Electronic Supplementary Material (ESI) for RSC Advances.

Supporting information

Bandgap Tuning Strategy by Cations and Halide Ions of lead Halide Perovskites Learned from Machine Learning

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1. Machine learning data and results

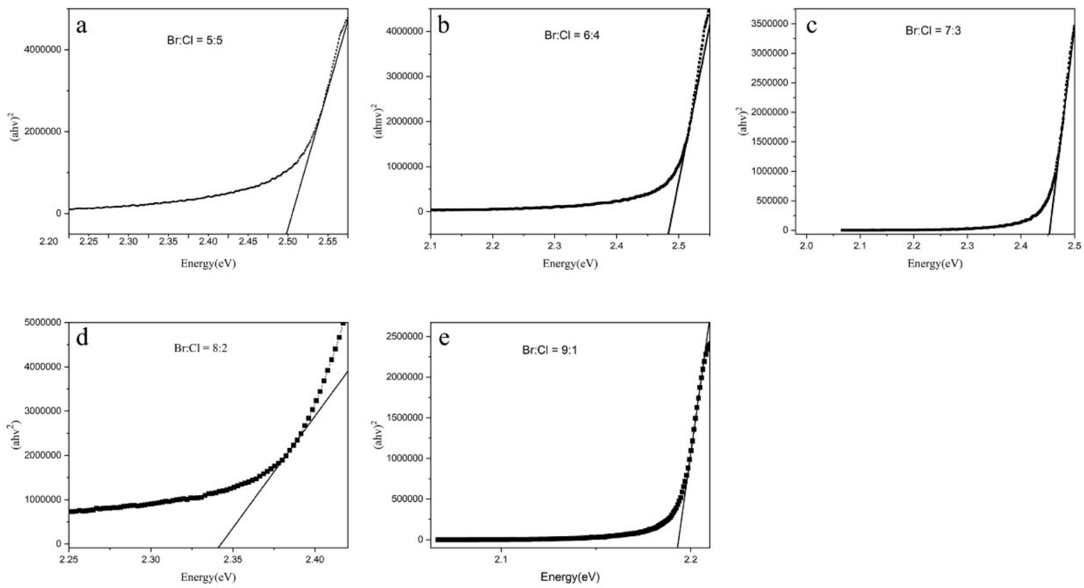


Fig. S1 Bandgaps of $CsPb(Cl_xBr_{1-x})_3$ (x=0.1-0.5) determined from their absorption profiles

Table S1 The compositions and the experimental bandgap values of the perovskites from literatures and our experiments (shown in Fig. S1). Some halide compositions in the literatures were normalized to make them fit the formula $MA_{(1-a-b)}FA_aCs_bPb(Cl_{(1-x-y)}Br_xI_y)_3$.[a]

ID	MA	FA	Cs	Cl	Br	I	Bandgap	Ref
1	1.00	0.00	0.00	0.00	0.00	1.00	1.60	[1]
2	0.70	0.20	0.10	0.00	0.00	1.00	1.56	[2]
3	0.50	0.40	0.10	0.00	0.00	1.00	1.54	[2]
4	0.40	0.50	0.10	0.00	0.00	1.00	1.52	[2]
5	0.25	0.75	0.00	0.00	0.00	1.00	1.55	[3]
6	0.20	0.70	0.10	0.00	0.00	1.00	1.49	[2]
7	0.17	0.83	0.00	0.00	0.00	1.00	1.53	[4]
8	0.00	0.80	0.20	0.00	0.00	1.00	1.57	[5]
9	0.00	0.83	0.17	0.00	0.00	1.00	1.56	[6]
10	0.00	0.85	0.15	0.00	0.00	1.00	1.54	[7]
11	0.00	0.90	0.10	0.00	0.00	1.00	1.53	[7]
12	0.00	0.95	0.05	0.00	0.00	1.00	1.52	[8]
13	0.00	1.00	0.00	0.00	0.00	1.00	1.48	[9]
14	0.15	0.85	0.00	0.00	0.05	0.95	1.54	[10]
15	0.00	0.80	0.20	0.00	0.06	0.94	1.58	[11]
16	1.00	0.00	0.00	0.00	0.07	0.93	1.68	[12]
17	1.00	0.00	0.00	0.00	0.10	0.90	1.61	[13]
18	0.15	0.85	0.00	0.00	0.10	0.90	1.57	[10]
19	0.10	0.85	0.05	0.00	0.10	0.90	1.55	[14]
20	0.05	0.85	0.10	0.00	0.10	0.90	1.57	[14]
21	0.05	0.90	0.05	0.00	0.10	0.90	1.52	[14]
22	0.00	0.90	0.10	0.00	0.10	0.90	1.53	[14]
23	0.00	0.95	0.05	0.00	0.10	0.90	1.48	[14]
24	1.00	0.00	0.00	0.00	0.12	0.88	1.62	[15]
25	0.12	0.83	0.05	0.00	0.13	0.87	1.60	[16]
26	0.15	0.79	0.06	0.00	0.15	0.85	1.75	[17]
27	0.14	0.81	0.05	0.00	0.15	0.85	1.61	[18]
28	0.13	0.76	0.10	0.00	0.15	0.85	1.61	[18]

