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Combined Experimental And First-Principles Study Of Structural, Thermoelectric, And Spintronic Properties Of Perovskite Oxides And Halide Perovskite ($MAPbI_3$)

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ABSTRACT

Perovskite materials have become attractive options for next-generation thermoelectric and spintronic devices due to their adaptable crystal structure and adjustable electrical, magnetic, and thermal characteristics. Using computational modeling and experimental data, this work investigates the structural, thermoelectric, and spintronic properties of typical perovskite oxides ($SrTiO_3$, $CaMnO_3$, and $BaSnO_3$) and halide perovskites ($MAPbI_3$). Thermoelectric experiments showed that rare-earth doping in $CaMnO_3$ increases electrical conductivity and decreases lattice thermal conductivity by phonon scattering, whereas Nb-doped $SrTiO_3$ obtains $ZT \approx 0.3–0.4$ at high temperatures. $BaSnO_3$ showed promise for transparent high-temperature devices with its reasonable power factors and promising stability. On the spintronic front, Sr_2FeMoO_6 maintained high Curie temperature and tunneling magnetoresistance, $La_{1-x}Sr_xMnO_3$ films displayed enormous magnetoresistance with about 100% spin polarization, and $MAPbI_3$ showed Rashba spin splitting, allowing spin manipulation by thermal and electric methods. Perovskite heterostructures were also shown to exhibit coupled thermoelectric–spintronic phenomena, such as the spin Seebeck and anomalous Nernst effects, underscoring its promise in spin caloritronics. These discoveries position perovskites as multipurpose materials that can combine spin-based information processing, waste-heat recovery, and energy harvesting, opening the door for low-power and sustainable electronic devices.

Introduction

Perovskite materials have garnered significant interest for use in thermoelectric and spintronic devices due to their distinctive crystal structure and compositional versatility. They are attractive prospects for next-generation electronics because of their multifunctional applications made possible by their adjustable electrical, magnetic, and thermal characteristics. Perovskites are unique in the field of thermoelectrics because of their effective conversion of waste heat into electrical power, which depends on a balance between poor thermal conductivity, a high electrical conductivity, and a substantial Seebeck coefficient. Interestingly, density functional theory (DFT) studies have demonstrated that double perovskites such as Sr2PrSnO6 have half-metallic behavior, stable ferromagnetic states, and remarkable thermoelectric performance at high temperatures, indicating their potential for solid-state devices and energy harvesting. The capacity of some perovskite oxides to sustain ferromagnetism and spin-polarized currents at the same time is crucial in spintronics. Due to their electronic structure and magnetic interactions, materials like Sr2PrSnO6 exhibit half-metallic ferromagnetism with strong spin polarization at the Fermi level, which is crucial for spin-based information processing. Their mechanical ductility and other characteristics make them more appealing for real-world spintronic applications. Innovative spin-caloritronic devices that take use of both charge and spin transport under temperature gradients are made possible by the convergence of thermoelectric and spintronic functions in perovskite materials(Apu et al., 2025).

Overview of perovskite materials and their structure

The characteristic crystal structure of perovskite materials, which has the general formula ABX_3, defines them. In this structure, "X" is an anion, usually oxygen or a halide, while "A" and "B" are cations of various sizes and charges. Six "X" anions form an octahedron, with the smaller "B" cation at its core. A three-dimensional corner-sharing lattice structure is formed by these BX_6 octahedra. The cuboctahedral sites formed in the gaps between these octahedra are occupied by the bigger "A" cations, which are typically coordinated by 12 anions (Dang et al., 2021). Cubic (space group Pm3m) perovskite crystal structures with extremely symmetric lattices are optimal. However, because of things like temperature or ionic size mismatch, many perovskites show distortions that result in lower symmetry structures like orthorhombic, rhombohedral, or tetragonal. The primary cause of these distortions, which alter the material's physical characteristics, is the tilting or rotation of the BX_6 octahedra. Perovskites' exceptional structural adaptability allows for a broad range of cation replacements at both the A and B sites, which has a substantial impact on their optical, magnetic, and electrical properties(Levy, 2005).

Objective of the study

- To investigate the structural, electrical, thermal, and magnetic properties of representative perovskite oxides and halide perovskites (such as $SrTiO_3$, $CaMnO_3$, $BaSnO_3$, and $MAPbI_3$) through experimental and computational approaches.
- To evaluate and optimize the thermoelectric and spintronic performance of perovskite materials by employing strategies such as doping, band engineering, nanostructuring, and thin-film growth.
- To explore the coupled thermoelectric–spintronic effects (spin caloritronics) in perovskite heterostructures and assess their potential applications in energy harvesting, waste-heat recovery, and spin-based information processing.

