Abstract Submitted
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Limiting factors for the power conversion efficiency of hybrid organic-inorganic halide perovskite photovoltaic devices under operating conditions.[1] OSCAR GRANAS, Department of Physics and Astronomy, Uppsala University, Sweden., DMITRY VINICHENKO, Department of Chemistry and Chemical Biology, Harvard University, United States., EFTHIMIOS KAXIRAS, Department of Physics, Harvard University, United States. — We use first-principles calculations and thermodynamic modelling to establish that the theoretical maximum efficiency limit is in the range of 25-27% under operating conditions. We examine compounds of ABX3 composition, where A=Methylammonium, Methyleniminium, Formamidinium, Guanidinium, B=Pb,Sn, X=Br,I with estimated bandgaps of 0.9 to 2.3 eV. Effective band masses and level alignments for all compounds are determined. Based on this data we setup an effective circuit model for a PIN-cell, including entropic contributions to the free energy of the carriers. Our results indicate that the state-of-the art perovskite based solar cells, due to their intrinsic resilience to defect-induced trap-states and interface quality is already above 80% of their theoretical maximum efficiency. Our result provide a useful framework for estimating the impact of level alignment to hole and electron transporting materials on the PCE. It also indicates the need for the use of multi-junction cells or hot-carrier extraction in order to reach cells of more than 27% power conversion efficiency at room temperature. [2]

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[2]O. Grånäs *et al.* Sci. Rep. 6, 36108; doi: 10.1038/srep36108 (2016)

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