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A possibility as a new type of thermoelectric application on organic-inorganic hybrid perovskite ABI$_3$ system: A density functional theory study$^1$ CHANGHOON LEE, JISOOK HONG, JI HOON SHIM, Pohang Univ of Sci & Tech, MYUNG-HWAN WHANGBO, NC State Univ., POSTECH TEAM — The electronic structures of organic-inorganic hybrid systems ABI$_3$ ($A$ = CH$_3$NH$_3$, NH$_2$CHNH$_2$; $B$ = Sn, Pb; $X$ = I) in the distorted phase from their patent cubic phase are systematically studied using the first-principles calculations. Here, we examine thermoelectric properties for ABI$_3$ compounds based on the DFT electronic structures of their optimized crystal structures. The ABI$_3$ compounds should be considered for good thermoelectric application. We reveal that good thermoelectric performance of ABI$_3$ systems originate from large seebeck coefficients and low thermal conductivities. As a consequence, we predict that ABI$_3$ system is a promising material for new thermoelectric application compared to thermoelectric properties of well-known thermoelectric material Bi$_2$Te$_3$.

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