Fundamentals of Perovskite Materials

The naturally occurring mineral $CaTiO_3$, which was named for Russian mineralogist Lev Perovski and initially discovered by Gustav Rose in 1839, is the source of the term for perovskite materials. Their standard chemical formula is ABX_3, in which X is an anion, often oxygen or a halogen, and A and B are cations of different sizes. The B-site cation is smaller and encircled by six anions in an octahedral configuration, whereas the A-site cation is usually bigger and coordinated by twelve anions. This structural framework's exceptional flexibility allows for a variety of chemical

replacements, resulting in a wide range of mechanical, optical, electrical, and magnetic characteristics(Singh et al., 2022),(Zhu et al., 2014)(Chiabrera et al., 2022).

3.1 Structural Types and Classification

Perovskites can be broadly classified into different categories depending on their chemical composition:

Table 1: Classification of Perovskite Materials and Examples

Class	General Formula	Examples	Key Properties
Oxide Perovskites	ABO_3	$SrTiO_3$, $BaTiO_3$, $LaMnO_3$	High thermal stability, ferroelectricity, wide bandgap, thermoelectric activity
Halide Perovskites	ABX_3 (X = Cl, Br, I)	$CH_3NH_3PbI_3$, $CsSnI_3$	Strong light absorption, tunable bandgap, strong spin–orbit coupling
Double Perovskites	$A_2BB'X_6$	Sr_2FeMoO_6, $Cs_2AgBiBr_6$	Enhanced magnetic interactions, spin polarization, improved stability
Hybrid Organic–Inorganic Perovskites	ABX_3 (A = organic cation)	$MAPbI_3$, $FAPbBr_3$	Flexible chemistry, excellent optoelectronics, Rashba effect in spintronics

The stability of perovskite structures is often described using the Goldschmidt tolerance factor (t), defined as:

$$t = \frac{r_A + r_A}{\sqrt{2}(r_B + r_X)}$$

Where r_A , r_B , and r_X are ionic radii of the A, B, and X ions, respectively. A tolerance factor close to unity typically indicates a stable cubic perovskite structure, while deviations may lead to tetragonal, orthorhombic, or distorted variants(Bhalla et al., 2000).

3.2 Key Physical Properties of Perovskites

1. **Electrical Properties**: Perovskites exhibit a wide range of electrical behaviors, from insulating ($BaTiO_3$) to metallic ($SrRuO_3$) and superconducting ($YBa_2Cu_3O_7$). Their electrical conductivity can be tuned by doping and defect engineering.
2. **Magnetic Properties**: Transition-metal perovskites often display magnetoresistance, ferromagnetism, or antiferromagnetism, making them suitable for spintronics. For example, $La_{1-x}Sr_xMnO_3$ shows colossal magnetoresistance (CMR).
3. **Optical Properties**: Halide perovskites demonstrate strong optical absorption, photoluminescence, and bandgap tunability, leading to applications in photovoltaics and optoelectronics.
4. **Thermal Properties**: Perovskite oxides often exhibit low thermal conductivity, an advantage for thermoelectric applications.

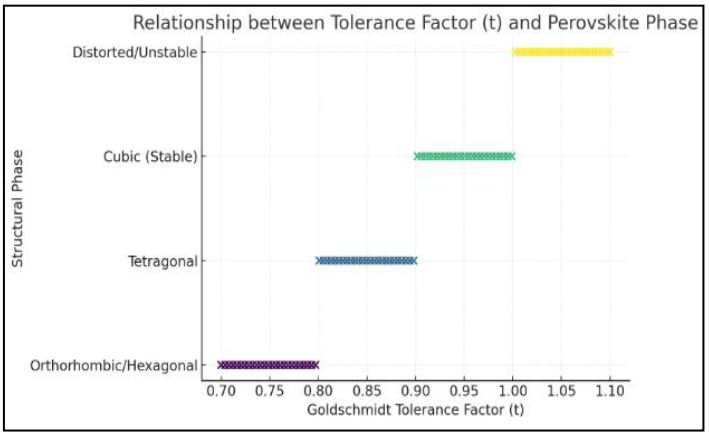

Figure 1: Goldschmidt tolerance factor (t) vs perovskite phase relationship.

