Electrical Properties of Organic-Inorganic Hybrid Tin Bromide Cubic Perovskites: Hole-Doping and Iodide Substitution Effects

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Supporting information

Computational methods

All band structures were calculated by the WIEN2K package.[23] The PBE (Perdew-Burke-Ernzerhof) version of the generalized gradient approximation (GGA) was adopted for the calculation of the exchange-correlation energy within density functional theory (DFT). In order to mimic the real system, where the $CH_3NH_3^+$ cation is randomly rotating and the system has cubic symmetry, Cs^+ (cubic symmetry) was used as the cation in the calculations, together with the observed lattice parameters (a = 6.243 Å for the tin iodide system, and a = 5.890 Å for the tin bromide system). We found that band dispersions around the band gap were not affected by the different cation.

Electronic properties measurements

Diffuse reflectance spectra were measured using a JASCO V-570 UV-VIS-NIR spectrometer with an integrating sphere unit. The samples were ground with KBr. The measured reflectivity was converted by the Kubelka-Munk function.

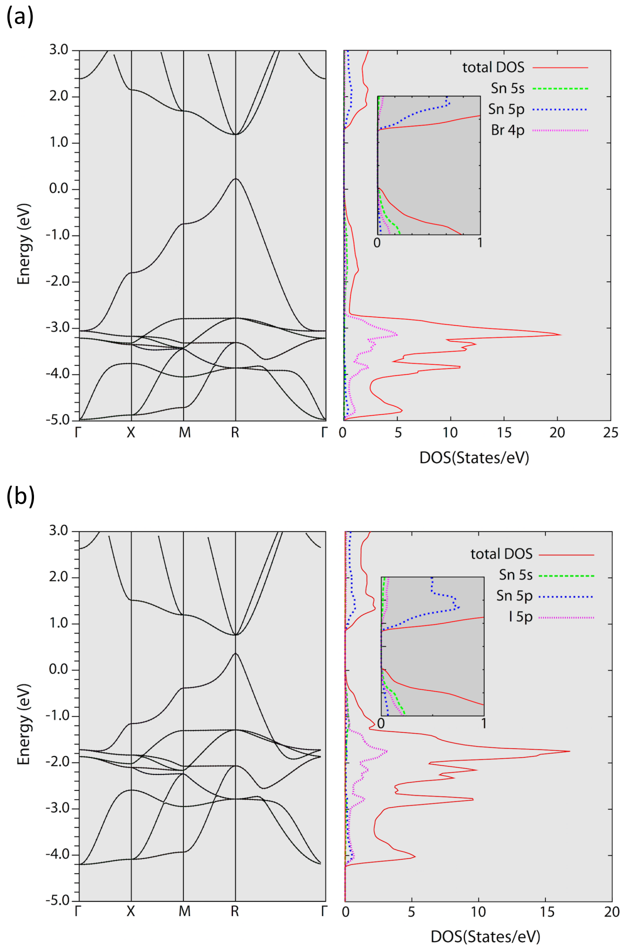

Figure S1. Band structures, total density of states (DOS), and projected density of states (PDOS) for the methylammonium tin (II) bromide (a) and iodide (b) cubic perovskites. The inset in the DOS plots for each perovskite is an enlargement of the region around the band gap.

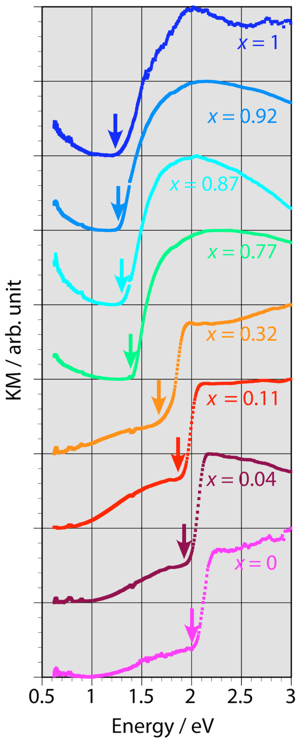

Figure S2. The diffuse reflectance spectra of $CH_3NH_3SnBr_{3(1-x)}I_{3x}$. The arrows mark the optical band gap for each substitution ratio.