Supporting Information

Structure free: compositionally-informed machine learning for solid-state electrolytes design

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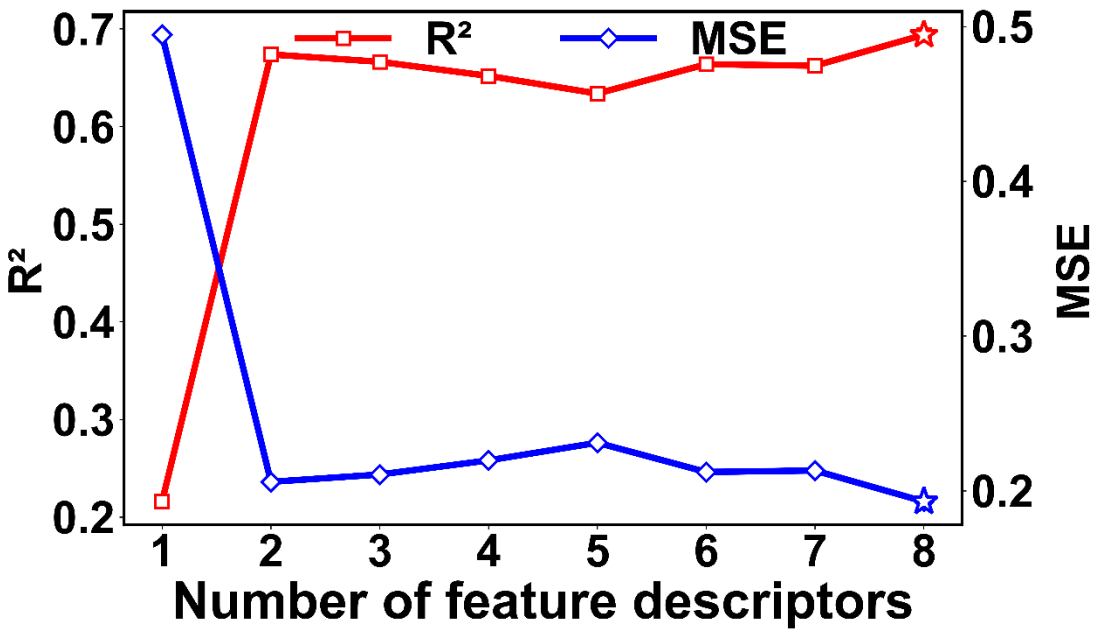

Figure S1. Impact of feature number on R^2 and mean squared error (*MSE*) in gradient boosting regression (XGBoost) models for halides.