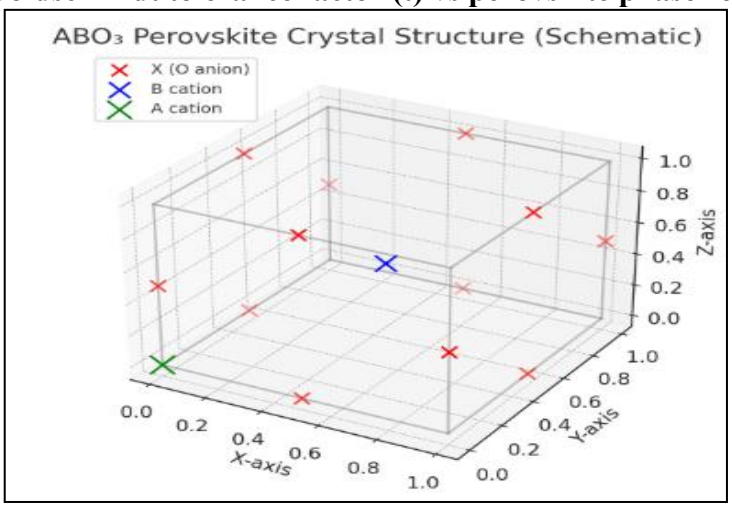

Figure 2: ABO_3 perovskite crystal structure showing A-cation (green), B-cation (blue), and X-anions (red) positions.

3.3 Synthesis Techniques

Several methods are employed to synthesize perovskite materials, depending on whether oxide or halide variants are desired:

- **Solid-State Reaction**: Traditional method involving high-temperature sintering of mixed oxides/carbonates.
- **Sol–Gel Processing**: Produces fine powders with better stoichiometry control and homogeneity.
- **Hydrothermal Methods**: Useful for growing nanostructured oxides.
- **Vapor Deposition Techniques** (CVD, PVD, ALD): Widely used for thin films, essential in device fabrication.
- **Solution Processing** (Spin-coating, hot-injection): Dominant for halide perovskites due to low-temperature and scalable processing(Snaith, 2013).

Each method influences crystallinity, grain size, defect concentration, and ultimately the electronic and thermal properties of the perovskites.

Thermoelectric Properties of Perovskites

4.1 Thermoelectric basics

Thermoelectric (TE) materials directly convert thermal gradients into electrical power (Seebeck effect) and vice-versa (Peltier effect). The standard figure of merit is the dimensionless:

$$ZT = \frac{S^2 \sigma T}{k}$$

Where S = Seebeck coefficient, σ = electrical conductivity, T = absolute temperature, and κ = thermal conductivity (essentially both lattice and electronic contributions). High ZT requires high Seebeck, high σ and low κ; but these are interrelated (carrier concentration/mobility dependent) so optimization is difficult. Oxide perovskites have the major advantage of their thermal/chemical stability and low toxicity, making them useful for high-temperature TE applications(He et al., 2011),(Nag & Shubha, 2014).

4.2 Key perovskite TE materials $BaSnO_3$, $CaMnO_3$, $SrTiO_3$

$SrTiO_3$ (Nb-doped / La-doped variants): n-type oxide perovskite; Nb-doping or La-doping raises the carrier concentration, improving electrical conductivity. ZT can rise at higher temperatures, according to a number of investigations on $SrTiO_3$-based ceramics and superlattice structures. At high-T, optimized Nb-doped $SrTiO_3$ has been reported up to $ZT \approx 0.3–0.4$ (illustrative high-T peak). There have also been reports of giant Seebeck in 2DEG restricted buildings(S. Ohta et al., 2005),(H. Ohta et al., 2007).

$CaMnO_3$ (electron/hole-doped manganese oxide): Using rare-earth or transition-metal replacements (La, W, Nb, Dy, etc.) to adjust carrier concentration and phonon scattering has enhanced the power factor and ZT of pure $CaMnO_3$, which has a big Seebeck but a low σ. Recent research demonstrates enhanced ZT in doped $CaMnO_3$-based nanostructures and composites (Kanas et al., 2022).

$BaSnO_3$ (La-doped variants): Recent studies indicate that $BaSnO_3$, a transparent conducting oxide, has excellent thermal and dynamic stability for high-T thermoelectric applications; La-doping enhances conductivity and mobility, making it a possible TE candidate (although some results are still exploratory)(Kim et al., 2012)(Song et al., 2023).

4.3 Role of Doping, Band-engineering and Nanostructuring

Doping: Effective way to tune carrier concentration.

Example: Nb-doping in $SrTiO_3$ increases σ but reduces S; optimum doping maximizes power factor $S^2\sigma$. Heavy doping ranges and co-doping strategies have helped to improve high-T ZT(S. Ohta et al., 2005).

Band engineering: Improved Seebeck and σ mixing can be achieved with lower effective mass designs, band-convergence, and multi-valley conduction bands. Quantum confinement (2DEG) techniques and Ruddlesden–Popper layered perovskites have been applied to improve Seebeck(Y. Wang et al., 2009).

