

Fig. S1. The model performance as a function of the number of features, evaluated by (a) R^2 , (b) MAE, and (c) RMSE. These analysis schemes were obtained from leave-one-out cross-validation, and the model performance was examined using a range of 12-112 features in increments of 20 features. With the increase of the number of features, the model is gradually over-fitted.

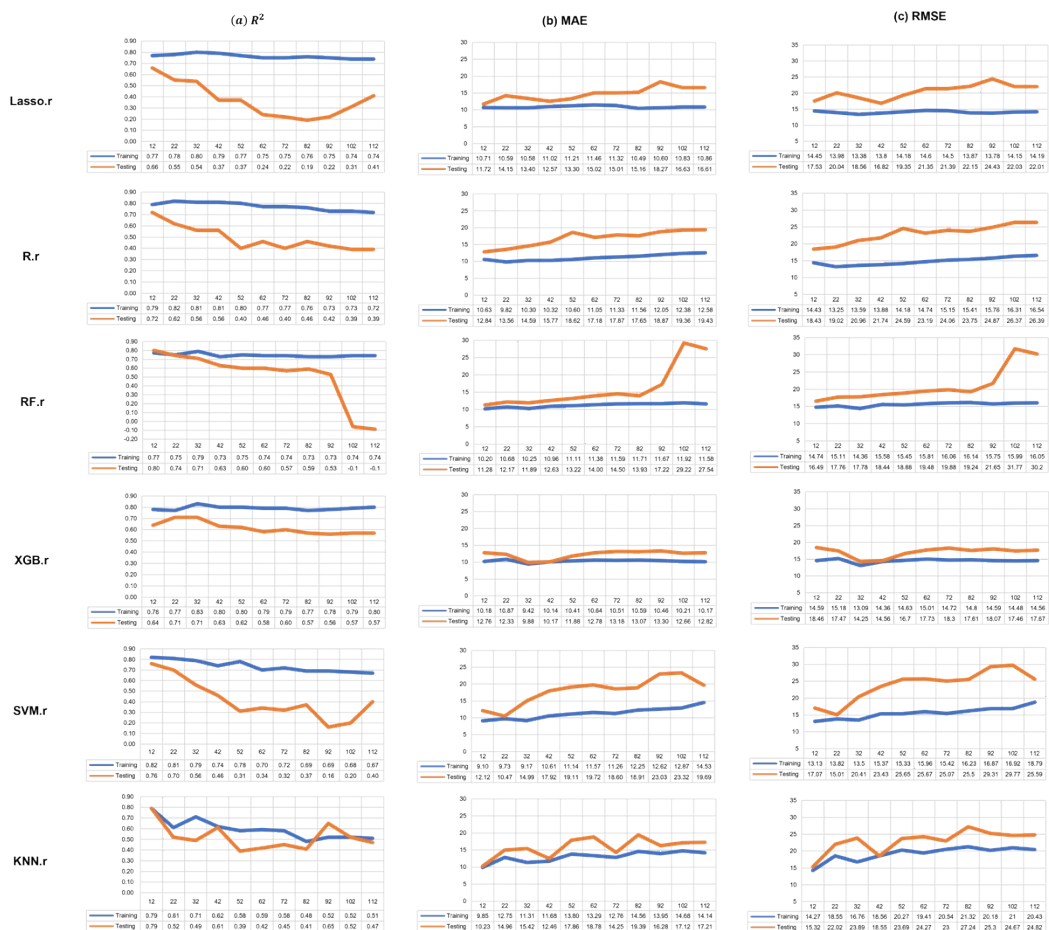


Fig. S2. XRD patterns of (a) $\text{Ba}_2\text{LaNbO}_6: 0.003\text{Mn}^{4+}$, (b) $\text{Ba}_2\text{YNbO}_6: 0.005\text{Mn}^{4+}$, (c) $\text{Sr}_2\text{LaSbO}_6: 0.008\text{Mn}^{4+}$, and (d) $\text{Mg}_2\text{TiO}_4: 0.004\text{Mn}^{4+}$. Above: standard pattern. Below: experimental data.

