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(Research Article)
Investigation of mechanical, thermal and acoustical properties of $CsPbX_3$ (X = Br, I) compounds using the density functional theory

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Abstract

Halide Perovskites have great energy conversion efficiency, but their structural degradation due to change in surface temperature arise from heat accumulation of solar radiation is one of their most important drawbacks. Analysis of structure and thermal transport can be useful in increasing their efficiency. in this paper mechanical, acoustical and thermal properties of CsPbI3 and CsPbBr3 in cubic phase were studied using density functional theory with PBE-GGA approximation. Elastic constants obtained with stress-strain methodology. Using elastic constants, mechanical stability, anisotropy, elastic coefficients, Debye temperature and various sound propagation modes in the materials investigated. Despite mechanical stability in static conditions, the existence of high anisotropy (~2.9) in these perovskites revealed that, they may become unstable in commercial applications. CsPbBr3 compared to CsPbI3 due to higher Debye temperature (120 and 101 K) and more speed of sound propagation (1774 and 1587 m/s), has stronger bonds between the components, in addition to, having higher phonon transport. Thermal conductivity was investigated using the Slack model, which obtained 0.349 and 0.274 W mK/s for CsPbI3 and CsPbBr3, respectively. Higher thermal conductivity of CsPbBr3 leads to less heat accumulation on the surface, so it can be introduce as better choice for use in solar cell applications.

Keywords: Perovskite, Sound velocity, Thermal conductivity, Anisortopic.

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