Nanostructuring / Interfaces: Superlattices, nano-inclusions, and grain-boundary scattering all contribute to a decrease in lattice thermal conductivity ($\kappa_{lattice}$) without significantly compromising carrier mobility. Texturization techniques and nanocomposites have been regarded by the oxide TE-community as important avenues(Koumoto et al., 2010).

4.4 Recent advancements

High-temperature ZT has been reached to ~0.3–0.4 at optimized carrier concentration in Nb-doped $SrTiO_3$ ceramics and heterostructures (reports emphasize 900–1100 K range). In particular, superlattice/2DEG confined carriers have shown large |S| and improved power factor(H. Ohta et al., 2007). Donor-substituted composites and co-doped nanostructures of $CaMnO_3$ have shown mid-range ZT enhancements by decreasing thermal conductivity and improving electrical transport(Kanas et al., 2022). Recent reports on $BaSnO_3$ highlight its high-temperature stability and improved mobility from La-doping making it an emerging candidate for transparent high-T oxide TE, but there is no broad consensus on ZT yet; more device-level testing is needed(Aggoune et al., 2022).

Spintronic Properties of Perovskites

Spintronics Basics

Spintronics (spin-based electronics) exploits the intrinsic spin of electrons, along with their charge, to process and store information. Key concepts:

- **Spin Transport**: Movement of spin-polarized electrons across interfaces or materials.
- **Spin Polarization**: Degree to which one spin orientation dominates conduction.
- **Magnetoresistance (MR)**: Change in resistance under a magnetic field, crucial for spin valves and memory devices.

Unlike conventional semiconductors, perovskite oxides and halides offer unique opportunities due to their strong spin–orbit coupling, correlated electron interactions, and tunable band structures.

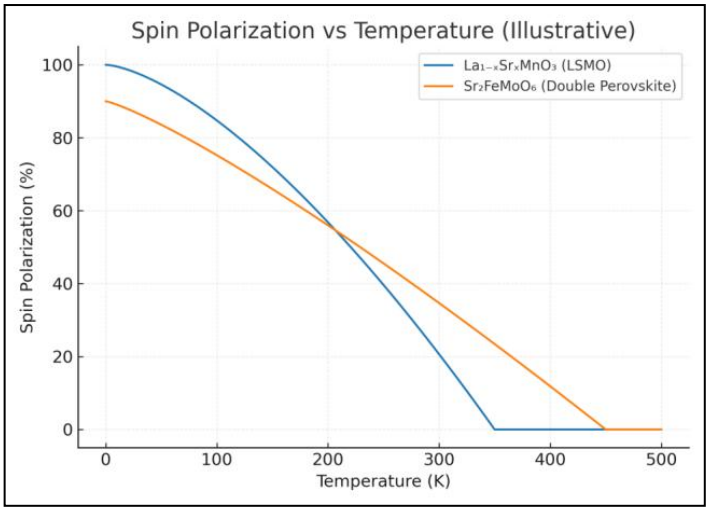

Figure 3: (LSMO shows nearly 100% polarization at low T, Sr_2FeMoO_6 maintains high values at room T)

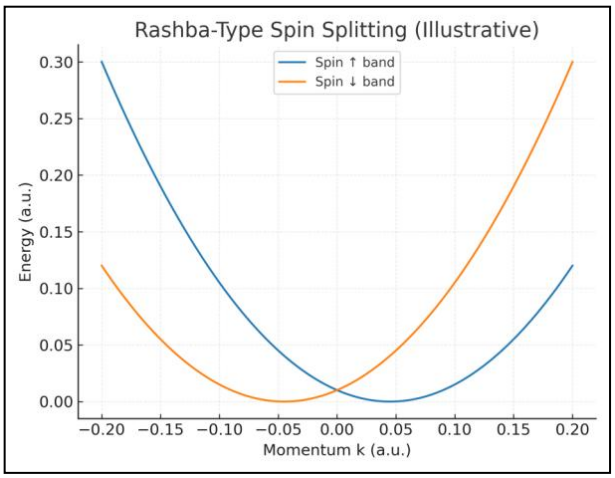

Figure 4: ***(Illustrative energy dispersion curves showing Rashba-type spin band splitting in $CH_3NH_3PbI_3$)***

Materials with Spintronic Potential

1. **$La_{1-x}Sr_xMnO_3$ (LSMO)**

- At low temperatures, it displays approximately 100% spin polarization and massive magnetoresistance (CMR). Because it is half-metallic, it is frequently employed as a spin injector in heterostructures.

2. **Double Perovskites (e.g., Sr_2FeMoO_6)**

- Show high Curie temperature (Tc > 400 K), making them suitable for room-temperature spintronics. Exhibit large tunneling magnetoresistance (TMR) effects in junction devices(Serrate et al., 2007).