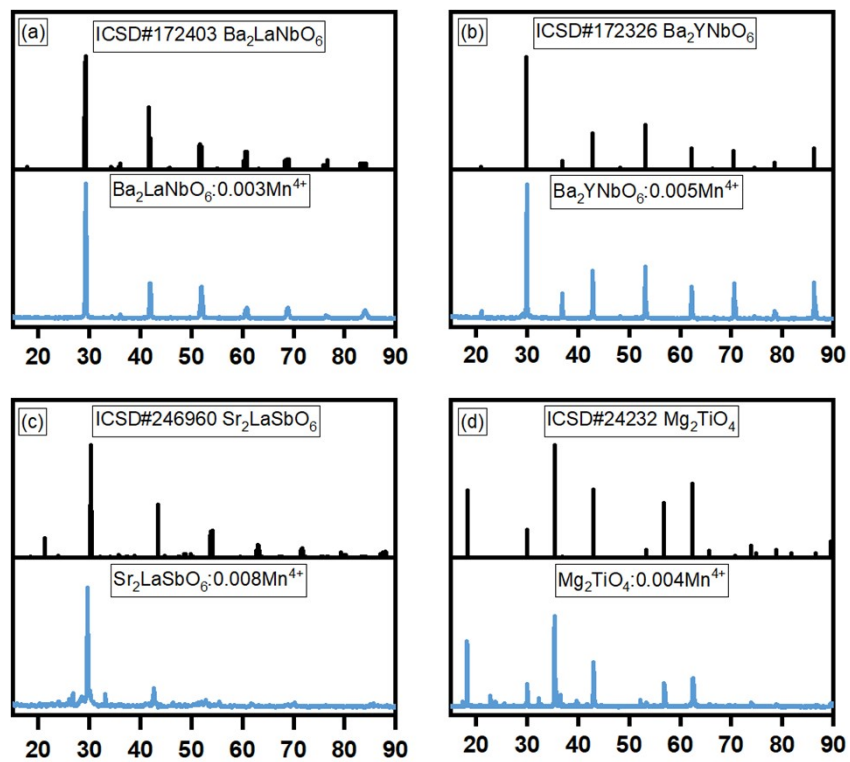


Fig. S3. photoluminescence excitation (PLE) and photoluminescence (PL) spectrum of (a) $\text{Ba}_2\text{LaNbO}_6: 0.003\text{Mn}^{4+}$, (b) $\text{Ba}_2\text{YNbO}_6: 0.005\text{Mn}^{4+}$, (c) $\text{Sr}_2\text{LaSbO}_6: 0.008\text{Mn}^{4+}$, and (d) $\text{Mg}_2\text{TiO}_4: 0.004\text{Mn}^{4+}$.

