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Enthalpy of formation of $CsSn(Cl_x(Br,I)_{1-x})_3$ and $CsPb(Cl_x(Br,I)_{1-x})_3$

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According to the third-generation of photovoltaic cell, the methylammonium lead iodide perovskite ($MAPbI_3$) has recently gained a great deal of interest. This is as, to date, the solar cell made of this material has been able to reach efficiencies 22.7% in 2017 and is very cost efficient to manufacture compared with that from the conventional silicon based. Such great efficiencies is attributed to their excellent features, most likely of which is the direct bandgap, high absorption coefficient and long carrier diffusion length [J. Mater. Chem. A 3, 8926-8942 (2015)]. However, the $MAPbI_3$ is somewhat structurally unstable under the ambient moisture, and more worse it contains the toxic lead (Pb) which is harmful to human health and environment. The existence of organic molecule in this material is a major obstacle to their stability. The effective way to remove this problem directly is to replace the organic cation with inorganic counterpart. According to the Goldschmidth tolerance factor rule, except for francium (Fr) which is a radioactive element, cesium might be the most appropriate substitution to organic site, because its atomic size is almost the largest in the periodic table to hole the stable perovskite structure. To remove the toxic effect of lead, tin metal cation is one of the most reasonable substituting for lead because it has the similar valence electronic configuration and has close ionic radius to lead, which makes it possible to form a perovskite structure [Monatsh. Chem. 148, 795-826 (2017)] In addition, mixing halide in perovskites has been verified as the effective way to refining the properties of perovskites such as tuning the bandgaps and enhancing stability. These then inspire us to pursue for families of perovskites possessing formula $CsSn(Cl_x(Br,I)_{1-x})_3$, which are nontoxic and could have better structural stability under ambient conditions. Therefore, in this work, we have investigated enthalpy of formation of $CsSn(Cl_x(Br,I)_{1-x})_3$ with x = 1/3, 2/3 and 1, in the cubic phase based on the density functional theory (DFT) with the Generalized Gradient Approcximation (GGA). The main objective is to seek for the characteristic of structural stability with respect to the composition x's. We found that the structural stability increases linearly with composition x's of halide atom from I to Br to Cl. These effects can be understood by considering at the trend of electronegativity of halide atoms which increases from I to Br to Cl. We found that the stability of $CsSn(Cl_x(Br,I)_{1-x})_3$ is slightly lower than $CsPb(Cl_x(Br,I)_{1-x})_3$. Thus $CsSn(Cl_x(Br,I)_{1-x})_3$ is still the promise candidate for photovoltaics. As we know that perovskites containing more Cl will have larger band gaps. Therefore, these studies could serve as a guidance to compromise the stability, by varying composition of halide atoms, with the optimal band gap or other solar-cell-desired properties.

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