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Cesium-Magnesium based cubic halide perovskites CsMgX3 (X = Cl,Br) with engrossing thermoelectric and optical properties suitable for energy conversion and solar cell based applications: A DFT speculation

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Abstract

We have performed a study on two cubic structured halide perovskites, CsMgX3 (X = Cl, Br) using ab-initio simulations in the outline of density functional theory. In this context, we extensively explored their structural, electronic, thermoelectric and optical properties. The cubic phases of these compounds were optimized and were found to be stable and energetically feasible. Their band structures implied that they are indirect wide gap semiconductors with band gaps of 6.35 and 4.26 eV for CsMgCl3 and CsMgBr3 respectively. Further, their thermoelectric properties comprised of high Seebeck coefficient and electrical conductivities with p-type as the majority charge carriers. Also their high figure of merit (ZT) of values 0.69 and 0.75 at room temperature, showed their efficient thermoelectric response along with the potential to be used for power generation and energy conversion applications. The wide band gaps and their optical behavior consisting of zero absorption, electron energy loss and negligible reflectance in visible region signified a important possibility to use these compounds as hole transport materials (HTM) in the solar cells, which can augment the efficiency of solar cell to a huge level. Moreover, the other calculated optical properties showed contrasting behavior in varying ranges of the electromagnetic spectrum. Thus, we speculate that the studied halide perovskites can emerge as very useful materials for thermoelectric energy conversion and solar cell applications.

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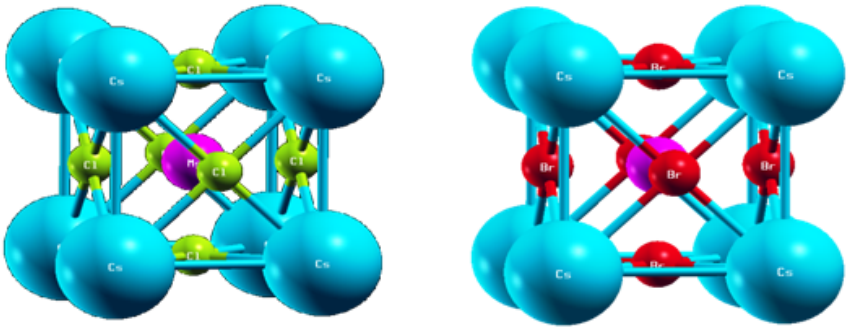