29	0.16	0.79	0.05	0.00	0.17	0.83	1.60	12
30	0.15	0.75	0.10	0.00	0.17	0.83	1.50	19
31	0.10	0.40	0.50	0.00	0.17	0.83	1.69	20
32	0.00	0.50	0.50	0.00	0.17	0.83	1.62	20
33	0.00	0.83	0.17	0.00	0.17	0.83	1.65	6
34	1.00	0.00	0.00	0.00	0.20	0.80	1.72	21
35	0.70	0.30	0.00	0.00	0.20	0.80	1.69	22
36	0.20	0.80	0.00	0.00	0.20	0.80	1.63	10
37	0.16	0.79	0.06	0.00	0.22	0.78	1.60	19
38	0.25	0.75	0.00	0.00	0.25	0.75	1.66	10
39	0.15	0.85	0.00	0.00	0.25	0.75	1.65	10
40	1.00	0.00	0.00	0.00	0.27	0.73	1.75	23
41	0.00	0.17	0.83	0.00	0.27	0.73	1.72	24
42	0.00	0.15	0.85	0.00	0.27	0.73	1.72	23
43	1.00	0.00	0.00	0.00	0.30	0.70	1.77	25
44	0.30	0.70	0.00	0.00	0.30	0.70	1.70	10
45	0.15	0.85	0.00	0.00	0.30	0.70	1.68	10
46	0.00	0.60	0.40	0.00	0.30	0.70	1.75	26
47	0.00	0.80	0.20	0.00	0.30	0.70	1.75	27
48	0.00	0.00	1	0.00	0.33	0.67	1.92	28
49	0.00	0.83	0.17	0.00	0.33	0.67	1.74	6
50	1.00	0.00	0.00	0.00	0.33	0.67	1.75	12
51	0.35	0.65	0.00	0.00	0.35	0.65	1.74	10
52	0.15	0.85	0.00	0.00	0.35	0.65	1.71	10
53	0.90	0.00	0.10	0.00	0.40	0.60	1.80	29
54	0.60	0.40	0.00	0.00	0.40	0.60	1.76	30
55	0.40	0.60	0.00	0.00	0.40	0.60	1.76	8
56	0.40	0.00	0.60	0.00	0.40	0.60	1.75	30
57	0.15	0.74	0.11	0.00	0.40	0.60	1.78	31

58	0.00	0.40	0.60	0.00	0.40	0.60	1.76	30
59	0.00	0.83	0.17	0.00	0.40	0.60	1.74	32
60	1.00	0.00	0.00	0.00	0.42	0.58	1.79	15
61	0.45	0.55	0.00	0.00	0.45	0.55	1.81	10
62	0.15	0.85	0.00	0.00	0.45	0.55	1.79	10
63	1.00	0.00	0.00	0.00	0.50	0.50	1.90	33
64	0.50	0.50	0.00	0.00	0.50	0.50	1.85	10
65	0.17	0.83	0.00	0.00	0.50	0.50	1.80	34
66	0.16	0.79	0.05	0.00	0.40	0.60	1.80	35
67	0.00	0.00	1.00	0.00	0.50	0.50	2.10	36
68	0.00	0.83	0.17	0.00	0.50	0.50	1.80	12
69	1.00	0.00	0.00	0.00	0.59	0.41	1.96	15
70	0.15	0.79	0.06	0.00	0.60	0.40	1.78	17
71	0.15	0.85	0.00	0.00	0.60	0.40	1.76	10
72	0.00	0.87	0.13	0.00	0.60	0.40	1.93	24
73	1.00	0.00	0.00	0.00	0.67	0.33	1.98	37
74	0.00	0.83	0.17	0.00	0.67	0.33	1.96	6
75	0.00	0.00	1.00	0.00	0.67	0.33	2.05	38
76	0.00	0.85	0.15	0.00	0.70	0.30	2.00	39
77	0.00	1.00	0.00	0.00	0.90	0.10	1.97	40
78	1.00	0.00	0.00	0.00	0.72	0.28	2.01	15
79	0.00	0.83	0.17	0.00	0.83	0.17	2.07	6
80	0.15	0.85	0.00	0.00	0.85	0.15	1.60	41
81	1.00	0.00	0.00	0.00	0.95	0.05	2.23	15
82	1.00	0.00	0.00	0.00	1.00	0.00	2.30	42
83	1.00	0.00	0.00	0.20	0.80	0.00	2.55	43
84	1.00	0.00	0.00	0.40	0.60	0.00	2.69	43
85	1.00	0.00	0.00	0.60	0.40	0.00	2.84	43
86	1.00	0.00	0.00	0.80	0.20	0.00	2.98	43

