Unveiling the Multifunctional Features of Cs2LiMoX6 (X = Cl and Br) for Green Energy Applications: A DFT Study

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Abstract Double-perovskite halides are believed to satisfy the requirements for resolving energy scarcity concerns and have the potential to be beneficial materials for the production of renewable energy. Density functional theory modeling was used to analyze the physical properties of Cs2LiMoX6 (X = Cl, Br), with electronic and optical features studied via Tran Blaha-modified Beche Johnson (TB-mBJ). Spin-resolved band structure and density of states confirmed their semiconductor nature. Cs2LiMoCl6 exhibited band gaps of 3.45 eV (spin-down) and 2.42 eV (spin-up), while Cs2LiMoBr6 had band gaps of 3.13 eV (spin-down) and 1.34 eV (spin-up). The stability of the studied composites was shown by their low ground state energy, elastic constants, and tolerance factor analyses. Both Poisson's and Pugh's ratios indicated that the materials are brittle. The materials absorbed light in the ultraviolet range, specifically from 212 to 327 nm for Cs2LiMoCl6 and from 171 to 385 nm for Cs2LiMoBr6, indicating that they could be useful for optoelectronic applications. The thermoelectric parameters as a function of temperature were calculated using the Boltztrap code, which has been integrated with the WIEN2K code. At 800 K, the thermoelectric figure of merit (zT) values were 0.75 for Cs2LiMoCl6 and 0.86 for Cs2LiMoBr6, demonstrating their potential for high-temperature thermoelectric applications.

Keywords **Author Keywords:** DFT; electronic properties; halide double perovskites; mechanical properties; optoelectronics
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Data availability statement

No datasets were generated or analyzed during the current study.

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