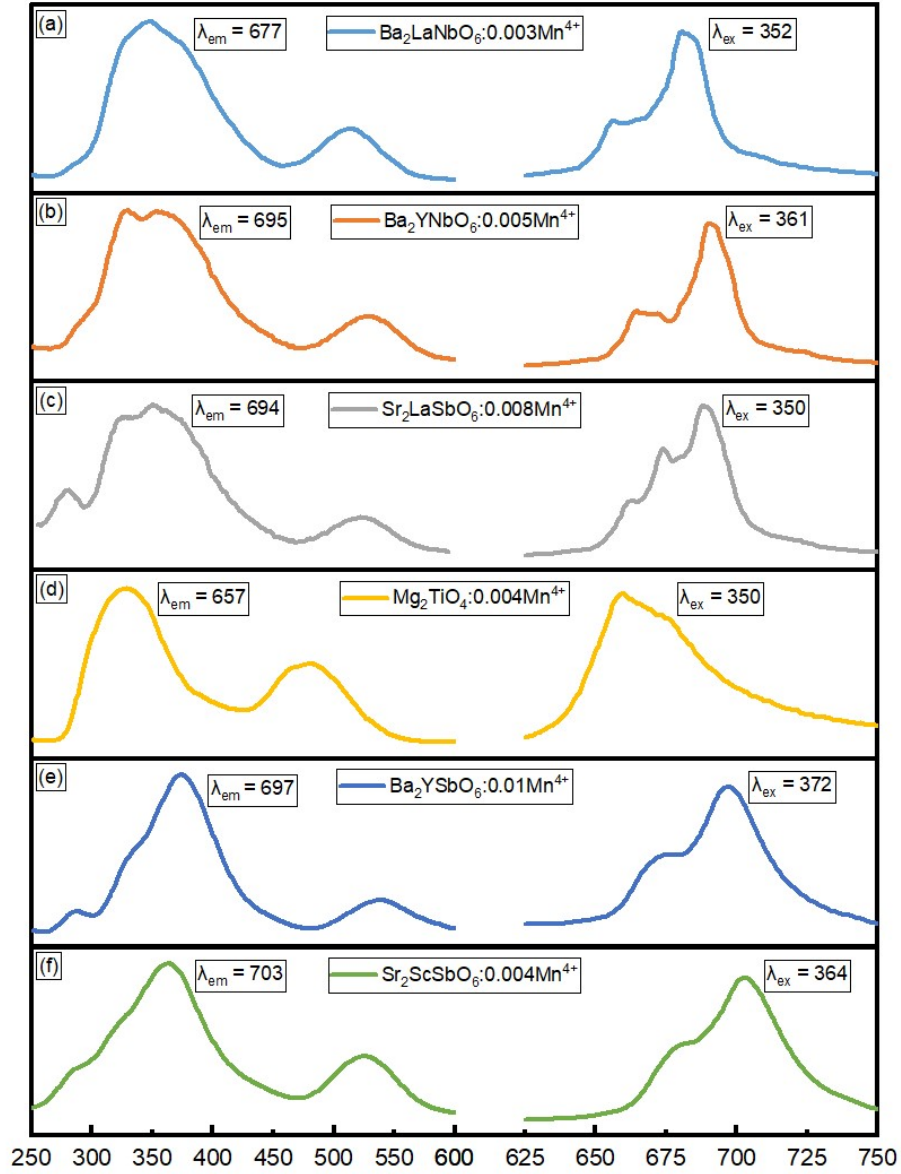


Table S1. Training labels.

Composition	Wavelength (nm)	Composition	Wavelength (nm)
(NH ₄) ₂ NaInF ₆	631	Ca ₂ ScSbO ₆	693
(NH ₄) ₂ SiF ₆	630	Ca ₂ WO ₂ F ₄	632
(NH ₄) ₂ SnF ₆	630	CaMg ₂ Al ₁₆ O ₂₇	655
(NH ₄) ₂ TiF ₆	630	CaMg ₂ Al ₁₆ O ₂₇	655
Ba ₂ CaWO ₆	680	Cs ₂ GeF ₆	633
Ba ₂ GdNbO ₆	676	Cs ₂ HfF ₆	630
Ba ₂ LaNbO ₆	685	Cs ₂ KCrF ₆	632
Ba ₂ LaSbO ₆	678	Cs ₂ NaAl ₃ F ₁₂	633
Ba ₂ LuNbO ₆	698	Cs ₂ SiF ₆	632
Ba ₂ LuTaO ₆	700	Cs ₂ ZrF ₆	633
Ba ₂ MgWO ₆	720	CsMoO ₂ F ₃	633
Ba ₂ MgWO ₆	725	Gd ₂ ZnTiO ₆	705
Ba ₂ YNbO ₆	695	Gd ₂ ZnTiO ₆	705
Ba ₂ YTaO ₆	690	K ₂ BaGe ₈ O ₁₈	666
BaGe ₄ O ₉	666	K ₂ GeF ₆	635
BaGeF ₆	634	K ₂ LiAlF ₆	635
BaLaMgNbO ₆	700	K ₂ NaInF ₆	631
BaLaZnTaO ₆	695	K ₂ SiF ₆	632
BaSn(PO ₄) ₂	660	K ₂ TiF ₆	632
BaSnF ₆	631	K ₃ AlF ₆	628
BaTiF ₆	632	KGaP ₂ O ₇	702
BaTiOF ₄	631	KNaSiF ₆	630
BaZn _{1.06} Al _{9.94} O ₁₇	665	KZnF ₃	636
Ca ₁₄ Al ₁₀ Zn ₆ O ₃₅	710	La(MgTiO ₆) _{0.5}	708
Ca ₁₄ Zn ₆ Ga ₁₀ O ₃₅	711	La ₂ ZnTiO ₆	708
Ca ₂ AlNbO ₆	712	La ₃ GaGe ₅ O ₁₆	659
Ca ₂ InSbO ₆	693	LaAlO ₃	731
Ca ₂ LaSbO ₆	680	LaScO ₃	703

