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Bandstructure, optical spectra, and mean free paths in the room-temperature structure of $\text{CH}_3\text{NH}_3\text{PbI}_3$ from many-body perturbation theory¹ DEREK VIGIL-FOWLER, MARCO BERNARDI, STEVEN G. LOUIE, University of California at Berkeley and Lawrence Berkeley National Lab — The organometallic halide perovskites have generated enormous interest due to the rapidly increasing efficiency of solar cells fabricated from these materials. Most research on the organometallic halide perovskites has been experimental due to the challenges posed by these materials to theoretical study, including the size of the unit cell, the presence of many defects, the orientational disorder in of the methyammonium (MA) cation, and the heavy atoms involved with the corresponding large spin-orbit coupling (SOC). We study the room-temperature tetragonal structure of $\text{CH}_3\text{NH}_3\text{PbI}_3$ using density functional theory (DFT) and a many-body Green's functions approach. We use DFT to study the effect of the dependence of the bandstructure on the orientation of the MA cation, while we perform GW and GW plus Bethe-Salpeter equation (GW-BSE) calculations to study the quasiparticle bandstructure and optical spectra, respectively, paying close attention to convergence and the effect of SOC. We particularly investigate the existence of a proposed charge-transfer state in this material. We also briefly discuss the mean free paths due to electron-phonon and electron-electron scattering in the ideal structure.

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