87	0.17	0.83	0.00	0.00	1.00	0.00	2.23	[4]
88	0.17	0.83	0.00	0.10	0.90	0.00	2.27	[4]
89	0.00	0.00	1.00	0.00	1.00	0.00	2.30	[44]
90	0.00	1.00	0.00	0.00	1.00	0.00	2.30	[45]
91	0.00	0.00	1.00	1.00	0.00	0.00	3.00	[46]
92	0.00	1.00	0.00	1.00	0.00	0.00	3.00	[47]
93	1.00	0.00	0.00	0.17	0.83	0.00	2.46	[48]
94	1.00	0.00	0.00	0.38	0.62	0.00	2.64	[48]
95	1.00	0.00	0.00	0.44	0.56	0.00	2.68	[48]
96	1.00	0.00	0.00	0.50	0.50	0.00	2.75	[48]
97	1.00	0.00	0.00	0.56	0.44	0.00	2.79	[48]
98	1.00	0.00	0.00	0.64	0.36	0.00	2.81	[48]
99	1.00	0.00	0.00	0.69	0.31	0.00	2.84	[48]
100	1.00	0.00	0.00	0.71	0.29	0.00	2.88	[48]
101	1.00	0.00	0.00	0.93	0.07	0.00	3.13	[48]
102	1.00	0.00	0.00	1.00	0.00	0.00	3.16	[48]
103	1.00	0.00	0.00	0.33	0.67	0.00	2.57	[49]
104	1.00	0.00	0.00	0.67	0.33	0.00	2.81	[49]
105	1.00	0.00	0.00	0.10	0.90	0.00	2.19	This work
106	0.00	0.00	1.00	0.20	0.80	0.00	2.33	This work
107	0.00	0.00	1.00	0.30	0.70	0.00	2.45	This work
108	0.00	0.00	1.00	0.40	0.60	0.00	2.47	This work
109	0.00	0.00	1.00	0.50	0.50	0.00	2.49	This work

a Summary of the data listed in Table S1

	MA	FA	Cs	Cl	Br	I	Bandgap
Min.	0.000	0.000	0.000	0.000	0.000	0.000	1.480
Median	0.150	0.5500	0.0000	0.0000	0.310	0.6000	1.760
Mean	0.383	0.4501	0.1669	0.1158	0.356	0.5283	1.952
Max.	1.0000	1.0000	1.0000	1.0000	1.0000	1.0000	3.160

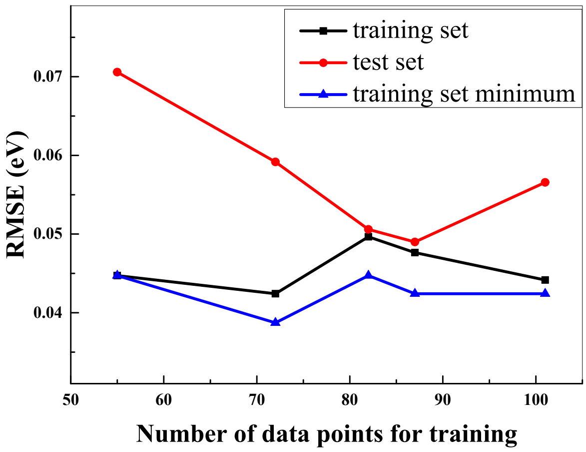


Fig. S2 The dependence of RMSE on the number of data points for training using NN algorithm. The RMSE values of training set and test set are obtained in the condition of the minimum RMSE on test set. The RMSE values of training set minimum represent for the minimum RMSE obtained by on the training set.

