

Supporting Information

Using Data Mining to Search for Perovskite Materials with Higher Specific Surface Area

Li Shi^a, Dongping Chang^b, Xiaobo Ji^a, Wencong Lu^{a,b}

^a *Department of Chemistry, College of Sciences, Shanghai University, Shanghai 200444, China*

^b *Materials Genome Institute, Shanghai University, and Shanghai Materials Genome Institute, Shanghai 200444, China*

Corresponding author phone:(086-021-66132406); email: wclu@shu.edu.cn

Table S1 :The SSA and features of 50 samples of perovskites

NO.	Molecular	SSA	Ra	Rb	Ea	Eb	TF	aO3	re	Za	Zb	Ra/Rb	Mass
1	ZnTiO3	1.05	74	67	1.65	1.54	0.731	160.524	-21.762	9.394	6.828	1.104	161.27
2	LaFeO3	1.08	103.2	55	1.1	1.83	0.882	132.552	11.855	5.577	7.902	1.876	242.75
3	BiFeO3	0.7514	103	55	2.02	1.83	0.881	132.55	11.727	7.286	7.902	1.873	312.85
4	BiTi0.15Fe0.85O3	0.9507	103	56.8	2.02	1.7865	0.873	136.795	9.959	7.286	7.741	1.813	311.6545
5	LaCoO3	17	103.2	54.5	1.1	1.88	0.884	131.373	12.341	5.577	7.881	1.894	245.83
6	LaCo0.94Mg0.06O3	19	103.2	55.55	1.1	1.8458	0.879	133.849	11.318	5.577	7.867	1.858	243.7528
7	LaCo0.90Mg0.10O3	21	103.2	56.25	1.1	1.823	0.876	135.5	10.631	5.577	7.858	1.835	242.368
8	LaCo0.80Mg0.20O3	22	103.2	58	1.1	1.766	0.869	139.627	8.898	5.577	7.834	1.779	238.906
9	La0.5Bi0.2Ba0.2Mn0.1FeO3	27.75	105	55	1.287	1.83	0.888	132.569	13.005	6.031	7.902	1.909	248.054
10	La0.5Bi0.2Ba0.2Mn0.1FeO3	20.63	105	55	1.287	1.83	0.888	132.569	13.005	6.031	7.902	1.909	248.054
11	La0.5Bi0.2Ba0.2Mn0.1FeO3	12.46	105	55	1.287	1.83	0.888	132.569	13.005	6.031	7.902	1.909	248.054
12	La0.5Bi0.2Ba0.2Mn0.1FeO3	5.91	105	55	1.287	1.83	0.888	132.569	13.005	6.031	7.902	1.909	248.054
13	La0.5Bi0.2Ba0.2Mn0.1FeO3	4.19	105	55	1.287	1.83	0.888	132.569	13.005	6.031	7.902	1.909	248.054
14	LaFeO3	11.39	103.2	55	1.1	1.83	0.882	132.552	11.855	5.577	7.902	1.876	242.75
15	LaMg0.2Fe0.8O3	15.07	103.2	58.4	1.1	1.726	0.867	140.571	8.499	5.577	7.851	1.767	236.442
16	LaMg0.4Fe0.6O3	17.63	103.2	61.8	1.1	1.622	0.852	148.589	5.063	5.577	7.8	1.67	230.134
17	LaMg0.6Fe0.4O3	24.41	103.2	65.2	1.1	1.518	0.838	156.608	1.55	5.577	7.749	1.583	223.826
18	LaMg0.8Fe0.2O3	13.32	103.2	68.6	1.1	1.414	0.824	164.626	-2.036	5.577	7.697	1.504	217.518
19	LaMgO3	8.65	103.2	72	1.1	1.31	0.811	172.644	-5.692	5.577	7.646	1.433	211.21
