Electronic structure calculations of Br-based halide perovskites

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Halide perovskites have gained large interest during the last years due to their rapidly growing solar cell photoconversion efficiency. However, it is still challenging to find a perovskite compound which provides high efficiency and good stability at the same time. In this work we investigate the electronic structure of several perovskites which are not much studied so far: perovskites with FA, Cs and Rb cations in combination with Br anions. For all of the compounds, we calculate band gaps with a PBE functional, both with and without spin-orbit interactions. We also calculate band gaps using GW calculations, which are shown to give band gaps closest to the experimental values. Additionally, we compare the electronic structures of FASnBr3 and FAPbBr3 and comment on the possible origins of the unusual gap inversion observed for these compounds.