Supporting information

Predicting the photon energy of quasi-2D lead halide perovskites from the precursor composition through machine learning

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Table S1 The compositions and the experimental photon energy values of the perovskites from literature.

The column named L represents the name of the organic spacer cation. The columns named MA, FA, Cs, Cl, Br are the ions ratios under the conditions the sum of MA, FA and Cs equals to 1 and the sum of Cl and Br equals 1. P2L and P2A represent the molar ratio of Pb^{2+} to organic spacer cation (abbreviated as P2L) and of Pb^{2+} to organic cation (abbreviated as P2A) in the precursor solution, respectively. The photon energy was calculated from the emission peak wavelength (most of them are electroluminescence wavelengths).

ID	L[a]	MA	FA	Cs	Cl	Br	P2L	P2A	Photon energy	Ref
1	PEA	0	0	1	0	1	2.5	0.77	2.40	1
2	PEA	0	0	1	0	1	2.5	0.63	2.39	1
3	PEA	0	0	1	0	1	2.5	0.53	2.40	1

4	PEA	0	0	1	0	1	2.5	0.45	2.40	1
5	BA	0	0	1	0	1	2.5	0.83	2.43	2
6	PEA	0.2	0	0.8	0	1	2	1.33	2.38	3
7	PEA	0	0	1	0	1	1.5	1.5	2.59	4
8	PEA	0	1	0	0	1	1	2	2.34	5
9	PEA	0	1	0	0	1	2.5	1.25	2.32	5
10	PEA	0	0	1	0	1	2.5	1	2.45	6
11	PEA	0	0	1	0	1	2.5	0.91	2.40	7
12	PEA	0	0	1	0	1	2	1	2.40	8
13	BA	0	0	1	0.58	0.42	1.387	0.86	2.66	9
14	BA	0	0	1	0.16	0.84	1.387	0.86	2.55	9
15	BA	0	0	1	0	1	1.387	0.86	2.45	9
16	PEA	0.5	0.5	0	0	1	2	1	2.38	10
17	PEA	0	0	1	0	1	2	0.97	2.42	11
18	PEA	0	0	1	0	1	0.91	1.1	2.62	12
19	PEA	0	0	1	0	1	0.83	1.25	2.68	12
20	PEA	0	1	0	0	1	2	1.33	2.36	13
21	PMA	0	1	0	0	1	1.5	1.5	2.32	14
22	$PEA_{0.67}NPA_{0.33}$	0	0	1	0	1	1	1.5	2.56	15
23	PA	0	0	1	0	1	1	1	2.55	16
24	PBA	0	1	0	0	1	2.22	0.83	2.31	17
25	$PBA_{0.87}PA_{0.13}$	0	1	0	0	1	1.92	0.83	2.32	17
26	$PBA_{0.76}PA_{0.24}$	0	1	0	0	1	1.69	0.83	2.32	17
27	$PBA_{0.62}PA_{0.38}$	0	1	0	0	1	1.37	0.83	2.37	17
28	PEA	0	1	0	0	1	1.75	1.4	2.34	18
29	BA	0	0	1	0	1	2	1	2.43	19
30	BA	0	0	1	0	1	1.25	1	2.45	19
31	BA	0	0	1	0	1	1	1	2.45	19
32	P-PDA	0	0	1	0	1	1	2	2.68	20

33	P-PDA	0	0	1	0	1	1.25	1.67	2.67	20
34	P-PDA	0	0	1	0	1	1.5	1.5	2.60	20
35	P-PDA	0	0	1	0	1	2	1.33	2.56	20
36	P-PDA	0	0	1	0	1	2.5	1.25	2.50	20
37	$P\text{-}PDA_{0.875}PEA_{0.125}$	0	0	1	0	1	1.25	1.67	2.67	20
38	$P\text{-}PDA_{0.75}PEA_{0.25}$	0	0	1	0	1	1.25	1.67	2.67	20
39	$P\text{-}PDA_{0.5}PEA_{0.5}$	0	0	1	0	1	1.25	1.67	2.63	20
40	$P\text{-}PDA_{0.75}PEA_{0.25}$	0	0	1	0	1	1.25	1.67	2.67	20
41	1-NMA	0	1	0	0	1	2	1	2.38	21
42	PEA	0	1	0	0	1	2	1	2.37	21
43	PBA	0	0.3	0.7	0	1	0.91	1	2.57	22
44	$PA_{0.15}PEA_{0.01}$	0	0	1	0	1	0.97	1.03	2.54	23
45	$PA_{0.15}PEA_{0.011}$	0	0	1	0	1	0.96	1.03	2.54	23
46	PEA	1	0	0	0	1	2	1	2.44	24
47	PEA	0.7	0.3	0	0	1	2	1	2.40	24
48	PEA	0.3	0.7	0	0	1	2	1	2.38	24
49	PEA	1	0	0	0	1	2	1.33	2.44	25
50	PEA	1	0	0	0	1	1.33	1.33	2.36	25
51	PEA	1	0	0	0	1	1	1.33	2.37	25
52	PEA	1	0	0	0	1	0.8	1.33	2.44	25
53	PEA	1	0	0	0	1	0.67	1.33	2.44	25
54	PEA	1	0	0	0	1	0.8	1	2.40	25
55	PEA	0	1	0	0	1	1.5	1.5	2.33	26
56	PEA	0	0	1	0	1	1.67	1	2.44	27
57	BA	0	1	0	0	1	1	2	2.34	28
58	BA	0	1	0	0	1	1.5	1.5	2.28	28
59	BA	0	1	0	0	1	2.5	1.25	2.28	28
60	BA	1	0	0	0	1	1.5	1.5	2.35	29
61	PEA	1	0	0	0	1	1.5	1.5	2.41	29

