCl_6 except for the slight movements towards the Fermi level with change in atoms at A-site which is attributed to the change in the strength of spin-orbit coupling of A-site atoms with the Cl atoms (Soulén Jr *et al.*, 1998).

A negative value for the exchange energy $\Delta(\text{pd})$ indicates that the spin-down ($\downarrow$) mode is contributing to the induction of ferromagnetic traits. The split phases at the boundaries of the bands, specifically the CBM (ΔE_c) and VBM (ΔE_v), are identifiable through the exchange constants ($N_o\alpha$ and $N_o\beta$). These coefficients quantify p-d and s-d exchanges and are presented below (Mahmood *et al.*, 2018):

$$N_o\alpha = \frac{\Delta E_c}{x\langle S \rangle}; N_o\beta = \frac{\Delta E_v}{x\langle S \rangle} \quad (4)$$

The negative (-ve) value of $N_o\beta$ directs that the down spin ($\downarrow$) mode promotes ferromagnetism (Zanib *et al.*, 2024). The exchange energy parameter values are detailed in Table 3.

Table 2 presents computed magnetic moments of distinct atoms and net magnetic moments (μ_e). The high T_c and vacancies at the A/Mn site

contribute to magnetic moment magnitude. Long-span ferromagnetism results from contact among local magnetic moment and unpaired electrons in a material, according to the Ruderman–Kittel–Kasuya–Yosida exchange interaction model (Brey *et al.*, 2006). This contact is a critical pointer often mentioned in the literature to comprehend the material's magnetic response. For example, Ishikawa *et al.* investigated SOC in Z₂TaCl₆ (Z = K, Rb, Cs), noting its dependence on the octahedron surrounding halide atoms, $J_{\text{eff}} = 3/2$ of 5d e's, and significant ionic behavior (Ishikawa *et al.*, 2019). In addition, the value of magnetic moment of 0.39, 0.22, and -0.86 μ_B for Mo, W, and Re were observed by Fang *et al.* in exploring the influence of 5d electrons on magnetoresistance and ferromagnetism in Sr₂Fe(Mo/W/Re)O₆. Related to 3d e's, 5d e's exhibit higher unquenched magnetic moments, leading to stronger coupling and boosted magnetic nature (Fang *et al.*, 2001). The integral values of the net μ_e confirm 100% SP (Brey *et al.*, 2006).

Fig. 7 (a) depicts σ/τ values of 0.24/0.02/0.22 $\times 10^{19}$ (1/ Ωm) at 200 K, increasing to 1.02/0.82/0.97 $\times 10^{19}$ (1/ Ωm) for K₂MnCl₆, Rb₂MnCl₆, and Cs₂MnCl₆, respectively with rising temperature up to 800 K. The computed Seebeck coefficient, plotted against temperature (T), is illustrated in Fig. 7 (b). The temperature-dependent trends of S expose a decreasing value from 770 at 200 K to 310 $\mu\text{V/K}$ at 800 K for Rb₂MnCl₆, and a constant value is observed for K₂MnCl₆ and Cs₂MnCl₆. This decline in Seebeck co-efficient may be attributed to the carrier's thermal excitation with increasing temperature. The κ_e/τ trends, illustrated in Fig. 7 (c), mirror those of σ/τ , although the values are notably low, emphasizing the significance of the studied composition for thermoelectric applications. The temperature-dependent behavior of κ_e/τ reveals an increase from 0.38/0.02/0.41 W/mK to 4.51/3.22/4.86 W/mK for K₂MnCl₆,

