Supporting Information

for

Understanding of the Formation of Shallow Level Defects from the Intrinsic Defects of Lead Tri-Halide Perovskites

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Table S1. Lattice structures (calculated lattice structures with the GGA exchange correlation), band gaps, and formation energies of the halide vacancy ($E_F(V_{Halide})$) and the Pb ($E_F(V_{Pb})$) of methylammonium lead trihalides. In this study, we used pseudo-tetragonal unit lattice structures for each perovskite.

	$MAPbI_3$	$MAPbBr_3$	$MAPbCl_3$
Lattice Constants	a=9.08 Å b=9.02Å c=12.77 Å	a=8.41 Å b=8.35 Å c=11.86 Å	a=8.14 Å b=8.00 Å c=11.28 Å
Band gap GGA (eV)	1.87	2.26	2.70
E_F (V_{Halide}) (eV)	2.21	2.93	3.28
E_F (V_{Pb}) (eV)	2.69	3.37	3.74