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Structural, electronic and optical properties of CH₃NH₃PbI₃

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Organic-inorganic halide perovskites are promising candidates for low cost, high-efficiency solar cells. We examined the structural, electronic, and optical properties of the low temperature tetragonal phase of the halide peroviskite CH₃NH₃PbI₃ using Density Functional Theory (DFT). Our numerically predicted structure is in agreement with existing experimental data. DFT electronic structure calculations show that relativistic effects are important for the heavy lead atom and spin-orbit coupling has to be included for accurate results. The experimental band gap of 1.63 to 1.66 eV is similar in magnitude to the DFT direct gap of 1.72 eV, which suggests that many-body and relativistic effects cancel in this compound. Our calculated fundamental gap, at the G₀W₀ level of approximation, is 2.48 eV. Optical anisotropy of tetragonal CH₃NH₃PbI₃ was investigated by including many-body effects at the time dependent Hartree Fock and the Bethe-Salpeter equation level of approximation, with input data from a range separated Heyd-Scuseria-Ernzerhof DFT functional calculation. The optical edge for radiation polarised parallel to the a- and b-axes differ by about 0.15 eV and for polarisation parallel to the b- and c-axes the difference is about 0.05 eV.

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