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Inverted band structure and excitons in halide perovskites[1] WALTER R.L. LAMBRECHT, LING-YI HUANG, Case Western Reserve University — The halide perovskites $CsSnX_3$, X=I, Br, Cl have recently received attention for their application in photovoltaics. The high hole-mobility and optimal band gap (1.3 eV) of γ-$CsSnI_3$ make it attractive as both absorber and hole transport material in all solid-state Grätzel cells. We present self-consistent GW-calculations of the electronic band structures of $CsSnI_3$, $CsSnBr_3$, $CsSnCl_3$ in different phases. The most important finding is that these materials have an "inverted" band structure in the sense that the CBM consists of p-like Sn states while the VBM consists of Sn-s antibonding with halide p-states. The reasons for the location in $\mathbf{k}$-space of the direct gap and the nature of the band edge states are explained. The intra SnI_6 cluster bonding is the origin of various anomalies, such as the low hole mass, the anomalous temperature dependence of the gap with lattice expansion, the relative insensitivity to the anion, and the strong dipole allowed optical transitions. We show that when the phonon contribution to the screening is included, the exciton binding energy is two orders of magnitude smaller than with electronic screening only. The observed luminescence with high binding energy is argued to be due to a defect bound exciton.

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Walter Lambrecht
Case Western Reserve University

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