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Quasiparticle band gap of organic-inorganic hybrid perovskites: Crystal structure, spin-orbit coupling, and self-energy effects[1] WEIWEI GAO, State Univ of NY - Buffalo, XIANG GAO, Beijing Computational Science Research Center, TESFAYE ABTEW, State Univ of NY - Buffalo, YIYANG SUN, SHENGBAI ZHANG, Rensselaer Polytechnic Institute, PEIHONG ZHANG, State Univ of NY - Buffalo — The quasiparticle band gaps of organic-inorganic hybrid perovskites are often determined (and can be controlled) by various factors, complicating predictive materials optimization. Here we report a comprehensive investigation on the band gap formation mechanism in $CH_3NH_3PbI_3$ by decoupling various contributing factors which ultimately determine their electronic structure and quasiparticle band gap. Four major factors, namely, quasiparticle self-energy, spin-orbit coupling, volume (lattice constant) effects, and structural distortions due to the presence of organic molecules, and their influences on the quasiparticle band structure of organometal hybrid perovskites are illustrated. We find that although methylammonium cations do not contribute directly to the electronic states near band edges, they play an important role in defining the band gap through a lattice distortion mechanism and by controlling the overall lattice constants (thus the chemical bonding of the optically active PbI_3^-). The spin-orbit coupling effects drastically reduce the electron and hole effective masses in these systems, which is beneficial for high carrier mobilities and small exciton binding energies.

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