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Phase stability, electronic structure and phonons in $CsGeI_3$[1]
LING-YI HUANG, WALTER LAMBRECHT, Case Western Reserve Univ — Because Ge is smaller than Sn and Pb, $CsGeI_3$ is promising to overcome the stability problems of the perovskite forms of $CsSnI_3$ and $CsPbI_3$ halides toward the denser yellow phase in which octahedra are edge as well as cornersharing in one dimensional chains. This phase has higher gaps and is unsuitable for photovoltaics. $CsGeI_3$ and other trihalide germanates are found to exist in the cubic perovskite phase at high temperature but in a rhombohedral phase in which the Ge is displaced toward three of the halogen neighbors in its surrounding octahedron, accompanied by a rhombohedral distortion of the lattice vectors. We will present density functional total energy calculations and band structures obtained within the quasi-particle self-consistent *GW* method for both the cubic and rhombohedral phase of $CsGeI_3$. For the latter, we find a gap of 1.6 eV in excellent agreement with recent experiments on its absorption edge. We will also present optical dielectric function and effective mass results for this material and discuss the trends for different types of distortions in halides depending on the chemical composition. The phonons at the Brillouin zone center are calculated and compared to experimental Raman spectra.

[1]NSF and DOE

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