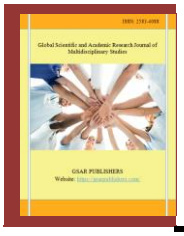

Global Scientific and Academic Research Journal of Multidisciplinary Studies
ISSN: 2583-4088 (Online)
Frequency: Monthly
Published By GSAR Publishers
Journal Homepage Link- https://gsarpublishers.com/journals-gsarjms-home/
DOI : 10.5281/zenodo.14770877

Advancing Double Perovskites: Tailoring Optoelectronic, Magnetic, and Transport Properties for Sustainable Energy and Next-Generation Technologies

By

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Received: 15 – 01 - 2025	Accepted: 28 – 01- 2025	Published: 30 – 01 -2025

Abstract

This study examines the structural, optoelectronic, magnetic, and transport properties of halide-based and oxide double perovskites, underscoring their potential in sustainable energy systems and advanced electronic applications. Using density functional theory (DFT) calculations, compositions such as Na_2AgTlX_6 (X = Cl, Br, I), Li_2AgTlX_6 (X = Cl, Br), and Pr_2NiMnO_6 were systematically analyzed to assess the impact of halide substitution and doping on lattice constants, electronic band structures, and thermodynamic stability. The findings reveal that these modifications induce significant changes in direct bandgap transitions, extending from the visible to the infrared spectrum, establishing these materials as strong candidates for photovoltaic and thermoelectric applications. Further evaluation of mechanical and transport properties indicated notable enhancements in bulk modulus, dielectric constants, Seebeck coefficients, and figure of merit, confirming their suitability for efficient energy harvesting and conversion. Magnetic analysis of Pr_2NiMnO_6 revealed robust properties, including spin-phonon coupling, magnetocaloric effects, and superexchange interactions driven by B-site cation ordering, making it a compelling choice for spintronic devices and magnetic refrigeration systems. This work emphasizes the adaptability and eco-friendly nature of double perovskites as lead-free alternatives to address global energy challenges. By tailoring their structural, electronic, and magnetic characteristics, these materials exhibit significant potential for integration into next-generation optoelectronic devices, sustainable energy technologies, and multifunctional applications. The results provide valuable insights into the strategic design of perovskite-based materials, paving the way for innovative solutions to modern technological demands.

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