Hydrogen bonds delicately restraining photoelectric performance in hybrid perovskite

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Supplementary Information

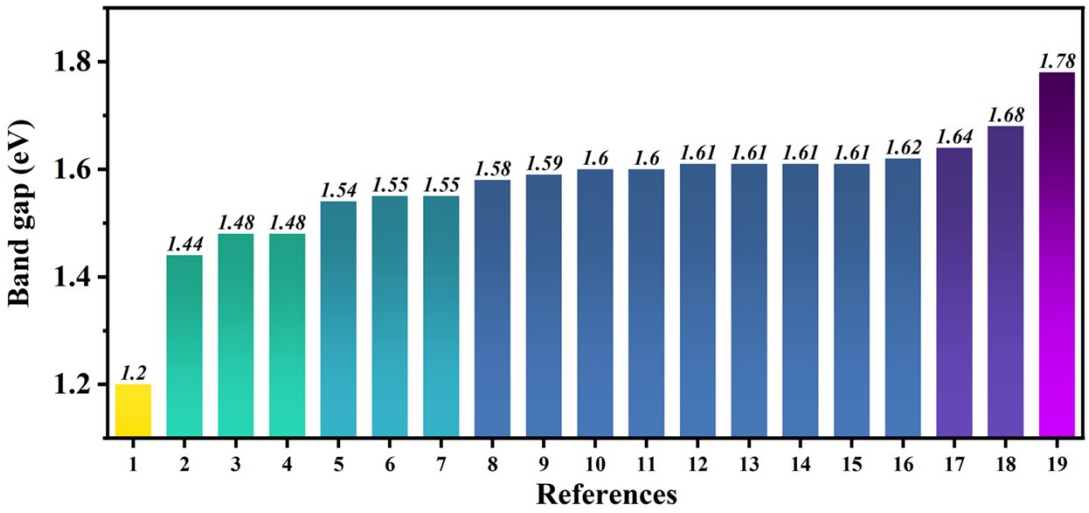

Fig. S1: Band gaps of tetragonal $MAPbI_3$ phase obtained from experimental and theoretical studies[1-19].

Table S1. The MA^+ orientation, lattice parameters and relative energy ΔE of the 61 tetragonal $MAPbI_3$ phase. ΔE is referenced to the lowest-energy structure of the 61 models.

Structure	MA^+ orientation	Lattice parameters a, b, c (Å)			ΔE (eV)
1	A+ A- A+ A-	8.9349	8.8135	13.0750	0.0247
2	A+ A+ A+ A-	8.8486	8.9103	13.0610	0.0045
3	A+ A+ A+ B+	8.7999	8.9569	13.0586	0.0846
4	A+ A- A+ B+	8.8420	8.9163	13.0716	0.0137