Rb₂MnCl₆, and Cs₂MnCl₆, respectively corresponding to the rise in thermally excited carriers with increasing temperature. Consequently, the κ/σ ratio, standing at 10^{-5} , aligns with the Weidman-Franz law, indicating an exceedingly small ratio (Albalawi *et al.*, 2022). At 200 K, K₂MnCl₆, Rb₂MnCl₆, and Cs₂MnCl₆ exhibit a susceptibility of 0.6×10^{-9} , 0.02×10^{-9} , and 0.8×10^{-9} ($\text{m}^3\text{mol}^{-1}$), respectively, which escalates to 1.1×10^{-9} for K₂MnCl₆, 0.5×10^{-9} for Rb₂MnCl₆, and 1.6×10^{-9} ($\text{m}^3\text{mol}^{-1}$) for Cs₂MnCl₆ at 800 K (Sajjad *et al.*, 2019). This increase could be attributed to the thermal effects on the spin movement of electrons, as depicted in Fig. 7 (d). Graphical representations in Fig. 7 (e) showcase the reported power factor against temperature. The value of power factor is recorded as 1.05×10^{11} for K₂MnCl₆, 0.04×10^{11} for Rb₂MnCl₆, and 1.08×10^{11} W/mK² for Cs₂MnCl₆ at 200 K which is increasing up to 4.3×10^{11} for K₂MnCl₆, 3.6×10^{11} for Rb₂MnCl₆, and 4.5×10^{11} W/mK² for Cs₂MnCl₆ at 800 K (Sajjad *et al.*, 2019). The ZT values are plotted in Fig. 7 (f) for temperature (K). Notably, ZT values at 200 K are 0.75/0.97/0.76, decreasing with rising temperature to 0.74/0.9/0.75 at 800 K for K₂MnCl₆, Rb₂MnCl₆, and Cs₂MnCl₆, respectively (Campi *et al.*, 2017).

The distinction between ductility and brittleness is discernible through Poisson's (ν) ratio, where the value is greater than 0.26 and the Pugh (B/G) ratio is greater than 1.75 demarcates ductile behavior (Cai *et al.*, 2017). Upon comparing critical values, all materials are ductile which reinforces the potential of the studied double perovskites for device fabrication. The elastic character of the composition is comprehensively presented in Table 4. The scrutiny of nominal actualities in solids underscores the significance of elastic anisotropy (Mahmood *et al.*, 2016a). Features of elastic anisotropy assume importance in enhancing the mechanical strength of the material (Feng, 2014).



Anisotropy calculations, including shear modulus (G), Poisson's (ν) ratio, linear compressibility (β), and Young's modulus (Y), have been executed for A_2MnCl_6 ($A = K, Rb, Cs$), as depicted in Fig. 8 and values are tabularized in Table 5. The asymmetrical nature of Young's modulus (Y), Poisson's (ν) ratio, shear modulus (G), and linear compressibility (β) in 3D is evident from the distorted shape, deviating from a circular or spherical form. The anisotropic nature of these parameters is further confirmed by the recorded minimum and maximum values in Table 6, underscoring the heightened anisotropy of K_2MnCl_6 (Kaderoglu *et al.*, 2017).

5. CONCLUSION

In the current report, we have explored the electronic, magnetic, structural, and thermoelectric response of A_2MnCl_6 ($A = K, Rb, Cs$) using density functional theory based on the WIEN2K package. Firstly, we scrutinize the structure in both AFM and FM states, conclusively establishing the higher stability of the FM state. The ferromagnetic phase of A_2MnCl_6 ($A = K, Rb, Cs$) exhibits formation energies of -1.64, -1.82, and -1.96 eV, affirming their Stable thermodynamic state. An increase in the value of lattice constant was witnessed from 9.61 to 9.69 and 9.82 Å when K has been replaced with Rb and Cs respectively. The value of bulk modulus was reduced from 39.91 to 39.29 and 38.71 GPa. The spin-polarized DOS confirms 100% spin polarization, while magnetic moment with high Curie temperature suggests fundamental hybridization. The hybridization of exchange energies and outermost shell electrons indicates that ferromagnetic behavior is driven by electronic spin in contrast to clustering. The significant effect of quantum confinement contributes to negative exchange co-efficient and $\Delta(pd)$ exchange energy values. Furthermore, the calculation of electrical ($0.2-1.02 \times 10^{19}/\Omega ms$) and thermal conductivity ($0-$

4.8×10^{14} W/mKs), Seebeck coefficient (>200 $\mu V/K$), power factor ($0-4.5 \times 10^{11}$ W/mK²s), magnetic susceptibility ($0-1.6 \times 10^{-9}$ m³/mol), and figure of merit (up to 0.97) highlighted the potential of these compositions in the field of thermoelectrics.