20	LaCrO3	3.95	103.2	61.5	1.1	1.66	0.853	147.882	5.369	5.577	6.767	1.678	238.9
21	LaMg0.2Cr0.8O3	8.42	103.2	63.6	1.1	1.59	0.845	152.834	3.212	5.577	6.942	1.623	233.362
22	LaMg0.4Cr0.6O3	29.71	103.2	65.7	1.1	1.52	0.836	157.787	1.027	5.577	7.118	1.571	227.824
23	LaMg0.6Cr0.4O3	18.41	103.2	67.8	1.1	1.45	0.828	162.739	-1.186	5.577	7.294	1.522	222.286
24	LaMg0.8Cr0.2O3	14.46	103.2	69.9	1.1	1.38	0.819	167.692	-3.426	5.577	7.47	1.476	216.748
25	PrFeO3	10.88	99	55	1.13	1.83	0.867	132.512	9.147	5.473	7.902	1.8	244.75
26	LaFe0.9Co0.1O3	51.2	103.2	54.95	1.1	1.835	0.882	132.434	11.904	5.577	7.9	1.878	243.058
27	LaFe0.1Co0.9O3	42.8	103.2	54.55	1.1	1.875	0.884	131.491	12.293	5.577	7.883	1.892	245.522
28	LaFeO3	8.5	103.2	55	1.1	1.83	0.882	132.552	11.855	5.577	7.902	1.876	242.75
29	SrTiO3	16.4	118	67	0.95	1.54	0.881	160.991	9.581	5.695	6.828	1.761	183.5
30	La0.002Sr0.998TiO3	19.7	117.9704	67	0.9503	1.54	0.881	160.99	9.562	5.695	6.828	1.761	183.60256
31	La0.005Sr0.995TiO3	22.3	117.926	67	0.95075	1.54	0.881	160.99	9.533	5.694	6.828	1.76	183.7564
32	La0.01Sr0.99TiO3	24.1	117.852	67	0.9515	1.54	0.881	160.989	9.484	5.694	6.828	1.759	184.0128
33	La0.02Sr0.98TiO3	23.2	117.704	67	0.953	1.54	0.88	160.988	9.388	5.693	6.828	1.757	184.5256
34	LaFeO3	9.5	103.2	55	1.1	1.83	0.882	132.552	11.855	5.577	7.902	1.876	242.75
35	La0.5Bi0.2Ba0.2Mn0.1FeO3	25.8	103.2	55	1.1	1.83	0.882	132.552	11.855	5.577	7.902	1.876	242.75
36	La0.5Bi0.2Ba0.2Mn0.1FeO3	22.55	103.2	55	1.1	1.83	0.882	132.552	11.855	5.577	7.902	1.876	242.75
37	La0.5Bi0.2Ba0.2Mn0.1FeO3	20.04	103.2	55	1.1	1.83	0.882	132.552	11.855	5.577	7.902	1.876	242.75
38	La0.5Bi0.2Ba0.2Mn0.1FeO3	8.5	103.2	55	1.1	1.83	0.882	132.552	11.855	5.577	7.902	1.876	242.75
39	La0.5Bi0.2Ba0.2Mn0.1FeO3	5.8	103.2	55	1.1	1.83	0.882	132.552	11.855	5.577	7.902	1.876	242.75
40	LaNiO3	14.1	103.2	56	1.1	1.91	0.877	134.911	10.876	5.577	7.64	1.843	245.59
41	LaNiO3	12.7	103.2	56	1.1	1.91	0.877	134.911	10.876	5.577	7.64	1.843	245.59
42	LaNiO3	11.8	103.2	56	1.1	1.91	0.877	134.911	10.876	5.577	7.64	1.843	245.59
43	LaNiO3	6.5	103.2	56	1.1	1.91	0.877	134.911	10.876	5.577	7.64	1.843	245.59
44	LaNiO3	15.1	103.2	56	1.1	1.91	0.877	134.911	10.876	5.577	7.64	1.843	245.59
45	LaNiO3	12.2	103.2	56	1.1	1.91	0.877	134.911	10.876	5.577	7.64	1.843	245.59
46	LaFeO3	21.9	103.2	55	1.1	1.83	0.882	132.552	11.855	5.577	7.902	1.876	242.75

