Abstract Submitted
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CsSnX3 (X= Cl, Br, I) band structure calculations by the QSGW method[1] LING-YI HUANG, WALTER R.L. LAMBRECHT, CWRU — $CsSnX_3$ (X=Cl,Br,I) perovskite compounds are of interest because of their strong photoluminescence and their potential application to solar cells. We present quasiparticle self-consistent GW (QSGW) calculations for the cubic (α-phase) including spin-orbit coupling and study the changes in band structures from the α-phase to the β- and γ-phases in LDA. The QSGW gaps are in good agreement with experiment. An analysis of the orbital character of the bands shows that they have an "inverted" band structure: the VBM has a non-degenerate s-like character (Sn-s and X-p antibonding), while the (CBM) has Sn-p character. The strongly intra-atomic dipole allowed nature of the direct gap explains the high photoluminescent intensity. The low hole mass indicates high hole mobility in agreement with experiment. The pressure dependence of the gap is found to be anomalous: the band gap decreases when the lattice constant is decreased. Effective masses and the Kohn-Luttinger type Hamiltonian of the CBM are extracted from the band structures and subsequently used to estimate exciton binding energies using our calculated dielectric constants. These indicate a much lower exciton binding energy for CsSnI3 than recently proposed.

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