Composition	Wavelength (nm)	Composition	Wavelength (nm)
$\text{Ca}_2\text{LaTaO}_6$	696	LaSrZnNbO_6	694
Ca_2MgWO_6	690	LaSrZnSbO_6	706
Ca_2MgWO_6	700	LaTiSbO_6	685
$\text{Li}_2\text{MgZrO}_4$	670	LiSrAlF_6	618
Li_2SnO_3	658	$\text{Mg}_7\text{Ga}_2\text{GeO}_{12}$	660
$\text{Li}_2\text{ZnTi}_3\text{O}_8$	681	$\text{Na}_{1.57}\text{Zn}_{0.57}\text{Al}_{10.43}\text{O}_{17}$	695
$\text{Li}_3\text{Mg}_2\text{NbO}_6$	668	Na_2GeF_6	620
$\text{Li}_5\text{La}_3\text{Nb}_2\text{O}_{12}$	715	$\text{Na}_2\text{MgAl}_{10}\text{O}_{17}$	695
$\text{Li}_5\text{La}_3\text{Ta}_2\text{O}_{12}$	714	$\text{Na}_2\text{NbF}_5\text{O}$	620
$\text{Li}_6\text{SrLa}_2\text{Sb}_2\text{O}_{12}$	705	Na_2SiF_6	620
$\text{LiLa}_2\text{SbO}_6$	725	Na_3AlF_6	628

Table S2. The prediction results (nm) of each model to the prediction set.

Composition	XGB.r	RF.r	Lasso.r	R.r	KNN.r	SVM.r
(GdNa) _{0.5} TiO ₃	642	666	685	689	688	688
(Na ₂ Mg)Si(SiO ₄) ₃	647	669	656	663	671	681
(NH ₄) ₃ GeF ₇	641	627	612	606	632	606
(NH ₄) ₃ InF ₆	629	646	630	631	642	618
(NH ₄) ₃ SnF ₇	641	627	613	607	632	601
Ba _{0.82} Mg _{.63} Al _{10.37} O ₁₇	679	672	684	688	675	678
Ba ₂ GdNbO ₆	696	696	713	717	697	707
Ba ₂ GdSbO ₆	681	698	716	720	704	657
Ba ₂ LaNbO ₆	701	691	708	710	696	710
Ba ₂ LuNbO ₆	696	699	715	716	696	709
Ba ₂ NaNb ₅ O ₁₅	669	674	681	678	682	667
Ba ₂ Nb ₁₅ O ₃₂	671	663	687	685	659	674
Ba ₂ Nb ₅ O ₉	696	695	704	703	694	709
Ba ₂ SnO ₄	707	692	704	703	696	697
Ba ₂ SrWO ₆	700	701	714	717	716	704
Ba ₂ TiZrO ₆	695	701	713	718	682	703
Ba ₂ YNbO ₆	702	696	704	707	694	709
Ba ₃ Al ₂ Si ₃ O ₁₂	707	682	684	681	661	688
Ba ₃ CaSb ₂ O ₉	704	693	700	704	692	688
Ba ₃ LaNb ₃ O ₁₂	694	693	706	706	693	700
Ba ₃ MgNb ₂ O ₉	696	697	708	712	698	707
Ba ₃ MgSb ₂ O ₉	696	695	710	714	701	699
Ba ₃ MgTa ₂ O ₉	692	702	723	726	716	706
Ba ₃ NaNbO ₆	703	694	693	692	691	700
Ba ₃ NaSbO ₆	703	694	695	695	691	699
Ba ₃ NaTaO ₆	701	694	701	700	692	696
Ba ₃ Nb ₆ Si ₄ O ₂₆	660	663	678	678	687	672
Ba ₃ SrSb ₂ O ₉	698	694	705	707	696	692
Ba ₃ Ta ₆ Si ₄ O ₂₆	670	678	696	693	694	679
Ba ₃ ZnTa ₂ O ₉	695	701	726	728	715	709
Ba ₄ Na ₂ W ₂ O ₁₁	688	695	709	706	716	694
Ba ₄ NaSb ₃ O ₁₂	678	681	670	673	683	677
Ba ₄ Sn ₂ Y ₂ O ₁₁	698	698	710	713	690	703
Ba ₅ Li ₂ W ₃ O ₁₅	685	686	709	704	713	691
Ba ₅ W _{3.04} Li _{0.96} O _{14.6}	702	695	710	706	716	695
Ba ₆ Nb ₁₄ Si ₄ O ₄₇	670	664	681	672	660	656
Ba ₉ Sc ₂ Si ₆ O ₂₄	711	687	686	684	661	684
BaAl ₁₂ O ₁₉	685	691	691	691	697	693
BaGeF ₆	629	631	632	624	632	632
BaLa ₂ Sc ₂ O ₇	697	697	705	707	703	711
BaNb ₁₀ SiO ₁₉	672	669	693	685	683	673
BaNb ₂ O ₆	676	666	680	678	659	669
BaNbO ₃	715	695	706	705	695	706
BaSi ₄ O ₉	645	649	668	671	672	675