Acknowledgment

The authors would like to acknowledge Researcher's Supporting Project Number (RSP2024R511), King Saud University, Riyadh, Saudi Arabia.

Conflict of Interest

The authors declare no conflict of interest.

Data Availability Statement

The data included in this paper can be provided on reasonable request.

REFERENCES

- Abdullah, D. and Gupta, D. C. 2023. Exploring the half-metallic ferromagnetism, dynamical and mechanical stability, optoelectronic and thermoelectric properties of K_2NaMI_6 ($M = Mn, Co, Ni$) for spintronic applications. *Scientific Reports*, 13:12795.
- Albalawi, H., Nazir, G., Younas, M., Al-Qaisi, S., Ashiq, M., Alzahrani, J., Sornail, H., Morsi, M. and Ghrib, T. 2022. Study of lead-free vacancy ordered double perovskites Cs_2TeX_6 ($X = Cl, Br, I$) for solar cells, and renewable energy. *Physica Scripta*, 97:095801.
- Ali, M. H., Islam, M. J., Kumer, A., Hossain, M. S., Chakma, U., Howlader, D., Islam, M. T. and Hossain, T. 2021. Investigation of structural, electronic and optical properties of $Na_2InAgCl_6$, $K_2InAgCl_6$, and $Rb_2InAgCl_6$ lead-free halide double perovskites regarding with $Cs_2InAgCl_6$ perovskites cell and a comparative study by dft functionals. *Materials Research*, 24:e20210086.



- Alnujaim, S., Bouhemadou, A., Chegaar, M., Guechi, A., Bin-Omran, S., Khenata, R., Al-Douri, Y., Yang, W. and Lu, H. 2022. Density functional theory screening of some fundamental physical properties of $Cs_2InSbCl_6$ and $Cs_2InBiCl_6$ double perovskites. *The European Physical Journal B*, 95:114.
- Amin, M. A., Nazir, G., Mahmood, Q., Alzahrani, J., Kattan, N. A., Mera, A., Mirza, H., Mezni, A., Refat, M. S. and Gobouri, A. A. 2022. Study of double perovskites X_2InSbO_6 ($X = Sr, Ba$) for renewable energy; alternative of organic-inorganic perovskites. *Journal of Materials Research and Technology*, 18:4403-4412.
- Ashiq, M., Mahmood, Q., Zelai, T., Hakami, O., Kattan, N. A., Albalawi, H., Aljameel, A., Bouzgarrou, S., Ghrib, T. and Hussein, K. I. 2023. The narrow band gap double perovskites $X_2CuInCl_6$ ($X = K, Rb, Cs$) for optoelectronics, and thermoelectric applications. *Materials Science and Engineering: B*, 296:116690.
- Brey, L., Calderón, M., Das Sarma, S. and Guinea, F. 2006. Mean-field theory for double perovskites: Coupling between itinerant electron spins and localized spins. *Physical Review B—Condensed Matter and Materials Physics*, 74:094429.
- Cai, Y., Xie, W., Ding, H., Chen, Y., Thirumal, K., Wong, L. H., Mathews, N., Mhaisalkar, S. G., Sherburne, M. and Asta, M. 2017. Computational study of halide perovskite-derived A_2BX_6 inorganic compounds: chemical trends in electronic structure and structural stability. *Chemistry of Materials*, 29:7740-7749.
- Campi, D., Paulatto, L., Fugallo, G., Mauri, F. and Bernasconi, M. 2017. First-principles calculation of lattice thermal conductivity in crystalline phase change materials: $GeTe$, Sb_2Te_3 , and $Ge_2Sb_2Te_5$. *Physical Review B*, 95:024311.
- Dar, S. A., Srivastava, V. and Sakalle, U. K. 2019. Structural, elastic, mechanical, electronic, magnetic, thermoelectric and thermodynamic investigation of half metallic double perovskite oxide Sr_2MnTaO_6 . *Journal of magnetism and magnetic materials*, 484:298-306.
- Dar, S. A. and Want, B. 2023. Predicting and understanding the structural stability, origin of half-metallic magnetic nature, and study of opto-electronic properties of Cs_2KXCl_6 : $X = Ti$ and V double perovskites. *Journal of Physics and Chemistry of Solids*, 174:111135.
- Faizan, M., Khan, S. H., Murtaza, G., Khan, A. and Laref, A. Computational Predictions of the Electronic and Magnetic Properties of Alkali Metal Chlorides A_2MCl_6 ($A =$ Alkali Metal, $M = Mn, Mo$): A Density Functional Theory Study.
- Fang, Z., Terakura, K. and Kanamori, J. 2001. Strong ferromagnetism and weak antiferromagnetism in double perovskites: Sr_2FeMO_6 ($M = Mo, W$, and Re). *Physical Review B*, 63:180407.
- Fedorovskiy, A. E., Drigo, N. A. and Nazeeruddin, M. K. 2020. The role of Goldschmidt's tolerance factor in the formation of A_2BX_6 double halide perovskites and its optimal range. *Small Methods*, 4:1900426.
- Feng, J. 2014. Mechanical properties of hybrid organic-inorganic $CH_3NH_3BX_3$ ($B = Sn, Pb$; $X = Br, I$) perovskites for solar cell absorbers. *Appl Materials*, 2.
- Flemban, T. H., Zelai, T., Mahmood, Q., Devi, A. A. S., Sajjad, M., Alhossainy, M., Somaily, H., Mera, A., Alharthi, S. and Amin, M. A. 2022. Half-metallic ferromagnetism and thermoelectric



