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Chemical trends in halide perovskite electronic properties[1] WALTER LAMBRECHT, LING-YI HUANG, Case Western Reserve University — The halide perovskites ABX_3 with B =Pb or Sn, X=I, and A=Cs or methylammionium (MA), have recently attracted attention as solar cell materials. We discuss the basic bonding, stability and electronic band structure of these materials for different chemical substitutions using first-principles calculations. An important feature of the Pb and Sn based halides is that these element's *s*-electrons strongly hybridize with the halogen *p*-orbitals leading to a valence band maximum with strong Sn or Pb-*s* character and small effective mass. The conduction band minimum is Sn or Pb *p*-like. We present trends in the electronic band structure with the halogen X =I, Br, Cl and the B cation Pb, Sn, Ge, Si. The gap is remarkably insensitive because of the opposing trends of the increased spin-orbit coupling for heavier elements (reducing the gap) and the decreased valence band width for heaver elements due to the larger B-X distance, which increases the gap. The stability of the perovskite structure *vs.* competing structures is influenced by the tolerance factor $t = R_{AC}/\sqrt{2}R_{BC}$. The smaller this factor, the least stable is the perovskite structure. $CsSiI_3$ is found to be a topological insulator. Its stability with respect to CsI and SiI_n is discussed.

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