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

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DOI: https://doi.org/10.1007/s00339-021-04504-x

Abstract

The orthorhombic phase of guanidinium tin halide perovskites C(NH2)3SnX3, 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(NH2)3SnCl3, C(NH2)3SnBr3, and C(NH2)3SnI3, 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 GUASnX3 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