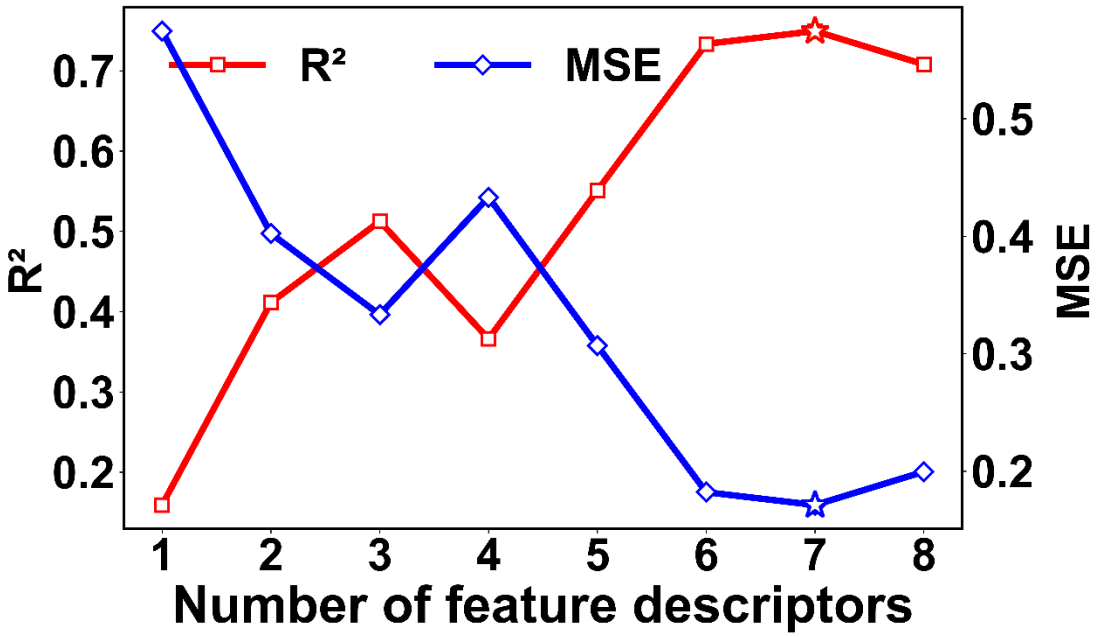

Figure S2. Impact of feature number on R^2 and mean squared error (*MSE*) in gradient boosting regression (XGBoost) models for ternary halides.

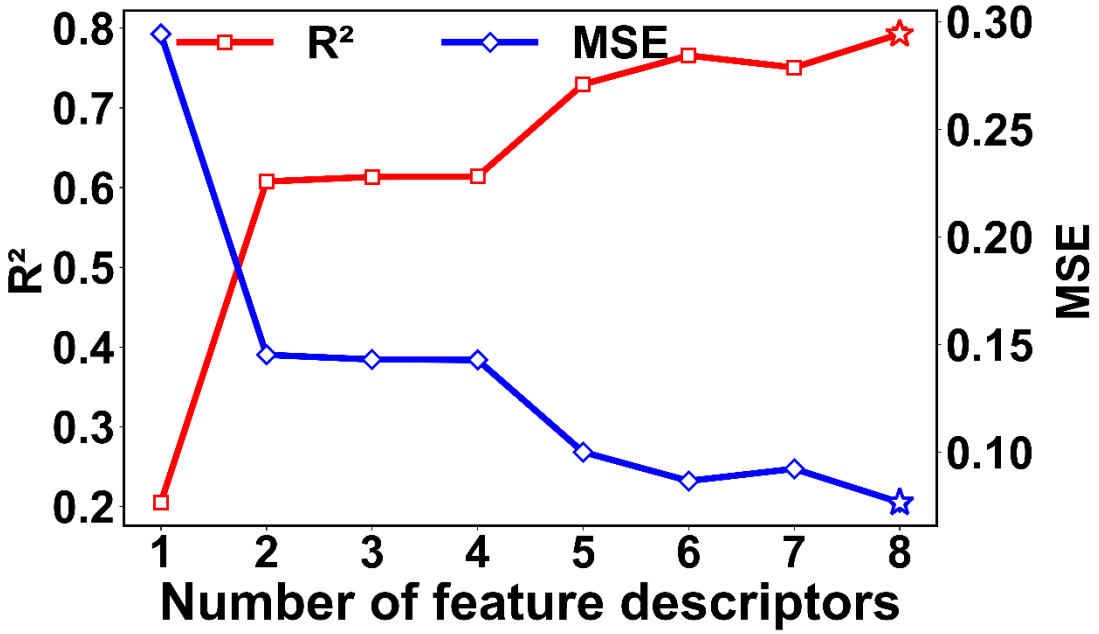

Figure S3. Impact of feature number on R^2 and mean squared error (*MSE*) in gradient boosting regression (XGBoost) models for quaternary halides.

Table S1 Complete list of 87 halide compounds used in this study, including chemical formula, room-temperature ionic conductivity (σ_{RT}) measured by electrochemical impedance spectroscopy (EIS), and corresponding literature source.

No.	Formula	σ_{RT} (ms/cm)	Reference
1	Li_3HoBr_6	1.1	1
2	$Li_{2.73}Ho_{1.09}Cl_6$	1.3	2
3	Li_3HoCl_6	0.29	2
4	$Li_{2.73}Dy_{1.09}Cl_6$	0.9	2
5	$Li_{2.73}Y_{1.09}Cl_6$	0.7	2
6	$Li_{2.73}Er_{1.09}Cl_6$	0.64	2
7	$Li_{2.73}Tm_{1.09}Cl_6$	0.89	2
8	Li_3TiCl_6	1.04	3
9	Li_3InCl_6	1.49	4
10	Li_3ScCl_6	3.02	5
11	$LiScCl_4$	0.123	5
12	$Li_{1.5}ScCl_{4.5}$	0.243	5
13	Li_2ScCl_5	0.624	5
14	$Li_{2.5}ScCl_{5.5}$	2.57	5
15	$Li_{3.5}ScCl_{6.5}$	2.42	5
16	Li_4ScCl_7	1.98	5