- properties of double perovskites $\text{Rb}_2\text{Z}(\text{Cl/Br})_6$ ($\text{Z} = \text{Ta}, \text{W}, \text{Re}$). *Journal of Alloys and Compounds*, 894:162313.
- Ishikawa, H., Takayama, T., Kremer, R. K., Nuss, J., Dinnebier, R., Kitagawa, K., Ishii, K. and Takagi, H. 2019. Ordering of hidden multipoles in spin-orbit entangled 5 d 1 Ta chlorides. *Physical Review B*, 100:045142.
- Kaderoglu, C., Surucu, G. and Erkisi, A. 2017. The investigation of electronic, elastic and vibrational properties of an interlanthanide perovskite: PrYbO_3 . *Journal of Electronic Materials*, 46:5827-5836.
- Khandy, S. A. and Gupta, D. C. 2021. Insight view of double perovskites Ba_2XNbO_6 ($\text{X} = \text{Ho}, \text{Yb}$) for spintronics and thermoelectric applications. *International Journal of Energy Research*, 45:13338-13354.
- Lamrani, A. F., Ouchri, M., Benyoussef, A., Belaiche, M. and Loulidi, M. 2013. Half-metallic antiferromagnetic behavior of double perovskite $\text{Sr}_2\text{OsMoO}_6$: First principle calculations. *Journal of magnetism and magnetic materials*, 345:195-200.
- Leng, K., Tang, Q., Wei, Y., Yang, L., Xie, Y., Wu, Z. and Zhu, X. 2020. Recent advances in Re-based double perovskites: Synthesis, structural characterization, physical properties, advanced applications, and theoretical studies. *AIP Advances*, 10.
- Li, Y.-F., Zhang, K.-C. and Liu, Y. 2019. Spin-orbital coupling and magnetic properties of Ir-based double perovskites with different 5d ($n = 3, 4, 5$) states. *Physics Letters A*, 383:558-565.
- Mahmood, Q., Alay-e-Abbas, S., Hassan, M. and Noor, N. 2016a. First-principles evaluation of Co-doped ZnS and ZnSe ferromagnetic semiconductors. *Journal of Alloys and Compounds*, 688:899-907.
- Mahmood, Q., Alhossainy, M., Rashid, M., Flemban, T. H., Althib, H., Alshahrani, T., Rashid, M. and Laref, A. 2021. First-principles study of lead-free double perovskites Rb_2TeX_6 ($\text{X} = \text{Cl}, \text{Br}, \text{and I}$) for solar cells and renewable energy. *Materials Science and Engineering: B*, 266:115064.
- Mahmood, Q., Ali, S., Hassan, M. and Laref, A. 2018. First principles study of ferromagnetism, optical and thermoelectric behaviours of AVO_3 ($\text{A} = \text{Ca}, \text{Sr}, \text{Ba}$) perovskites. *Materials Chemistry and Physics*, 211:428-437.
- Mahmood, Q., Alshahrani, T., Ul Haq, B., Gulfam, Q.-u.-A., Tahir, Y., Kattan, N. A., Fatima, M. and Laref, A. 2020. Role of 5d orbital of Re in ferromagnetism and thermoelectric characteristics of $\text{Cs}_2\text{ReCl/Br}_6$ double-perovskites: a density functional theory study. *The European Physical Journal Plus*, 135:1-13.
- Mahmood, Q., Hassan, M. and Noor, N. 2016b. Systematic study of room-temperature ferromagnetism and the optical response of $\text{Zn}_{1-x}\text{TM}_x\text{S/Se}$ ($\text{TM} = \text{Mn}, \text{Fe}, \text{Co}, \text{Ni}$) ferromagnets: first-principle approach. *Journal of Physics: Condensed Matter*, 28:506001.
- Mahmood, Q., Nazir, G., Bouzgarrou, S., Rashid, M., Algrafy, E., Alharthi, S., Amin, M. A., Rehman, A., Mera, A. and Hegazy, H. 2022a. Room temperature half metallic ferromagnetism due to Os/Ir (5d) in double perovskites. *Journal of Alloys and Compounds*, 896:163130.
- Mahmood, Q., Nazir, G., Rahim, A., Alzahrani, J., Aljameel, A., Murtaza, G., Aldayyat, A., Albalawi, H., Mera, A. and Haq, B. U. 2022b. Impact of 5d electrons