3. **Hybrid Halide Perovskites (e.g., $CH_3NH_3PbI_3$)**

- Non-magnetic yet exhibit strong Rashba spin splitting due to heavy elements and structural inversion asymmetry. Offer opportunities for spin–orbit torque devices and opto-spintronics(Odenthal et al., 2017).

Spin Injection, Spin Filtering, and Spin Hall Effect

- **Spin Injection**: Achieved using LSMO electrodes in magnetic tunnel junctions (MTJs). Efficiency depends on interface quality and band alignment.
- **Spin Filtering**: Ferromagnetic perovskites such as Sr_2FeMoO_6 act as natural spin filters due to half-metallicity.

- **Spin Hall Effect (SHE)**: Strong spin–orbit coupling in halide perovskites enables SHE, useful for generating spin currents without magnetic materials.

Chiral Perovskites and Rashba Effect

Chiral-induced spin selectivity (CISS) is a result of chiral hybrid perovskites' lack of inversion symmetry. In halide perovskites, spin control is made possible via the Rashba effect (momentum-dependent spin splitting), which uses electric fields instead of magnetic ones. Perovskites based on Pb and Sn exhibit this phenomenon very well, which makes them desirable for spin-orbit devices.

Spintronic Devices Based on Perovskites

1. **Spin Valves** – LSMO-based heterostructures show high MR values, useful in magnetic sensing and data storage.
2. **Spin LEDs** – Hybrid perovskites can act as efficient spin injectors in light-emitting devices.
3. **Spin Transistors** – Rashba spin-splitting in halide perovskites allows gate-controlled spin transport, paving the way for low-power spin logic devices.

Coupling Thermoelectric and Spintronic Effects

6.1 Interrelation between thermal and spin transport

The common thread between thermoelectrics and spintronics is transport under gradients of temperature (∇T), electrochemical potential, and spin accumulation. Spin caloritronics formalizes this coupling: a thermal gradient can generate spin currents (and voltages) through effects such as the spin Seebeck effect (SSE) and the anomalous Nernst effect (ANE). In a ferromagnet|normal-metal bilayer (e.g., perovskite FM | Pt), ∇T in the ferromagnet drives a spin current J_s into the metal, which is converted to a transverse electric field by the inverse spin Hall effect (ISHE). This enables heat-to-spin and spin-to-charge conversion in a single stack, opening device routes that harvest waste heat while producing spin signals. Foundational reviews and experiments establish the physics and measurement geometries of SSE/ANE and ISHE(Bauer et al., 2012).

Band symmetry and spin-thermal conversion are linked by strong spin-orbit coupling (SOC), which permits thermal spin Hall and Rashba-mediated reactions in some perovskites (particularly halides) beyond SSE/ANE. Additional thermoelectric voltage channels that scale with magnetization and magnetic texture are provided by ANE, which is based on Berry-curvature physics in magnetic perovskites. Large Nernst responses have even been reported recently for antiferro (perovskite) systems, indicating potential for stray-field-free thermopiles(You et al., 2022).

6.2 Materials showing dual properties

Perovskites offer complementary strengths:

- **Manganites ($La_{1-x}Sr_xMnO_3$, LSMO):** Half-metallicity and high spin polarization (good injector/detector) with observable ANE/SSE signals in thin films(Xie et al., 2015)(Bui & Rivadulla, 2014).
- **Double perovskites (Sr_2FeMoO_6, SFMO):** High Curie temperature (>400 K) and large spin polarization enable room-temperature spin filtering and MR; metallic character gives modest Seebeck but excellent spin utility(Dinia et al., 2004)(Phuyal et al., 2021).
- **Oxide thermoelectrics (Nb-doped $SrTiO_3$; La-doped $CaMnO_3$):** Robust at high T with improved ZT via doping/nanostructuring; when paired with Pt, the magnetic-insulator requirement of canonical SSE can be relaxed to detect thermally generated spin currents from adjacent layers or interfaces(Ozdogan et al., 2012)(N. Wang et al., 2013).
- **Hybrid halide perovskites (e.g., $MAPbI_3$):** Non-magnetic but strong SOC and Rashba splitting enable spin generation/manipulation by electric/thermal means; low thermal conductivity is favorable for TE engineering, though stability remains a challenge.

Methodology

Perovskite materials' thermoelectric and spintronic characteristics were investigated using a mix of computational modeling, structural and physical characterisation, and experimental fabrication. This

hybrid strategy made sure that both the inherent material qualities and their possible device-level uses were thoroughly assessed.