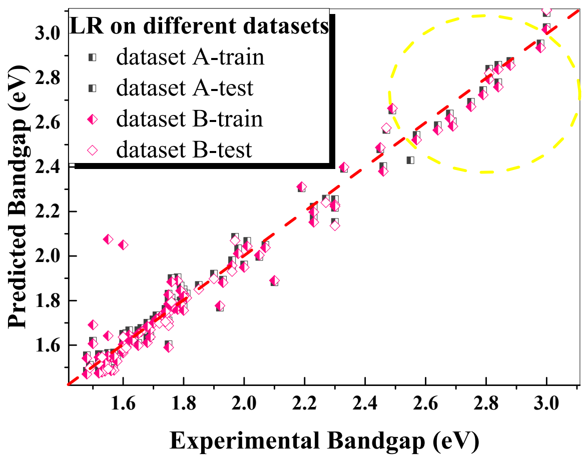


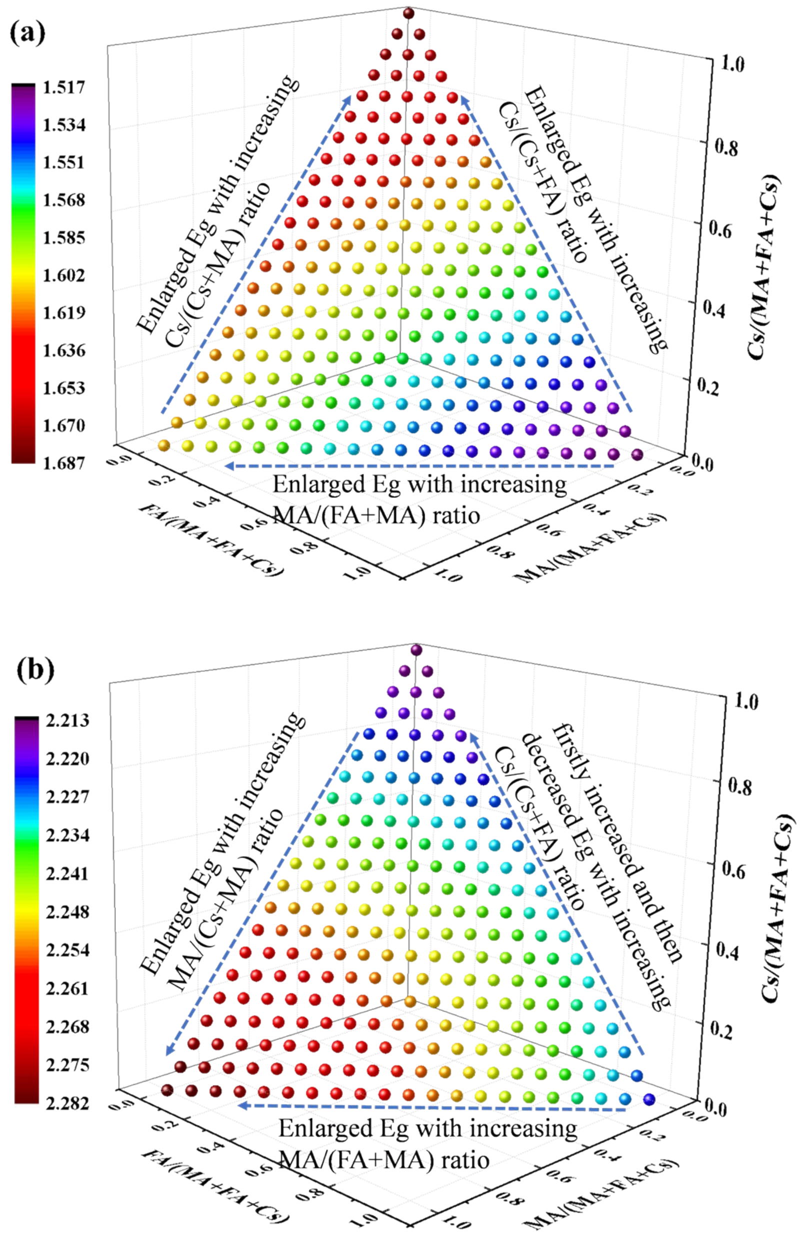
Fig.S3 Comparison of the performance of linear regression algorithm on different datasets. The red dash line presents the condition in which the predicted value equals to the experimental value. Dataset A includes all the data points listed in Table S1, while dataset B includes dataset A and three additional data points ($MAPb(Cl_{0.05}I_{0.95})_3$ (E_g=1.55eV[50]), $MAPb(Cl_{0.33}I_{0.67})_3$ (E_g=1.55eV[51]), $FA_{0.3}MA_{0.7}Pb(Cl_{0.1}I_{0.9})_3$ (E_g=1.5eV[52])).

