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A possibility as a new type of thermoelectric application on organic-inorganic hybrid perovsike 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_3NH_3, NH_2CHNH_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_2Te_3.

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