Supplementary Information for:

Ab Initio Static and Dynamic Study of CH₃NH₃PbI₃ Degradation in the Presence of Water, Hydroxyl Radicals, and Hydroxide Ions

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The computational errors from using finite k-point sampling in our calculations of different bulk crystals were assessed. For each bulk crystal, we calculated the energies of the relaxed structures using two sets of k-point mesh. Table SI1 shows the simulation details and the energy differences (ΔE) per formula unit obtained using the following equation: $\Delta E = (E_2 - E_1)/Z$. E_1 is the total energy with the smaller k-point mesh, E_2 is the total energy using the larger k-point mesh, and Z is the number of formula units in the simulation cell. The absolute values of the energy differences are within 0.13 kcal/mol for all the crystals considered. The errors from our choice of the k-point meshes for different crystals are insignificant. The energetic results reported in this work were all calculated from the energies using the larger k-point meshes.

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Table SI1 The simulation details and the energy difference per formula unit (in kcal/mol) between the smaller k-point mesh and the larger k-point mesh for different crystals.

Crystal	Simulation cell (Å)	Number of formula units	K-point mesh		ΔE (kcal/mol)
			(1)	(2)	
$MAPbI_3$	$8.85 \times 8.85 \times 12.64$	4	$4 \times 4 \times 4$	$6 \times 6 \times 6$	-0.02
$MAPbI_3 \cdot H_2O$	$10.39 \times 4.64 \times 11.11$	2	$5 \times 8 \times 5$	$7 \times 9 \times 7$	-0.06
$MA_4PbI_6 \cdot 2H_2O$	$10.39 \times 11.31 \times 10.55$	2	$4 \times 4 \times 4$	$6 \times 6 \times 6$	-0.13
MAI	$5.12 \times 5.12 \times 9.01$	2	$8 \times 8 \times 6$	$10 \times 10 \times 8$	0.01
PbI_2	$4.56 \times 4.56 \times 6.98$	1	$6 \times 6 \times 6$	$8 \times 8 \times 8$	-0.01
α-PbO	$3.96 \times 3.96 \times 5.01$	2	$8 \times 8 \times 8$	$10 \times 10 \times 10$	0.07
β-PbO	$5.88 \times 5.48 \times 4.74$	4	$6 \times 6 \times 6$	$8 \times 8 \times 8$	0.01
I_2	$7.27 \times 9.79 \times 4.79$	4	$8 \times 7 \times 10$	$10 \times 8 \times 12$	0.01