Composition	XGB.r	RF.r	Lasso.r	R.r	KNN.r	SVM.r
BaSnO ₃	709	695	707	706	696	700
BaSnSi ₃ O ₉	645	657	677	677	669	669
BaTi ₇ MgO ₁₆	668	683	684	690	680	685
BaTiF ₆	641	630	627	618	632	628
BaTiSi ₃ O ₉	658	660	674	674	682	674
BaY ₂ SbO ₆	707	692	707	710	694	708
BaZrO ₃	705	694	701	699	696	697
Ca(TiO)(SiO ₄)	650	671	660	659	668	671
Ca _{0.5} TaO ₃	689	695	696	693	700	689
Ca ₂ Gd ₃ Sb ₃ O ₁₄	661	686	667	674	682	682
Ca ₂ La ₃ Sb ₃ O ₁₄	683	688	687	689	686	700
Ca ₂ LaSbO ₆	706	692	686	688	689	693
Ca ₂ LuNbO ₆	703	696	692	694	693	705
Ca ₂ Nb ₂ O ₇	686	661	656	650	657	642
Ca ₂ Sb ₂ O ₇	689	670	668	665	659	664
Ca ₂ Y ₃ Sb ₃ O ₁₄	683	692	685	688	691	699
Ca ₂ ZrSi ₄ O ₁₂	641	663	648	647	668	654
Ca ₃ Al ₂ O ₆	683	662	657	657	672	675
Ca ₃ Al ₂ Si ₃ O ₁₂	688	675	656	655	667	674
Ca ₃ Ga ₂ Ge ₄ O ₁₄	663	679	674	678	676	675
Ca ₃ Ga ₂ Si ₃ O ₁₂	676	676	661	659	669	674
Ca ₃ Sc ₂ Si ₃ O ₁₂	685	675	656	654	667	673
Ca ₃ SnSi ₂ O ₉	686	671	660	659	668	656
Ca ₃ WO ₆	703	677	678	676	687	675
CaMg ₂ Al ₆ O ₁₂	683	683	673	677	669	688
CaNb ₂ O ₆	667	662	669	669	696	669
CaNbO ₃	706	668	669	669	671	676
CaSc ₂ O ₄	664	658	656	654	654	651
CaSi ₂ O ₅	655	653	653	655	694	669
CaSiO ₃	689	671	673	673	701	685
CaSnO ₃	714	678	676	675	699	676
CaTiGeO ₅	661	672	668	667	667	683
CaYAlO ₄	674	697	685	688	702	705
CaZr ₄ O ₉	686	675	666	662	659	651
CaZrGeO ₅	663	673	669	666	677	673
CaZrO ₃	704	672	674	673	702	680
Cs ₂ GeF ₆	639	630	623	615	632	623
Cs ₂ KTiF ₆	633	638	637	639	631	623
Cs ₂ NaInF ₆	631	636	618	622	626	599
Cs ₂ NaScF ₆	632	637	613	616	626	601
Cs ₂ NaTiF ₆	634	636	641	641	631	621
Cs ₂ Nb ₄ O ₁₁	665	654	649	645	648	647
CsSbTeO ₆	687	665	690	686	695	683
CsTiF ₄	640	630	629	619	632	624
K(SbO)(SiO ₄)	658	659	663	660	689	664