- on half metallic ferromagnetism, and thermoelectric properties of Cs_2Z (Cl/Br) 6 (Z= Os, Ir) for spintronic applications. *Materials Chemistry and Physics*, 288:126414.
- Mahmood, Q., Rashid, M., Hassan, M., Yaseen, M., Laref, A. and Haq, B. U. 2019. Engineering of the band gap and optical properties of In_xGa_{1-x} (As/Sb) via across composition alloying for solar cell applications using density functional theory-based approaches. *Physica Scripta*, 94:105812.
- Manzoor, M., Iqbal, M. W., Noor, N. A., Ullah, H., Sharma, R. and Alarfaji, S. S. 2023. Exploring the structural, electronic, optical, and thermoelectric properties of potassium-based double perovskites K_2AgX_6 (X= Sb, Bi) compounds: A DFT study. *Materials Science and Engineering: B*, 287:116122.
- Mera, A., Nazir, G., Mahmood, Q., Kattan, N. A., Alshahrani, T., Rehman, A., Sultana, H., Amin, M. A. and Ali, H. E. 2023. The bandgap engineering of double perovskites Cs_2CuSbX_6 (X= Cl, Br, I) for solar cell and thermoelectric applications. *Inorganic Chemistry Communications*, 148:110303.
- Mir, S. A. and Gupta, D. C. 2020. New ferromagnetic half-metallic perovskites for spintronic applications: $BaMO_3$ (M= Mg and Ca). *RSC advances*, 10:36241-36252.
- Moews Jr, P. 1966. The crystal structure, visible, and ultraviolet spectra of potassium hexachloromanganate (IV). *Inorganic Chemistry*, 5:5-8.
- Mustafa, G. M., Hassan, M., Aloufi, N. M., Saba, S., Al-Qaisi, S., Mahmood, Q., Albalawi, H., Bouzgarrou, S., Smaili, H. and Mera, A. 2022. Half metallic ferroamgnetism, and transport properties of vacancy ordered double perovskites Rb_2 (Os/Ir) X_6 (X= Cl, Br) for spintronic applications. *Ceramics International*, 48:23460-23467.
- Nishio-Hamane, D., Shimizu, A., Nakahira, R., Niwa, K., Sano-Furukawa, A., Okada, T., Yagi, T. and Kikegawa, T. 2010. The stability and equation of state for the cotunnite phase of TiO_2 up to 70 GPa. *Physics and Chemistry of Minerals*, 37:129-136.
- Noor, N., Hassan, M., Rashid, M., Alay-e-Abbas, S. and Laref, A. 2018a. Systematic study of elastic, electronic, optical and thermoelectric properties of cubic $BiBO_3$ and $BiAlO_3$ compounds at different pressure by using ab-initio calculations. *Materials Research Bulletin*, 97:436-443.
- Noor, N., Mahmood, Q., Rashid, M., Haq, B. U., Laref, A. and Ahmad, S. 2018b. Ab-initio study of thermodynamic stability, thermoelectric and optical properties of perovskites $ATiO_3$ (A= Pb, Sn). *Journal of Solid State Chemistry*, 263:115-122.
- Radja, K., Farah, B. L., Ibrahim, A., Lamia, D., Fatima, I., Nabil, B., Mohamed, A., Al-Douri, Y. and Abd El-Rehim, A. 2022. Investigation of structural, magneto-electronic, elastic, mechanical and thermoelectric properties of novel lead-free halide double perovskite $Cs_2AgFeCl_6$: First-principles calcuations. *Journal of Physics and Chemistry of Solids*, 167:110795.
- Ramawat, S., Kukreti, S., Kale, A. J., Dutt, R., Chakrabarti, A. and Dixit, A. 2023. Cs_2KMnCl_6 : A possible half-metallic double perovskite for spintronics. *Journal of Applied Physics*, 133.
- Sajjad, M., Singh, N., Sattar, S., De Wolf, S. and Schwingenschlöggl, U. 2019. Ultralow