17	$LiAlCl_4$	0.001	6
18	Li_2ZrCl_6	0.81	6
19	Li_3YCl_6	0.51	7
20	Li_3ErCl_6	0.087	7
21	Li_3YBr_6	0.72	8
22	$Li_{1.52}Mn_{1.24}Cl_4$	0.015	9
23	$Li_{1.6}Mg_{1.2}Cl_4$	0.035	9
24	$Li_2Sc_{2/3}Cl_4$	1.5	10
25	Li_3YbCl_6	0.19	11
26	$Li_{2.61}Y_{1.13}Cl_6$	0.38	12
27	Li_3ScBr_6	1.4	13
28	Li_3ErI_6	0.65	14
29	$LiAlF_4$	0.001	15
30	$Li_{2.7}AlF_{5.4}$	0.075	16
31	Li_3InBr_6	1	17
32	$LiGaBr_4$	0.007	18
33	Li_2VCl_4	0.006	19
34	Li_2MnCl_4	0.004	19
35	$Li_{1.6}Fe_{1.2}Cl_4$	0.013	20

36	Li_3FeCl_6	0.13	21
37	Li_6FeCl_8	0.22	22
38	Li_6CoCl_8	0.062	22
39	Li_3TbCl_6	0.2	23
40	Li_3DyCl_6	0.1	23
41	Li_3TmCl_6	0.1	23
42	Li_3YI_6	0.1	24
43	Li_3GaF_6	0.088	25
44	$Li_{2.65}YCl_{5.65}$	0.205	26
45	$Li_{2.83}Y_{1.06}Cl_6$	0.57	27
46	$Li_{2.727}Y_{1.091}Cl_6$	0.69	27
47	Li_3LaI_6	0.96	28
48	Li_3TbBr_6	1.7	29
49	$Li_{1.4}MgCl_{3.4}$	0.00869	30
50	Li_4YI_7	1.04	31
51	$Li_{2.7}In_{0.7}Hf_{0.3}Cl_6$	1.28	32
52	$Li_{2.5}Y_{0.5}Zr_{0.5}Cl_6$	1.4	33
53	$Li_{2.633}Er_{0.633}Zr_{0.367}Cl_6$	1.1	33
54	$Li_{2.9}Er_{0.9}Zr_{0.1}Cl_6$	0.36	33

55	$Li_{2.8}Er_{0.8}Zr_{0.2}Cl_6$	0.77	33
56	$Li_{2.25}Zr_{0.75}Fe_{0.25}Cl_6$	0.98	34
57	$Li_{2.6}Yb_{0.6}Hf_{0.4}Cl_6$	1.5	35
58	$Li_{2.8}Yb_{0.8}Zr_{0.2}Cl_6$	1.2	35
59	$Li_{2.7}Zr_{0.3}In_{0.7}Cl_6$	2.1	36
60	$Li_3Y(Br_3Cl_3)$	1.6	37
61	$Li_3HoBr_3I_3$	2.7	38
62	$Li_3YBr_{5.7}F_{0.3}$	1.8	39
63	$13Li_3InCl_{4.8}F_{1.2}$	0.51	40
64	$Li_{2.7}In_{0.4}Hf_{0.6}Cl_6$	0.71	40
65	$Li_{2.7}In_{0.3}Hf_{0.7}Cl_6$	0.31	40
66	$Li_{2.9}In_{0.9}Hf_{0.1}Cl_6$	0.97	40
67	$Li_{2.8}In_{0.8}Hf_{0.2}C_{l6}$	1.05	40
68	$Li_{2.5}Er_{0.5}Zr_{0.5}Cl_6$	0.9	41
69	$Li_{2.5}Sc_{0.5}Zr_{0.5}Cl_6$	2.23	42
70	$20Li_{2.1}Zr_{0.95}Mg_{0.05}Cl_6$	0.67	43
71	$Li_{2.6}In_{0.6}Zr_{0.4}Cl_6$	1.25	44
72	$Li2In_{1/3}Sc_{1/3}Cl_4$	2	45
73	$Li_3Ho_{0.6}In_{0.4}Cl_6$	2.5	46