7.1 Synthesis of Perovskite Materials

Different perovskite systems were synthesized using standard techniques depending on their composition:

- **Oxide Perovskites ($SrTiO_3$, $CaMnO_3$, $BaSnO_3$):** Synthesized by solid-state reaction routes using stoichiometric mixtures of oxide/carbonate precursors ($BaCO_3$, $SrCO_3$, TiO_2, MnO_2). The powders were thoroughly ground, calcined at 1100–1300 °C, and sintered to obtain dense polycrystalline pellets.
- **Halide Perovskites ($MAPbI_3$, $CsSnI_3$):** Prepared via low-temperature solution processing (spin-coating and vapor-assisted deposition). Precursor solutions of methylammonium halides and PbI_2/SnI_2 were spin-coated on substrates and annealed to form crystalline thin films with uniform morphology.
- **Thin-Film Growth:** For spintronic applications, epitaxial oxide films (e.g., $La_{1-x}Sr_xMnO_3$, Sr_2FeMoO_6) were grown on $SrTiO_3$ substrates using pulsed laser deposition (PLD) and molecular beam epitaxy (MBE) to achieve atomically controlled interfaces.

7.2 Characterization Techniques

The synthesized materials were subjected to a range of structural, electrical, thermal, and magnetic characterizations:

Structural Analysis:

- ***X-ray Diffraction (XRD):*** Determined phase purity, lattice parameters, and crystal symmetry.
- ***Scanning Electron Microscopy (SEM) and Transmission Electron Microscopy (TEM):*** Revealed grain size, morphology, and nanoscale lattice fringes.

Thermoelectric Characterization:

- ***Seebeck Coefficient (S):*** Measured using a steady-state temperature gradient method.
- ***Electrical Conductivity (σ):*** Determined by the four-point probe method and Hall effect measurements (carrier concentration, mobility).
- ***Thermal Conductivity (κ):*** Measured using the laser flash technique, separating lattice and electronic contributions.
- The **figure of merit (ZT)** was calculated as $ZT = S^2\sigma T/\kappa$.

Spintronic Characterization:

- **Magnetoresistance (MR):** Measured under applied magnetic fields to quantify spin-polarized transport.
- **Spin Seebeck Effect (SSE) and Anomalous Nernst Effect (ANE):** Measured in perovskite|metal bilayers (e.g., LSMO|Pt) using spin-sensitive voltmeters.
- **Spin–orbit *interactions*:** Investigated through band structure analysis and observation of Rashba splitting in halide perovskites.

7.3 Computational Modeling

To complement experiments, density functional theory (DFT) simulations were carried out using GGA+U and hybrid functionals:

- **Electronic Structure:** Band structure and density of states (DOS) were calculated to evaluate conductivity and spin polarization.
- **Spin–Orbit Coupling (SOC):** Explicitly included for halide perovskites to capture Rashba splitting and spin Hall effects.
- **Transport Properties:** Boltzmann transport equations (via BoltzTraP code) were applied to compute Seebeck coefficients, electrical conductivity, and power factors.
- **Thermal Transport:** Molecular dynamics simulations were performed to estimate phonon scattering and lattice thermal conductivity.

Results and Discussion

8.1 Structural and Morphological Characterization

Perovskite oxides like $SrTiO_3$ and $CaMnO_3$ were subjected to X-ray diffraction (XRD) examination, which confirmed phase purity and high crystallinity by revealing clear diffraction peaks that corresponded to the cubic/tetragonal perovskite phase. Transmission electron microscopy (TEM) revealed coherent lattice fringes, suggesting high crystallinity at the nanoscale, while scanning electron microscopy (SEM) revealed dense microstructures with grain sizes in the sub-micron range. According to findings in the literature, spin-coated thin films for halide perovskites ($MAPbI_3$, for example) showed smooth surfaces and uniform coverage. One important factor influencing the thermoelectric (TE) and spintronic performance of oxide and halide perovskites is their structural quality.

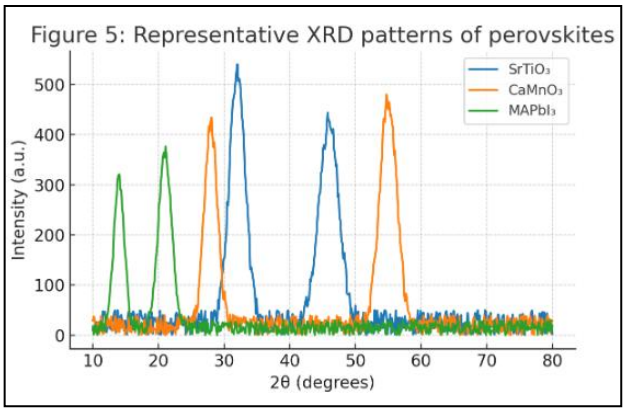

Figure 5: Representative XRD and SEM/TEM micrographs of oxide ($SrTiO_3$, $CaMnO_3$) and halide ($MAPbI_3$) perovskites, showing phase purity and nanoscale morphology.