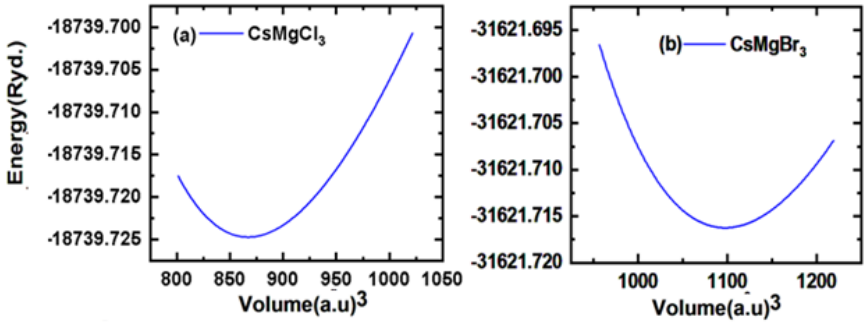

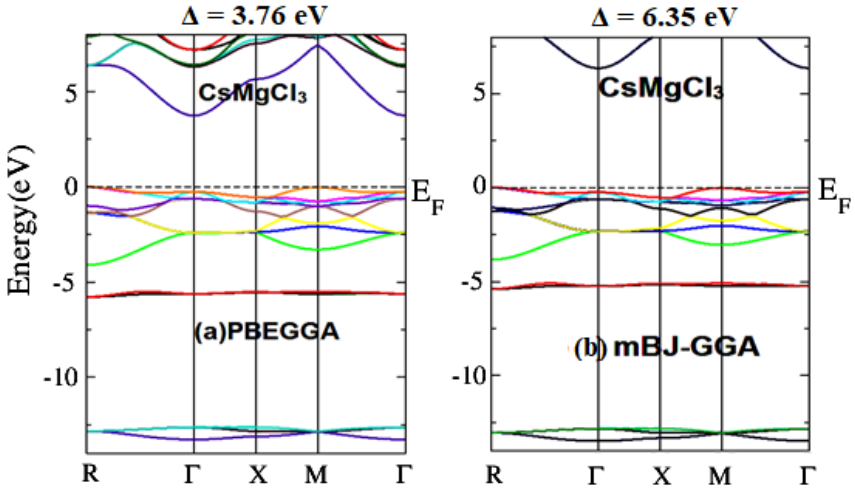

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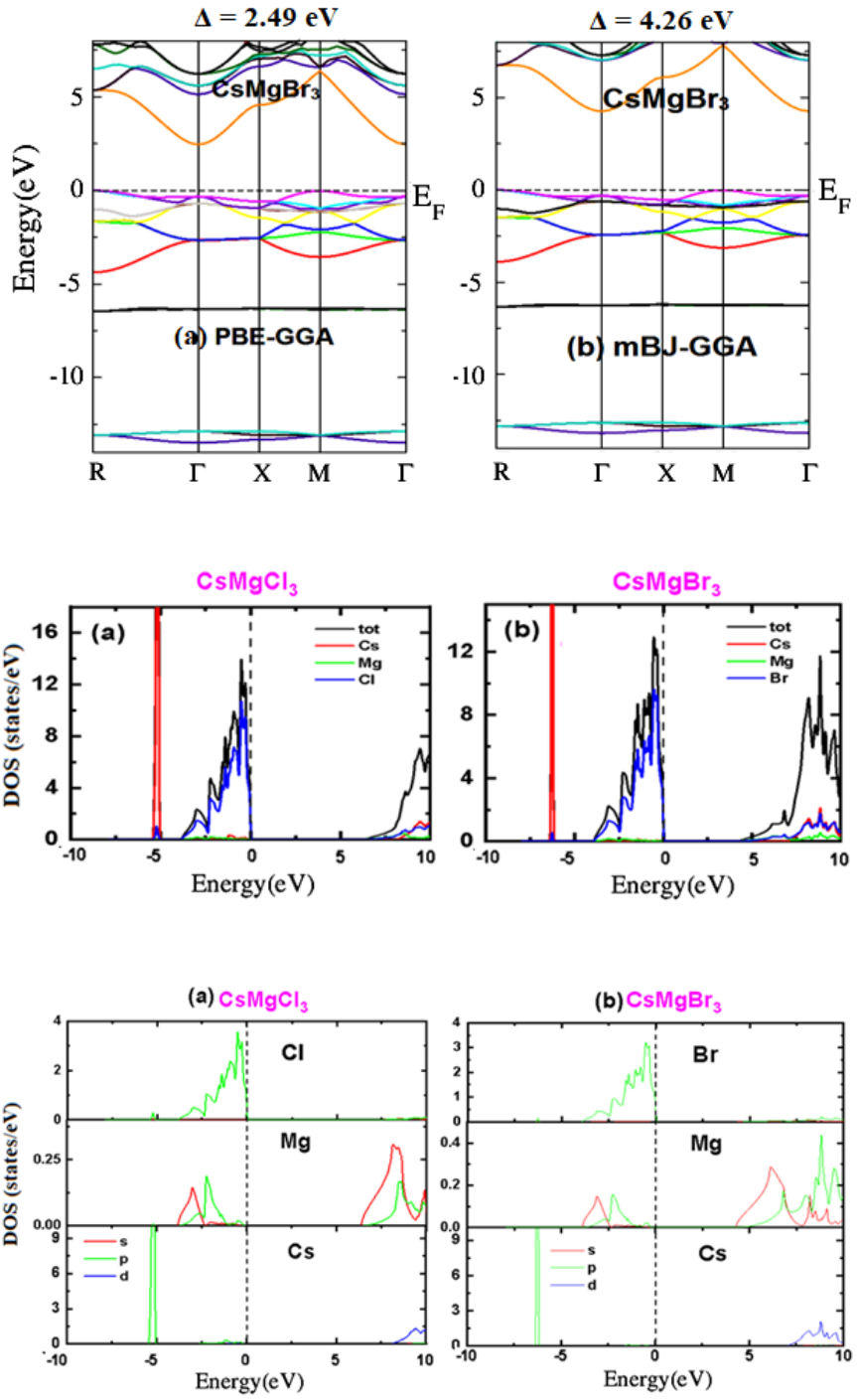