Table S2 Importance of the input features presented by different algorithms

Input feature	RF	LR
	% increase in mean squared error	Coefficient in equation (1)
FA	22.1	-0.102

Cs	12.8	-0.039
Br	19.6	0.669
Cl	36.6	1.543

2. Prediction results by neuronal network algorithm



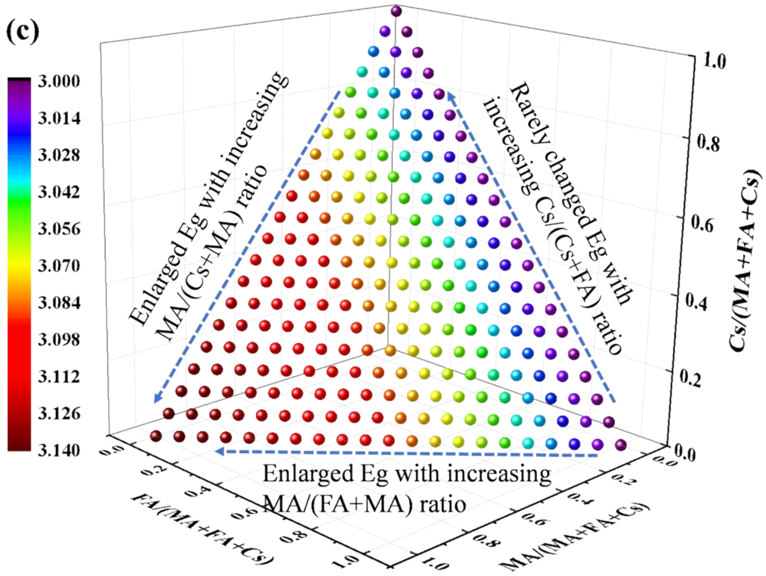


Fig. S5 4D plots of the predicted bandgap (unit: eV) of $Cs_aFA_bMA_{(1-a-b)}PbX_3$, X=I, Br and Cl, respectively, with different cation ratios by neutral net algorithm trained by the experimental data listed in Table S1.

Table S3 The compositions of the $FACsPb(Cl_{(0.2-x)}Br_xI_{0.8})_3$ perovskites with the predicted bandgaps of 1.650-1.710 eV and 1.780-1.840 eV by neutral net algorithm trained by the experimental data listed in Table S1.

Bandgap	FA/(FA+MA+Cs)	Cs/(FA+MA+Cs)	Br/(Cl+Br+ I)	Cl/(Cl+Br+ I)
1.784	0	1	0.20	0
1.651	0.7	0.3		
1.827	0	1	0.15	0.05
1.818	0.05	0.95		
1.808	0.1	0.9		
1.798	0.15	0.85		
1.788	0.2	0.8		
1.697	0.7	0.3		
1.688	0.75	0.25		
1.680	0.8	0.2		
1.672	0.85	0.15		
1.664	0.9	0.1		
1.657	0.95	0.05		
1.801	0.4	0.6	0.10	0.10
1.792	0.45	0.55		
1.783	0.5	0.5		
1.838	0.2	0.8		

1.828	0.25	0.75
1.819	0.3	0.7
1.699	0	1
1.810	0.35	0.65

Table S4 Experimental and theoretical efficiencies of the TSCs based on perovskite

TSC type	Bottom cell	Theoretical efficiency limit and the optimized bandgap of perovskite	Perovskite bandgap	efficiency
4T	Si	45.3% and 1.81 eV from detailed balance theory[54]	1.74	19.8[32]
			1.75	21.18[55]
			1.63	28.2[56]
			1.72	27.1[57]
			1.63	26.4[58]
			1.55	25.2[59]
	CIGS	Similar to above	1.6	20.7[60]
			1.62	23.9[61]
			1.68	25.9[62]
			1.75	23.4[61]
2T	Si	45.1% and 1.73 eV from detailed balance theory[54]	1.60	25.2[63]
			1.68	25.0[63]
			1.66	25.5[64]
			1.64	25.4[65]
	CIGS	Similar to above	1.72	10.98[66]
			1.59	22.43[67]

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