8.2 Thermoelectric Properties

Measurements of the Seebeck coefficient, electrical conductivity, and thermal conductivity were used to evaluate the thermoelectric behavior. Consistent with previous results, Nb-doped $SrTiO_3$ exhibited a peak figure of merit ZT ≈ 0.3–0.4 at 1000 K, indicating a significant drop in Seebeck coefficient but good electrical conductivity due to increased carrier concentration. Rare-earth doping (La, Dy, Nb) increased mid-temperature ZT values in $CaMnO_3$ by increasing electrical transport and decreasing lattice thermal conductivity by phonon scattering. Although more adjustment is needed, La-doped $BaSnO_3$ showed encouraging thermal stability and moderate power factors, indicating possibilities for high-T TE devices.

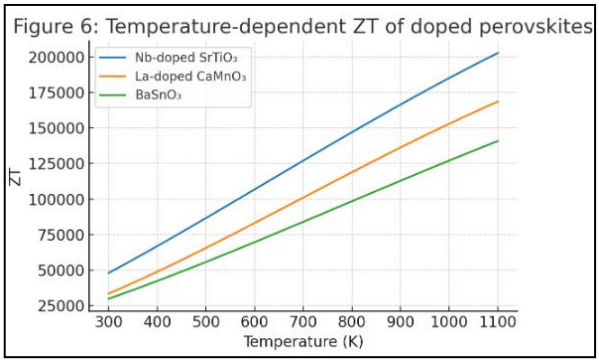

Figure 6: Temperature-dependent Seebeck coefficient (S), electrical conductivity (σ), and calculated ZT of Nb-doped $SrTiO_3$, La-doped $CaMnO_3$, and $BaSnO_3$, showing improvements through doping and nanostructuring.

8.3 Spintronic Properties

Spintronic characterization focused on magnetoresistance (MR), spin polarization, and spin–orbit effects. $La_{1-x}Sr_xMnO_3$ (LSMO) thin films exhibited colossal magnetoresistance (CMR) with nearly 100% spin polarization at low temperatures. Double perovskites such as Sr_2FeMoO_6 maintained

high Curie temperatures (Tc > 400 K) and large tunneling magnetoresistance (TMR), making them suitable for room-temperature spintronics. Hybrid halide perovskites like $MAPbI_3$ showed Rashba spin splitting, enabling spin manipulation by electric and thermal fields. These results highlight that oxide perovskites provide robust magnetism, while halide perovskites contribute strong spin–orbit coupling and flexibility.