Composition	XGB.r	RF.r	Lasso.r	R.r	KNN.r	SVM.r
K _{1.58} Al ₁₁ O ₁₇	694	663	658	657	666	656
K ₂ BaGe ₈ O ₁₈	639	659	665	664	661	656
K ₂ Ge ₄ O ₉	658	652	654	653	657	653
K ₂ GeSi ₆ O ₁₅	630	656	651	652	670	658
K ₂ LaTa ₅ O ₁₅	678	693	694	692	690	683
K ₂ LiAlF ₆	633	636	604	607	632	607
K ₂ NaAlF ₆	633	637	603	606	632	606
K ₂ NaInF ₆	633	637	608	611	632	600
K ₂ NaSb ₃ O ₉	682	679	664	664	693	664
K ₂ NaScF ₆	633	637	613	615	632	610
K ₂ SnSi ₃ O ₉	644	657	657	657	676	661
K ₂ SrTa ₂ O ₇	699	700	697	701	694	690
K ₂ Ta ₄ O ₁₁	682	685	698	695	699	682
Ca ₂ LaSbO ₆	706	692	686	688	689	693
Ca ₂ LuNbO ₆	703	696	692	694	693	705
Ca ₂ Nb ₂ O ₇	686	661	656	650	657	642
Ca ₂ Sb ₂ O ₇	689	670	668	665	659	664
Ca ₂ Y ₃ Sb ₃ O ₁₄	683	692	685	688	691	699
Ca ₂ ZrSi ₄ O ₁₂	641	663	648	647	668	654
Ca ₃ Al ₂ O ₆	683	662	657	657	672	675
Ca ₃ Al ₂ Si ₃ O ₁₂	688	675	656	655	667	674
Ca ₃ Ga ₂ Ge ₄ O ₁₄	663	679	674	678	676	675
Ca ₃ Ga ₂ Si ₃ O ₁₂	676	676	661	659	669	674
Ca ₃ Sc ₂ Si ₃ O ₁₂	685	675	656	654	667	673
Ca ₃ SnSi ₂ O ₉	686	671	660	659	668	656
Ca ₃ WO ₆	703	677	678	676	687	675
CaMg ₂ Al ₆ O ₁₂	683	683	673	677	669	688
CaNb ₂ O ₆	667	662	669	669	696	669
CaNbO ₃	706	668	669	669	671	676
CaSc ₂ O ₄	664	658	656	654	654	651
CaSi ₂ O ₅	655	653	653	655	694	669
CaSiO ₃	689	671	673	673	701	685
CaSnO ₃	714	678	676	675	699	676
CaTiGeO ₅	661	672	668	667	667	683
CaYAlO ₄	674	697	685	688	702	705
CaZr ₄ O ₉	686	675	666	662	659	651
CaZrGeO ₅	663	673	669	666	677	673
CaZrO ₃	704	672	674	673	702	680
Cs ₂ GeF ₆	639	630	623	615	632	623
Cs ₂ KTiF ₆	633	638	637	639	631	623
Cs ₂ NaInF ₆	631	636	618	622	626	599
Cs ₂ NaScF ₆	632	637	613	616	626	601
Cs ₂ NaTiF ₆	634	636	641	641	631	621
Cs ₂ Nb ₄ O ₁₁	665	654	649	645	648	647