62	PEA	0	0	1	0	1	1	1	2.52	30
63	PBA	0	0	1	0.3	0.7	1.39	0.8	2.53	31
64	PBA	0	0	1	0.4	0.6	1.39	0.8	2.58	31
65	PBA	0	0	1	0.5	0.5	1.39	0.8	2.62	31
66	PBA	0	0	1	0	1	1.39	0.8	2.45	31
67	PBA	0	0	1	0.05	0.95	1.39	0.8	2.47	31
68	PBA	0	0	1	0.1	0.9	1.39	0.8	2.48	31
69	PBA	0	0	1	0.15	0.85	1.39	0.8	2.49	31
70	PBA	0	0	1	0.2	0.8	1.39	0.8	2.51	31
71	PBA	0	0	1	0.25	0.75	1.39	0.8	2.52	31
72	PBA	0	0	1	0.35	0.65	1.39	0.8	2.56	31
73	PBA	0	0	1	0.45	0.55	1.39	0.8	2.61	31
74	PEA	0	0	1	0.3	0.7	2.5	1	2.56	32
75	PEA	0	0	1	0.3	0.7	1.67	1	2.56	32
76	PEA	0	0	1	0.3	0.7	1.25	1	2.57	32
77	PEA	0	0	1	0.3	0.7	1	1	2.58	32
78	PEA	0	0	1	0.3	0.7	0.83	1	2.59	32
79	PEA	0	0	1	0.25	0.75	1	1	2.60	33
80	$PEA_{0.17}PA_{0.83}$	0	0	1	0	1	1	1.2	2.55	34
81	PEA	0	0	1	0.1	0.9	1.25	1	2.59	35
82	PBA	0	0	1	0	1	0.6	3	2.84	36
83	PBA	0	0	1	0	1	0.6	1.98	2.67	36
84	PBA	0	0	1	0	1	0.67	1.67	2.55	36
85	PBA	0	0	1	0	1	0.75	1.5	2.52	36
86	PEA	0.2	0	0.8	0.1	0.9	1.5	1.5	2.42	37
87	PEA	0.2	0	0.8	0.2	0.8	1.5	1.5	2.48	37
88	PEA	0.2	0	0.8	0.3	0.7	1.5	1.5	2.48	37
89	PEA	0.2	0	0.8	0	1	1.5	1.5	2.54	37
90	p-F-PEA	0	0.11	0.89	0.5	0.5	2	0.52	2.64	38

91	PEA	0.17	0	0.83	0	1	1.25	1.67	2.42	39
92	$PEA_{0.4}IPA_{0.1}$	0.17	0	0.83	0	1	1.11	1.67	2.43	39
93	$PEA_{0.4}IPA_{0.2}$	0.17	0	0.83	0	1	1	1.67	2.45	39
94	$PEA_{0.4}IPA_{0.4}$	0.17	0	0.83	0	1	0.83	1.67	2.51	39
95	$PEA_{0.4}IPA_{0.6}$	0.17	0	0.83	0	1	0.71	1.67	2.62	39
96	$PEA_{0.4}IPA_{0.4}$	0.25	0	0.75	0	1	0.83	1.67	2.53	39
97	$PEA_{0.4}IPA_{0.4}$	0.33	0	0.67	0	1	0.83	1.67	2.62	39
98	PEA	0	0	1	0	1	1.5	1.15	2.44	40
99	PEA	0	0	1	0	1	1.5	0.93	2.46	40
100	PEA	0	0	1	0	1	1.5	0.83	2.50	40
101	EA	1	0	0	0	1	1.18	1.54	2.56	41
102	EA	1	0	0	0	1	1.33	1.33	2.41	41
103	POEA	1	0	0	0	1	2.5	0.33	2.46	42
104	POEA	1	0	0	0	1	1.67	0.33	2.38	42
105	POEA	1	0	0	0	1	1.25	0.33	2.44	42
106	POEA	1	0	0	0	1	0.83	0.33	2.68	42

a: Abbreviations of the large spacer cations: phenylethylamine (PEA), butylamine (BA), N-(2-Bromoethyl)-1,3-propanediamine (NPA), Propylamine (PA), 4-Phenylbutylamine (PBA), 1,2-Bis(bromomethyl)benzene (P-PDA), 1-naphthylmethylamine (1-NMA), 4-Fluorophenethylamine (p-F-PEA), iso-propylammonium (IPA), 2-phenoxyethylamine (POEA).

Table S2 Summary of the data listed in Table S1

	XLogP3	FA ratio	Cs ratio	Br ratio	P2L	P2A	Photon energy
Min.	0.620	0.0000	0.0000	0.4200	0.600	0.33	2.280
Median	2.370	0.0000	1.0000	1.0000	1.390	1.00	2.465
Mean	2.432	0.1595	0.6619	0.9392	1.474	1.17	2.487
Max.	3.370	1.0000	1.0000	1.0000	2.500	3.00	2.840

Table S3 Parameter settings for quasi-2D perovskite precursor compositions

Features	P2L	P2A	XLogP3	Cs	FA	Br

Settings	0.6-1.6, step 0.1	1.4-2.4, step 0.2	1.6-4.0, step 0.3	0.75-1.0, step 0.05	=1-(Cs ratio)	0-1, step 0.1

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