

Supplementary Material

The feasibility of hybrid halide perovskites using mixed Ga and In as Pb alternatives

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Table S1: Calculated lattice parameters and band gaps (E_g) of the reference OIHP material.

Compound	Functionals	Theoretical				Experimental			
		a(Å)	b(Å)	c(Å)	E_g (eV)	a(Å)	b(Å)	c(Å)	E_g (eV)
MASnI ₃	LDA	6.55	13.66	9.44	0.82	8.556	12.428	8.326	1.3
	PBE	7.30	13.92	9.60	1.31				
	PBEsol	8.50	13.15	9.14	1.26				
	PBE0	8.53	13.17	9.16	2.10				
	HSE06	8.51	13.16	9.15	1.96				

Table S2: Band gap values of the reference compound with different k-point mesh for convergence test.

Compound	k-point mesh	Band gap (eV)
CH ₃ NH ₃ SnI ₃	2 x 2 x 2	1.30
	4 x 4 x 4	1.31

Relative phase compositions of the designed materials:

