Supplementary Information

Lead-Free 2D MASnBr₃ and Ruddlesden-Popper BA₂MASn₂Br₇ as Light Harvest Materials

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Solar Cell Efficiency Parameter

Moreover, we have investigated that 2D MASnBr₃ perovskite materials have strong optical absorption which is useful to improve solar cell efficiency. To find the performance of the 2D MASnBr₃ layer structure in the solar cell device. To better understand the performance of the solar cell, we have calculated open-circuit voltage (Voc), fill factor (FF), power conversion efficiency (η), short circuit current density (Jsc). As we know, Shockley and Quessier (SQ) model depend on the band gap (E_g) of material to calculate the performance of solar cell efficiency which gives A(E) = 1 if E>E_g and A(E) = 0 for E< E_g [5,41]. With all this calculation of solar cells, parameters are good agreement with the previously reported in experimental as well as theoretical results [5,41,43].

Table S1: Represents calculated solar cell parameters for tensile strain open circuit voltage, Fill Factor, short circuit current density, power conversion efficiency of of MASnBr₃ monolayer.

MASnBr ₃	0 %	2 %	4 %	6 %	8 %	10%
Voc (eV)	2.64	2.64	2.68	2.70	2.71	2.75
FF	0.9453	0.9453	0.9459	0.9462	0.9465	0.9471
Jsc (mA/cm ²)	9.40	9.03	8.35	7.31	6.94	5.56
η(%)	23.46	22.54	21.43	18.64	17.83	14.83

Table S2: Represents calculated solar cell parameters for compressive strain open circuit voltage, Fill Factor, short circuit current density, power conversion efficiency of of MASnBr₃ monolayer.

MASnBr ₃	0 %	2 %	4 %	6 %	8 %	10%
Voc (eV)	2.64	2.64	2.66	2.68	2.71	2.75
FF	0.9453	0.9453	0.9456	0.9459	0.9465	0.9471
Jsc (mA/cm ²)	9.40	8.64	8.25	7.31	6.22	5.07
η(%)	23.46	21.56	21.74	18.51	15.98	13.21

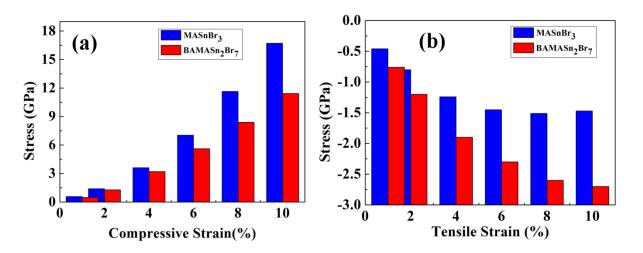


Fig. S1. Applied (a) Compressive and (b) Tensile strain varses Stress of MASnBr₃ and BAMASn₂Br₇.