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Guanidinium tin halide perovskites: structural, electronic, and thermodynamic properties by quantum chemical study

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Abstract

The orthorhombic phase of guanidinium tin halide perovskites $C(NH_2)_3SnX_3$, $X = Cl, Br, I$ has been studied by quantum chemical method. The lattice parameters are optimized to obtain the minimum energy using the density functional theory with the generalized gradient approximation, GGA-PBE. The Kohn–Sham electronic band structures have been computed; the materials have direct bandgaps of 3.00, 2.47, and 1.78 eV for the $C(NH_2)_3SnCl_3$, $C(NH_2)_3SnBr_3$, and $C(NH_2)_3SnI_3$, respectively, situated at the gamma symmetry points. The projected densities of states are analyzed and the contribution of the p- and s-states of the tin and halogen atoms evaluated. For the $GUASnX_3$ compounds, thermodynamic stability to different decomposition routes has been assessed and standard enthalpies of formation obtained.

Keywords

Guanidinium; Lead-free; Enthalpy of formation; The density of states; Orthorhombic; Bandgap