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Density-functional theory calculations of hybrid perovskites for photovoltaics KUNTAL TALIT, DAVID A. STRUBBE, Univ of California - Merced — Hybrid organometallic perovskites ($CH_3NH_3PbI_3$), are a promising material for solar cell applications as the power conversion efficiencies for perovskite devices have risen significantly in recent years. If we are able to make the structure stable at ambient conditions, it may provide a grid-competitive efficiency at low manufacturing cost. We have performed first-principles density-functional theory (DFT) calculations on the cubic phase of $CH_3NH_3PbI_3$ using different exchange-correlation functionals to find optimized structures and noticed that the Van der Waals interaction plays a role for structural optimization. Band-structure calculations for different orientations (100 and 111) of the methylammonium ion within the unit cell indicates that the orientation does not change the overall shape of the band structure. By contrast, spin-orbit coupling significantly modifies the conduction bands, reducing the band gap. Calculated effective masses are compared with some previously published results. These preliminary calculations will help us to study light induced degradation mechanism in $CH_3NH_3PbI_3$.

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