5	A+ A- A+ B-	8.8753	8.8950	13.0401	0.1032
6	A+ A+ A- B-	8.8462	8.9312	13.0439	0.0321
7	A+ B+ B- A-	8.8700	8.9626	12.9875	0.0757
8	B+ B+ A+ A-	8.8323	8.9320	13.0505	0.1024
9	B+ B- A+ A+	8.8339	8.9297	13.0528	0.0986
10	B+ B- A- A-	8.9294	8.8308	13.0459	0.1322
11	B+ B- A- A+	8.8628	8.8751	13.0848	0.0026
12	B+ A+ B+ A+	8.8149	8.9273	13.0848	0.0175
13	B+ A- B+ A-	8.8308	8.9630	13.0202	0.1324
14	B+ A+ B+ A-	8.8830	8.8801	13.0646	0.1363
15	B+ A+ B- A+	8.8457	8.9171	13.0652	0.1385
16	B+ A- B- A-	8.8259	8.9200	13.0830	0.0000
17	A+ A+ A+ C-	8.8611	8.8913	13.0983	0.0431
18	A- A+ A+ C+	8.8968	8.9113	13.0173	0.1404
19	A+ A+ A- C+	8.9286	8.9573	12.9651	0.1686
20	A+ A- A+ C-	8.8792	8.8687	13.0935	0.0470
21	A+ C+ C+ A-	8.9021	8.8742	13.0657	0.1546
22	A+ C+ C- A+	8.9346	8.8756	13.0252	0.1534
23	A- C+ C- A-	8.9000	8.8730	13.0639	0.1713
24	A- C+ C- A+	8.9629	8.8545	13.0438	0.0993
25	C+ C+ A+ A-	8.8981	8.8720	13.0860	0.1087
26	C+ C- A+ A+	8.9049	8.8545	13.0579	0.0381
27	C+ C- A- A-	8.8761	8.8836	13.0907	0.1062
28	C+ C- A+ A-	8.8962	8.8427	13.0995	0.0056
29	C+ C- A- A+	8.9009	8.8380	13.0936	0.0072
30	C+ A- C+ A-	8.8944	8.8738	13.1084	0.0923
31	C+ A+ C+ A-	8.9439	8.9103	13.0422	0.2063
32	C+ A+ C- A+	8.9448	8.9207	13.0134	0.1802
33	C+ A- C- A-	8.9565	8.9459	12.9966	0.2181
34	C+ A+ C- A-	8.9387	8.9377	12.9832	0.2506
35	A+ A+ B+ C+	8.8787	8.9412	13.0252	0.0934
36	A+ B+ A+ C+	8.8755	8.9104	13.0787	0.0926
37	A+ A+ B- C-	8.8937	8.8983	13.0287	0.0461
38	A+ B- A+ C-	8.9329	8.8245	13.0807	0.1231
39	A+ B+ A+ C-	8.8459	8.9152	13.0822	0.0532
40	A+ A- B+ C+	8.8582	8.8951	13.0751	0.0224
41	A+ A- B- C-	8.9485	8.8853	12.9648	0.1566
42	A+ A- B- C+	8.9582	8.7811	13.0802	0.1285
43	A+ A- B+ C-	8.8769	8.8734	13.0651	0.0950
44	A+ B+ A- C-	8.8863	8.9285	13.0461	0.1501
45	A+ B- A- C+	8.8560	9.0227	12.9442	0.1773
46	A+ B- C+ A-	8.9010	8.9432	12.9944	0.1577
47	A+ C+ B+ D+	8.8999	8.8714	13.0582	0.1598
48	A- B+ C+ D+	8.9276	8.8414	13.0647	0.0128

49	A+ B+ C- D+	8.8663	8.9065	13.0486	0.0990
50	A+ B+ C+ D-	8.8936	8.8252	13.0974	0.1499
51	A+ C- B+ D+	8.8880	8.9646	13.0046	0.1559
52	A+ C+ B+ D-	8.9137	8.9576	12.9915	0.1567
53	A- B+ C- D+	8.8828	8.8810	13.0543	0.0960
54	A- B+ C+ D-	8.8829	8.8396	13.0983	0.1735
55	A+ B- C- D+	8.8877	8.8312	13.1038	0.1501
56	A+ B- C+ D-	8.8648	8.9251	13.0756	0.2484
57	A+ B+ C- D-	8.9146	8.9666	12.9043	0.2181
58	A- C+ B+ D-	8.9516	8.8169	13.0366	0.1040
59	A+ C- B- D+	8.9598	8.8122	13.0420	0.0824
60	A- B- D+ C+	8.9539	8.8831	12.9689	0.1038
61	A+ B+ D- C-	8.7794	9.0157	13.0196	0.0954
Average	-	8.8897	8.8968	13.0470	-

Table S2. Calculated and experimental structural parameters for tetragonal $MAPbI_3$ phase.

Methods	a (Å)	b (Å)	c (Å)	Average deviation (%)
PBE	9.03	9.03	13.36	3.25
PBE+optB86-vdW	8.88	8.88	13.05	1.31
PBE+D3	8.76	8.76	12.95	1.50
Experiment[20]	8.85	8.85	12.64	/

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