74	$Li_2ZrCl_{5.2}F_{0.8}$	0.2	47
75	$Li_{2.375}Sc_{0.375}Zr_{0.625}Cl_6$	2.2	48
76	$Li_{2.375}Sc_{0.375}Hf_{0.625}Cl_6$	1.1	48
77	$Li_2ZrCl_{5.6}F_{0.4}$	0.321	49
78	Li_3YCl_5F	0.22	50
79	$29Li_{2.6}Sc_{0.6}Zr_{0.4}Cl_6$	1.61	51
80	$Li_{2.556}Yb_{0.492}Zr_{0.492}Cl_6$	1.58	52
81	$Li_{2.9}In_{0.9}Zr_{0.1}Cl_6$	1.54	53
82	$Li_3YBr_2Cl_4$	1.27	54
83	$Li_3AlF_{5.87}Cl_{0.13}$	0.2	55
84	$Li_{2.8}Zr_{0.2}In_{0.8}Cl_6$	1.39	56
85	$Li_{1.7}Zr_{0.7}Ta_{0.3}C_{l6}$	1.42	57
86	$Li_4YBr_{3.5}I_{3.5}$	1.5	58
87	$Li_3HoBr_{3.1}I_{2.9}$	2.7	59

Table S2 Pairwise Spearman rank correlation coefficients between XGBoost and other top-performing models (GBR, RF, and DT).

Dataset	Model Pair	Spearman ρ
Ternary Halides	XGBoost vs GBR	0.9348
	XGBoost vs RF	0.8681
	XGBoost vs DT	0.8430
	Mean	0.8820

Quaternary Halides	XGBoost vs GBR	0.9541
	XGBoost vs RF	0.9736
	XGBoost vs DT	0.8579
	Mean	0.9285

Note: A higher ρ value indicates better ranking consistency between models. All Spearman correlation coefficients exceed 0.84, indicating strong consistency in material rankings across different ML models. This stability supports the reliability of XGBoost as the core model for mechanistic interpretation and the identification of promising halide candidates.

Note S1. Detailed discussion of candidates in Tables S3 and S4

This note provides additional details on the promising SSEs identified in Tables S3 and S4.

1. Previously unreported candidates. Many of these candidates have not been previously reported as SSEs, which represents targets for future experimental validation. Representative examples are ternary compounds such as $CsLiBr_2$, $CsLi_2Br_3$, and $CsLi_3Br_4$ (predicted $\sigma_{RT} \approx 2.23$ mS/cm), and quaternary compounds such as $Rb_2LiTaBr_6$ (2.40 mS/cm), $Cs_2LiTaBr_6$ (2.31 mS/cm) and $LiRb_2MoBr_6$ (2.28 mS/cm).

2. Model consistency and resolution limits. Among the top ternary candidates, several Cs-Li-Br compounds share nearly identical predicted conductivities (≈2.23 mS/cm) and similarly low IonicRad_Mis values (<0.09 Å). This reflects the model's internal consistency, as compounds with analogous descriptor values are predicted to exhibit comparable performance. As an initial screening tool, the model is not designed to resolve fine-grained differences among such closely related compositions. These candidates are therefore prioritized for subsequent experimental validation and structure-dependent analyses, which will determine the optimal stoichiometry for SSEs.

3. External validation for $CsLi_2Cl_3$. Among these candidates, $CsLi_2Cl_3$ has been studied by AIMD simulations, which report a room-temperature ionic conductivity of 4.5 mS/cm (US Patent App. 2025/0140906 A1). The agreement confirms the predictive

capability of our approach.

Table S3. Representative ternary halide systems identified by the ML model, showing predicted σ_{RT} and corresponding key descriptors (i.e. ionic radius mismatch and van der Waals mismatch).

