$CsSnX_3$ Band Structure Calculations by the QSGW Method

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$CsSnX_3$ perovskite compounds are of interest because of their strong photoluminescence. Their electronic properties are not yet well understood. Here, we carry out quasiparticle self-consistent GW (QSGW) calculation for cubic (α-phase) $CsSnX_3$, where X can be a Cl, Br or I ion. Our results show larger band gaps then previous calculations using only local density approximation (LDA) or generalized gradient approximation (GGA) [1, 2]. Our QSGW gaps are in good agreement with experiment. An analysis of the orbital character of the bands, shows that the valence band maximum has a strong Sn-s X-p antibonding character, while the conduction band minimum has Sn-p character. The direct gap thus has a strong intra-atomic Sn-s to Sn-p character which explains to first order why these materials have strong luminescence. Our calculations for Cl, Br and I show that the variation of the anion only has a moderate effect on the band gaps. We also performed GW calculations for the tetragonal (β-phase) $CsSnI_3$ in order to study the band gap changes during the structural phase transition. It turns out that the QSGW correction from LDA are only weakly dependent on the structure. We thus can estimate the band gap of the orthorhombic (γ-phase) $CsSnI_3$ using the LDA results. The spin-orbit coupling effect is included in our calculations.

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