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Electronic structure and stability of $RbGeCl_3$[1] SANTOSH KUMAR RADHA, WALTER R . L LAMBRECHT, Case Western Reserve Univ — Metal halide pervoskites have recently received significant attention, including recently the Ge based $AGeX_3$. First-principles calculations of $RbGeCl_3$ stability and structure were performed using the full-potential linearized muffin-tin orbital (FP-LMTO) method. The band structures were calculated using the quasi-particle self-consistent (QS)*GW* method. We find that the perovskite structure exhibits octahedral rotations rather than the ferro-electric distortion, in contrast to $CsGeCl_3$, as expected from the tolerance factor ≈ 1. The relative stability of the perovskite form and the monoclinic form is found to be very sensitive to the exchange-correlation functional used. LDA predicts the Pervoskite to be the lower energy while GGA predicts the monoclinic. GGA is significantly better at predicting the lattice constants of these materials than LDA. The band structure in the perovskite phase has significantly lower band gap than the monoclinic phase.

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