- lattice thermal conductivity and thermoelectric properties of monolayer Ti_2O . *ACS Applied Energy Materials*, 2:3004-3008.
- Siad, A. B., Baira, M., Dahou, F. Z., Bettir, K. and Monir, M. E. A. 2021a. Insight into structural, elastic, optoelectronic, magnetic, and thermoelectric properties of the double perovskite compound $\text{Pb}_2\text{FeTaO}_6$: First principle study. *Journal of Solid State Chemistry*, 302:122362.
- Siad, A. B., Baira, M. and Siad, M. 2021b. Structural, mechanical, optoelectronic and thermoelectric properties of double perovskite compounds Cs_2TeX_6 ($\text{X} = \text{Br}, \text{I}$) for energy storage applications: first principles investigations. *Journal of Physics and Chemistry of Solids*, 152:109955.
- Souidi, A., Bentata, S., Benstaali, W., Bouadjemi, B., Abbad, A. and Lantri, T. 2016. First principle study of spintronic properties for double perovskites Ba_2XMoO_6 with $\text{X} = \text{V}, \text{Cr}$ and Mn . *Materials Science in Semiconductor Processing*, 43:196-208.
- Soulen Jr, R., Byers, J., Osofsky, M., Nadgorny, B., Ambrose, T., Cheng, S., Broussard, P. R., Tanaka, C., Nowak, J. and Moodera, J. 1998. Measuring the spin polarization of a metal with a superconducting point contact. *Science*, 282:85-88.
- Tang, Q. and Zhu, X. 2022. Half-metallic double perovskite oxides: recent developments and future perspectives. *Journal of Materials Chemistry C*, 10:15301-15338.
- Wang, H.-C., Pistor, P., Marques, M. A. and Botti, S. 2019. Double perovskites as p-type conducting transparent semiconductors: a high-throughput search. *Journal of Materials Chemistry A*, 7:14705-14711.
- Zanib, M., Mustafa, G. M., Iqbal, M. W., Younas, B., Mahmood, A. and Iqbal, M. 2024. Half metallic ferromagnetism in Ba_2XIrO_6 ($\text{X} = \text{Y}, \text{La}, \text{Sc}$) double perovskites for energy storage applications. *Materials Science in Semiconductor Processing*, 169:107890.