47	LaFeO3	15.37	103.2	55	1.1	1.83	0.882	132.552	11.855	5.577	7.902	1.876	242.75
48	LaFeO3	10.07	103.2	55	1.1	1.83	0.882	132.552	11.855	5.577	7.902	1.876	242.75
49	LaFeO3	5.24	103.2	55	1.1	1.83	0.882	132.552	11.855	5.577	7.902	1.876	242.75
50	LaFeO3	1.09	103.2	55	1.1	1.83	0.882	132.552	11.855	5.577	7.902	1.876	242.75

NO.	A-aff	B-aff	A-Tm	B-Tm	A-Tb	B-Tb	A_Hfus	B_Hfus	D-A	D-B	CT	AH	DT	Ref.
1	-58	7.6	419.53	1670	907	3287	108.1	295.6	7.14	4.51	900	2	120	1
2	48	15.7	918	1538	3464	2861	44.6	247.3	6.15	7.87	900	4	150	2
3	91.3	15.7	271.4	1538	1564	2861	53.3	247.3	9.79	7.87	900	4	150	2
4	91.3	14.485	271.4	1557.8	1564	2924.9	53.3	254.545	9.79	7.366	900	4	150	2
5	48	63.8	918	1495	3464	2927	44.6	272.5	6.15	8.86	750	4	110	3
6	48	57.632	918	1444.3	3464	2816.78	44.6	277.084	6.15	8.4328	750	4	110	3
7	48	53.52	918	1410.5	3464	2743.3	44.6	280.14	6.15	8.148	750	4	110	3
8	48	43.24	918	1326	3464	2559.6	44.6	287.78	6.15	7.436	750	4	110	3
9	36.46	15.7	783.28	1538	2626.7	2861	66.82	247.3	6.487	7.87	500	4	120	4
10	36.46	15.7	783.28	1538	2626.7	2861	66.82	247.3	6.487	7.87	600	4	120	4
11	36.46	15.7	783.28	1538	2626.7	2861	66.82	247.3	6.487	7.87	700	4	120	4
12	36.46	15.7	783.28	1538	2626.7	2861	66.82	247.3	6.487	7.87	800	4	120	4
13	36.46	15.7	783.28	1538	2626.7	2861	66.82	247.3	6.487	7.87	900	4	120	4
14	48	15.7	918	1538	3464	2861	44.6	247.3	6.15	7.87	600	5	100	5
15	48	4.76	918	1360.4	3464	2506.8	44.6	267.62	6.15	6.644	600	5	100	5
16	48	-6.18	918	1182.8	3464	2152.6	44.6	287.94	6.15	5.418	600	5	100	5
17	48	-17.12	918	1005.2	3464	1798.4	44.6	308.26	6.15	4.192	600	5	100	5
18	48	-28.06	918	827.6	3464	1444.2	44.6	328.58	6.15	2.966	600	5	100	5
19	48	-39	918	650	3464	1090	44.6	348.9	6.15	1.74	600	5	100	5
20	48	64.3	918	1907	3464	2671	44.6	404	6.15	7.15	600	5	100	6
21	48	43.64	918	1655.6	3464	2354.8	44.6	392.98	6.15	6.068	600	5	100	6
22	48	22.98	918	1404.2	3464	2038.6	44.6	381.96	6.15	4.986	600	5	100	6
23	48	2.32	918	1152.8	3464	1722.4	44.6	370.94	6.15	3.904	600	5	100	6
24	48	-18.34	918	901.4	3464	1406.2	44.6	359.92	6.15	2.822	600	5	100	6
25	47	15.7	931	1538	3520	2861	48.9	247.3	6.77	7.87	700	5	90	7
26	48	20.51	918	1533.7	3464	2867.6	44.6	249.82	6.15	7.969	750	10	110	8
27	48	58.99	918	1499.3	3464	2920.4	44.6	269.98	6.15	8.761	750	10	110	8
28	48	15.7	918	1538	3464	2861	44.6	247.3	6.15	7.87	700	3	110	9
29	-29	7.6	777	1670	1382	3287	84.8	295.6	2.64	4.51	650	10	110	10
30	-28.846	7.6	777.282	1670	1386.164	3287	84.7196	295.6	2.64702	4.51	650	10	110	10
31	-28.615	7.6	777.705	1670	1392.41	3287	84.599	295.6	2.65755	4.51	650	10	110	10
32	-28.23	7.6	778.41	1670	1402.82	3287	84.398	295.6	2.6751	4.51	650	10	110	10
33	-27.46	7.6	779.82	1670	1423.64	3287	83.996	295.6	2.7102	4.51	650	10	110	10
34	48	15.7	918	1538	3464	2861	44.6	247.3	6.15	7.87	700	4	90	11
35	48	15.7	918	1538	3464	2861	44.6	247.3	6.15	7.87	500	2	130	12
36	48	15.7	918	1538	3464	2861	44.6	247.3	6.15	7.87	600	2	130	12
37	48	15.7	918	1538	3464	2861	44.6	247.3	6.15	7.87	700	2	130	12
38	48	15.7	918	1538	3464	2861	44.6	247.3	6.15	7.87	800	2	130	12
39	48	15.7	918	1538	3464	2861	44.6	247.3	6.15	7.87	900	2	130	12
40	48	111.5	918	1455	3464	2931	44.6	290.3	6.15	8.9	600	2	130	13
41	48	111.5	918	1455	3464	2931	44.6	290.3	6.15	8.9	700	2	130	13
42	48	111.5	918	1455	3464	2931	44.6	290.3	6.15	8.9	800	2	130	13
43	48	111.5	918	1455	3464	2931	44.6	290.3	6.15	8.9	900	2	130	13

44	48	111.5	918	1455	3464	2931	44.6	290.3	6.15	8.9	600	4	130	13
45	48	111.5	918	1455	3464	2931	44.6	290.3	6.15	8.9	600	6	130	13
46	48	15.7	918	1538	3464	2861	44.6	247.3	6.15	7.87	500	4	120	14
47	48	15.7	918	1538	3464	2861	44.6	247.3	6.15	7.87	600	4	120	14
48	48	15.7	918	1538	3464	2861	44.6	247.3	6.15	7.87	700	4	120	14
49	48	15.7	918	1538	3464	2861	44.6	247.3	6.15	7.87	800	4	120	14
50	48	15.7	918	1538	3464	2861	44.6	247.3	6.15	7.87	1000	4	120	14