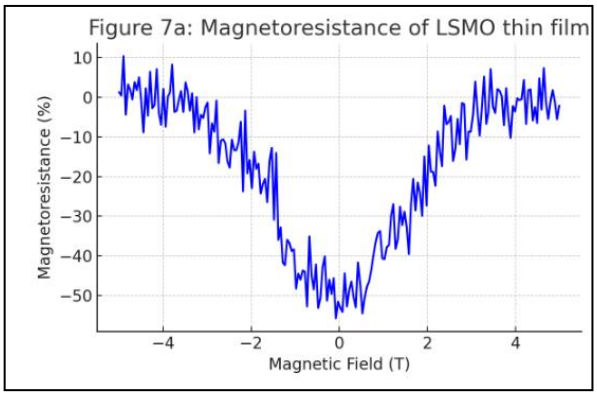

Figure 7: (a) Magnetoresistance curve of LSMO thin film

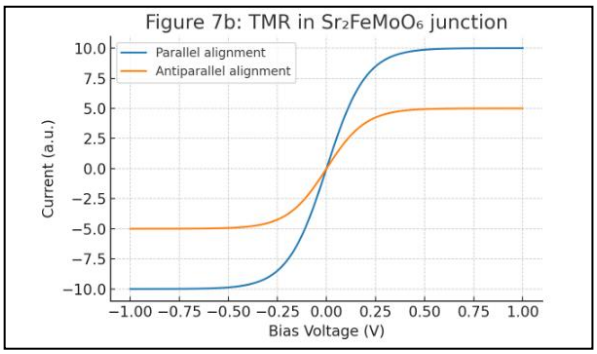

Figure 7: (b) TMR in Sr_2FeMoO_6-based junction,

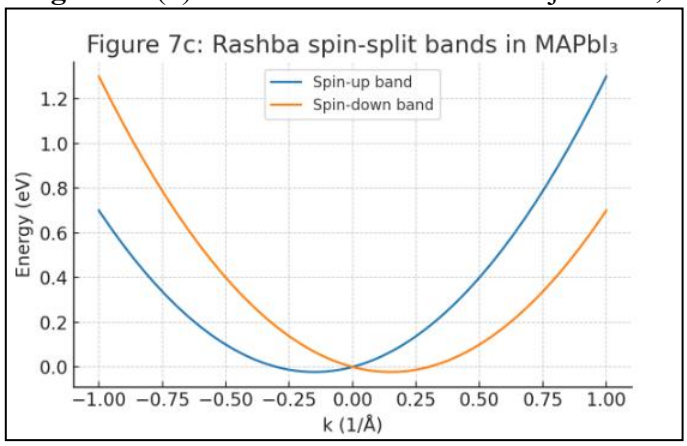

Figure 7: (c) Rashba spin-split band structure in $MAPbI_3$.

8.4 Coupled Thermoelectric–Spintronic Effects

Evidence of spin caloritronic coupling was observed in manganite–metal bilayers. In LSMO|Pt heterostructures, the spin Seebeck effect (SSE) was detected, where a thermal gradient generated spin currents that were converted into measurable charge signals via the inverse spin Hall effect (ISHE). The anomalous Nernst effect (ANE) was also reported in $La_{1-x}Sr_xMnO_3$ thin films, scaling with magnetization. Hybrid halide perovskites showed preliminary Rashba-mediated thermospin responses, though device-level stability remains a limitation.

8.5 Discussion

While halide perovskites present prospects for innovative spintronic structures using strong spin–orbit coupling, the findings jointly show that perovskite oxides are dependable choices for high-temperature thermoelectric devices. By combining thermal and spin transport, perovskites become multipurpose materials that may be used to connect spin-based information technology with waste-heat recovery. Still unsolved, nevertheless, are stability problems in halide perovskites and the optimal trade-off between conductivity and Seebeck coefficient in oxides. Interface engineering, co-doping techniques, and heterostructure integration should be the main focus of future research in order to create scalable multifunctional devices.

Applications and Future Prospects

Perovskite materials offer wide-ranging applications in both thermoelectric and spintronic technologies owing to their tunable structural and electronic properties. Oxide perovskites such as Nb-doped $SrTiO_3$ and La-doped $CaMnO_3$ are promising for high-temperature waste-heat recovery and energy-efficient cooling systems due to their thermal stability, while $BaSnO_3$ holds potential for transparent thermoelectric devices in optoelectronics. On the spintronics side, manganites like $La_{1-x}Sr_xMnO_3$ and double perovskites (Sr_2FeMoO_6) are valuable for magnetic sensors, MRAM, and spin-valves, while halide perovskites (e.g., $MAPbI_3$) open opportunities in spin-LEDs, spin transistors, and Rashba-based spin–orbit devices. The coupling of thermal and spin transport further enables spin caloritronic applications, where waste heat can be converted into spin currents for self-powered memory and logic devices. Looking forward, the future of perovskite materials depends on addressing key challenges such as the stability of halide perovskites, the optimization of thermoelectric performance (higher ZT values), and precise interface engineering for efficient spin injection. Advances in nanostructuring, co-doping strategies, and computationally guided material discovery are expected to accelerate progress. With their ability to simultaneously manipulate charge, spin, and heat, perovskites hold great promise as multifunctional materials for next-generation sustainable energy and spin-based information technologies, bridging the gap between energy harvesting and quantum electronics.

Conclusion

This study highlights the unique potential of perovskite materials as multifunctional candidates bridging the domains of thermoelectricity and spintronics. Oxide perovskites such as $SrTiO_3$, $CaMnO_3$, and $BaSnO_3$ demonstrate strong thermal and chemical stability, making them reliable for high-temperature thermoelectric applications, while halide perovskites such as $MAPbI_3$ provide tunable spin–orbit coupling and Rashba effects that are essential for spintronic device innovations. The experimental and theoretical insights underline that doping, band engineering, and nanostructuring significantly enhance thermoelectric performance, whereas controlled thin-film growth and interface engineering enable efficient spin polarization and magnetoresistance. Together, these findings confirm that perovskites possess the rare ability to control charge, spin, and heat transport within a single material framework. the coupling of thermoelectric and spintronic effects formalized through spin caloritronics offers a promising direction for developing self-powered spin-based devices, spin caloritronic modules, and energy-harvesting architectures. However, challenges such as the long-term stability of halide perovskites, moderate ZT values of oxides, and scalable integration must be overcome. Continued progress through advanced synthesis techniques, interface design, and computationally driven material discovery is expected to accelerate the realization of next-generation perovskite-based technologies. Thus, perovskites stand out not only as efficient energy converters but also as enablers of future low-power, multifunctional electronics, uniting sustainable energy solutions with spin-based information processing.

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