MP ID	Formula	IonicRad_Mis (Å)	VdWRad_Mis (Å)	Predicted σ_{RT} (mS/cm)
mp-23057	$CsLiBr_2$	0.068938766	0.130568221	2.226537
mp-571409	$Cs_2Li_3Br_5$	0.074347975	0.131154689	2.226537
mp-606680	$CsLi_2Br_3$	0.078175446	0.130416212	2.226537
mp-580554	$CsLi_3Br_4$	0.083256432	0.127153108	2.226537
mp-1080005	$Cs_3Li_2Br_5$	0.063858571	0.128874283	2.1507561
mp-1189357	Cs_3LiBr_4	0.056709937	0.125393637	2.1507561
mp-1095674	Cs_2LiBr_3	0.060620879	0.127416142	2.150756
mp-1120734	Cs_3LiCl_4	0.041812848	0.113042506	2.1237724
mp-28243	$RbLiCl_2$	0.082141484	0.129157631	2.1237724
mp-7594	$CsLiF_2$	0.068021152	0.137326821	2.1237723
mp-559766	Cs_3LiF_4	0.043914271	0.117713424	2.1237723
mp-558728	$Cs_3Li_2F_5$	0.057804265	0.128528569	2.1237723
mp-553988	Cs_2LiF_3	0.051497258	0.123416029	2.1237723
mp-23364	$CsLiCl_2$	0.063009036	0.126522366	2.1237723
mp-571390	Cs_2LiCl_3	0.048608623	0.117211738	2.1237723
mp-570756	$Cs_3Li_2Cl_5$	0.054177837	0.120783511	2.1237723
mp-606604	$CsLi_2F_3$	0.088719638	0.155981033	2.0587742
mp-555439	$CsLi_3F_4$	0.102102998	0.167617478	2.0587742
mp-560088	$Cs_2Li_3F_5$	0.079697703	0.147824	2.0587742
mp-7593	$RbLiF_2$	0.088467569	0.151864102	2.0587742
mp-569117	$CsLi_2Cl_3$	0.080048028	0.136586896	2.0587742
mp-571666	$CsLi_3Cl_4$	0.090380206	0.140838786	2.0587742
mp-28237	$RbLiBr_2$	0.087300247	0.120649031	1.961933

Table S4. Representative quaternary halide systems identified by the ML model, showing predicted σ_{RT} and corresponding major descriptors (i.e. IonicRad_Mis and **Pol_m/n**).

MP ID	Formula	IonicRad_Mis (Å)	Pol_m/n	Predicted σ_{RT} (mS/cm)
mp-1110707	$Rb_2LiTaBr_6$	0.162072229	26.57142857	2.4023396
mp-1111834	$Cs_2LiTaBr_6$	0.150188636	30.42857143	2.3136315
mp-1110711	$Rb_2LiMoBr_6$	0.12858525	27.19047619	2.2804255
mp-1206187	$Rb_2LiRhCl_6$	0.161123863	37.67123288	2.2325229
mp-1206553	$Rb_2LiRuCl_6$	0.156926753	38.08219178	2.2325229
mp-1110680	$Rb_2LiSbCl_6$	0.144708558	36.09589041	2.2325229
mp-1110708	$Rb_2LiSbBr_6$	0.132131932	25.0952381	2.1992716
mp-1110706	Rb_2LiYBr_6	0.106667077	30.76190476	2.1592814
mp-1111835	$Cs_2LiSbBr_6$	0.120768942	28.95238095	2.1177573
mp-1110668	$Rb_2LiMoCl_6$	0.143888012	39.10958904	2.0853662
mp-989405	$Cs_2LiInBr_6$	0.114161609	30	2.0290501
mp-1111847	$Cs_2LiMoBr_6$	0.116897729	31.04761905	2.0290501
mp-567628	$Rb_2LiDyBr_6$	0.12807629	30.90476191	2.0290501
mp-1111833	Cs_2LiYBr_6	0.095674145	34.61904762	2.0290501
mp-1110746	Rb_2LiSbI_6	0.129313479	16.01823708	1.992416
mp-1113000	Cs_2LiTaI_6	0.146695149	19.4224924	1.9277602
mp-1110745	Rb_2LiTaI_6	0.155533461	16.96048632	1.8972519
mp-	Rb_2LiMoI_6	0.124536763	17.3556231	1.8020976

1110749				
mp-989583	$Rb_2LiInCl_6$	0.135898917	37.60273973	1.7325861
mp-1112836	Cs_2LiMoI_6	0.116492526	19.81762918	1.6431778
mp-1112673	Cs_2LiSbI_6	0.121189539	18.48024316	1.6431778
mp-1112663	Cs_2LiYI_6	0.100903921	22.09726444	1.6431778
mp-1111439	$Cs_2LiSbCl_6$	0.13209266	41.64383562	1.5502586
mp-1206399	Rb_2LiVCl_6	0.155654403	39.10958904	1.1124629
mp-1113928	$Rb_2LiScCl_6$	0.105451333	39.79452055	0.8715433

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