

## Supporting Information for

### In silico Optimization of Organic-inorganic Hybrid Perovskites for Photocatalytic Hydrogen Evolution Reaction in Acidic Solution

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**Table S1.** The geometry and energy differences calculated by a force convergence criteria of 0.05 eV/Å and 0.03 eV/Å, respectively.

Force convergence	Initial structure		Intermediate structure		Final structure ΔE
	ΔE	H...Pb distance	ΔE	H-Pb bond length	
0.05 eV/Å	0	3.917 Å	-1.349 eV	1.970 Å	-3.645 eV
0.03 eV/Å	0	3.921 Å	-1.379 eV	1.973 Å	-3.656 eV