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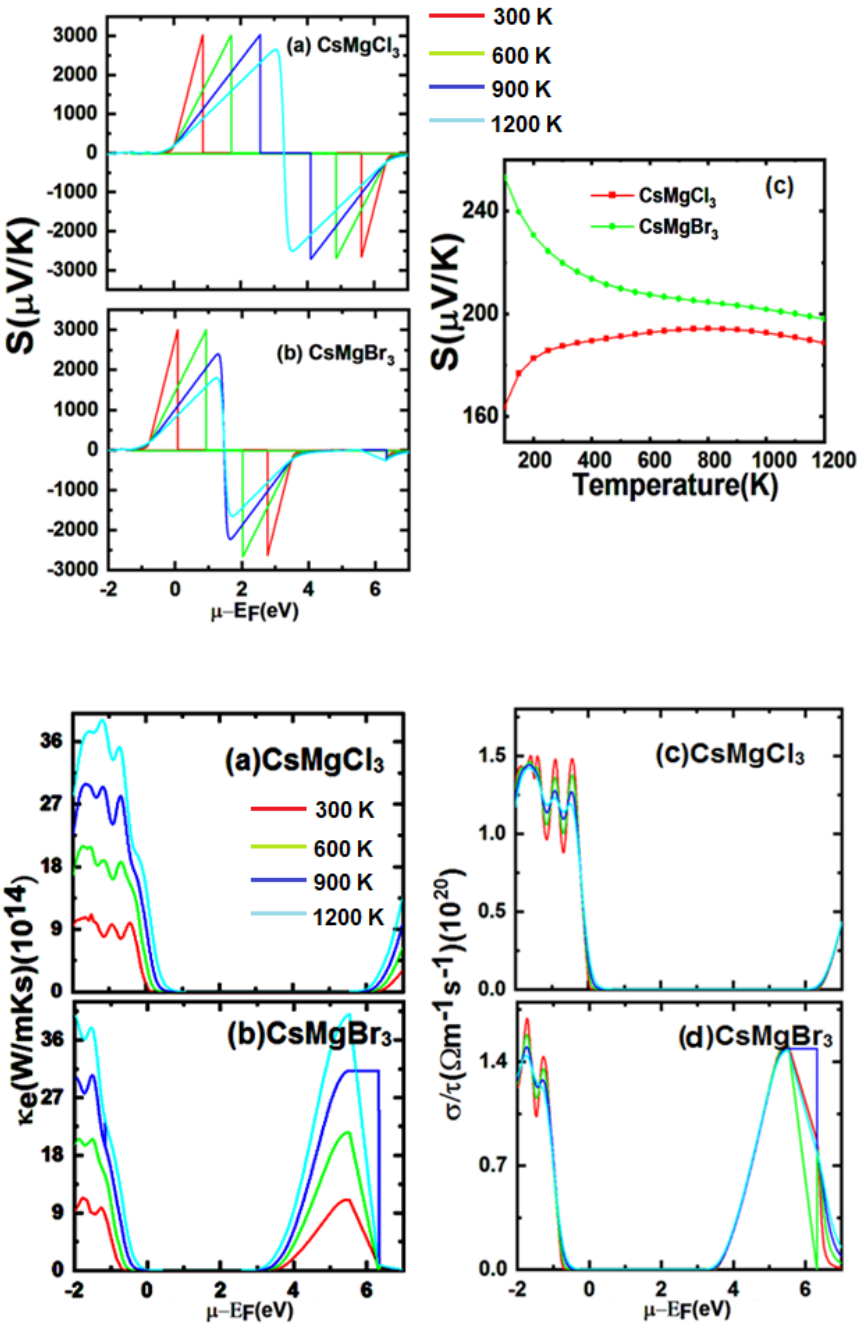

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