Composition	XGB.r	RF.r	Lasso.r	R.r	KNN.r	SVM.r
CsSbTeO ₆	687	665	690	686	695	683
CsTiF ₄	640	630	629	619	632	624
K(SbO)(SiO ₄)	658	659	663	660	689	664
K _{1.58} Al ₁₁ O ₁₇	694	663	658	657	666	656
K ₂ BaGe ₈ O ₁₈	639	659	665	664	661	656
K ₂ Ge ₄ O ₉	658	652	654	653	657	653
K ₂ GeSi ₆ O ₁₅	630	656	651	652	670	658
K ₂ LaTa ₅ O ₁₅	678	693	694	692	690	683
K ₂ LiAlF ₆	633	636	604	607	632	607
K ₂ NaAlF ₆	633	637	603	606	632	606
K ₂ NaInF ₆	633	637	608	611	632	600
K ₂ NaSb ₃ O ₉	682	679	664	664	693	664
K ₂ NaScF ₆	633	637	613	615	632	610
K ₂ SnSi ₃ O ₉	644	657	657	657	676	661
K ₂ SrTa ₂ O ₇	699	700	697	701	694	690
K ₂ Ta ₄ O ₁₁	682	685	698	695	699	682
K ₂ TiO ₃ (SiO ₂) ₆	628	657	643	643	668	658
K ₂ TiSi ₃ O ₉	680	661	648	646	674	654
K ₂ ZrSi ₃ O ₉	673	663	652	651	668	657
K ₃ (Nb ₃ O ₆)(Si ₂ O ₇)	681	660	660	659	679	668
K ₃ ScSi ₂ O ₇	683	675	658	658	688	669
K ₄ Sn ₂ Si ₆ O ₁₈	643	656	651	649	674	646
K ₄ Zr ₅ O ₁₂	697	666	668	668	699	672
KLuTa ₂ O ₇	701	696	707	707	696	706
KNaSiF ₆	637	639	608	609	632	619
KNb ₈ O ₁₄	695	670	672	671	659	675
KNbO ₃	691	663	668	668	696	676
KScO ₂	683	668	666	666	699	674
KTaO ₃	710	695	695	692	700	688
KYT ₂ O ₇	702	695	696	698	687	700
La ₂ MgGeO ₆	692	697	712	716	700	710
La ₂ NaTaO ₆	701	694	708	707	698	696
La ₂ SrAl ₂ O ₇	688	706	710	715	701	722
La ₃ LiTi ₄ O ₁₂	704	693	696	695	689	702
LaCaGaO ₄	688	705	708	712	701	706
LaK ₂ (Nb ₅ O ₁₅)	657	669	677	678	688	668
LaMgAl ₁₁ O ₁₉	675	683	690	694	675	684
LaSrScO ₄	700	705	703	708	703	710
Li _{0.5} La _{0.5} TiO ₃	699	691	677	679	688	702
Li _{0.5} TiO ₂	687	661	655	654	674	664
Li ₂ GeF ₆	634	628	599	588	624	612
Li ₂ La ₂ Ti ₃ O ₁₀	689	699	680	680	674	703
Li ₂ MgSi ₂ (SiO ₄) ₃	634	666	651	659	668	678
Li ₂ MgTi ₃ O ₈	682	685	663	668	671	677

Composition	XGB.r	RF.r	Lasso.r	R.r	KNN.r	SVM.r
Li ₂ TiO ₃	669	660	651	648	655	652
Li ₂ ZrF ₆	635	631	607	598	632	618
Li ₃ InF ₆	633	630	608	595	624	600
Li ₃ Na ₃ In ₂ F ₁₂	632	636	602	604	631	604
Li ₃ TiF ₆	621	626	591	580	624	600
Li ₆ Zr ₂ O ₇	666	661	656	655	697	656
Li ₈ SnO ₆	681	664	655	655	698	655
LiAl ₅ O ₈	655	652	647	646	655	651
LiAlO ₂	682	668	655	655	697	674
LiBaAlF ₆	631	645	599	606	632	610
LiCaAlF ₆	631	644	615	623	632	628
LiGaO ₂	711	691	674	672	703	685
LiGaSi ₂ O ₆	639	661	653	652	671	666
LiMgAlF ₆	633	642	609	614	632	617
LiScGe ₂ O ₆	650	668	663	662	686	670
LiScGeO ₄	681	673	663	662	702	665
LiScO ₂	681	666	658	657	698	664
LiSrAlF ₆	631	645	615	622	631	624
LiTaSiO ₅	658	671	669	666	700	670
LiTi ₂ O ₄	690	661	655	654	694	666
LiTiO ₂	695	667	664	663	700	678
LiTiSi ₂ O ₆	637	663	649	649	662	661
Mg ₂ SnO ₄	701	665	666	665	695	664
Mg ₄ Nb ₂ O ₉	698	671	667	667	697	663
MgNb ₂ O ₆	667	665	668	668	697	668
MgScAlO ₄	676	688	673	676	665	688
MgTiO ₃	685	666	665	664	700	664
Na(SbO)(SiO ₄)	642	655	659	656	689	663
Na _{1.77} Al ₁₁ O ₁₇	691	663	655	654	667	659
Na ₂ Ba ₄ W ₂ O ₁₁	697	701	699	699	716	696
Na ₂ Ca ₂ Nb ₄ O ₁₃	668	687	674	678	695	652
Na ₂ Ca ₂ Ta ₃ O ₁₀	701	700	697	700	696	700
Na ₂ GeF ₆	636	625	598	588	624	608
Na ₂ MgAlF ₇	632	646	605	613	632	614
Na ₂ Nb ₄ O ₁₁	661	655	664	662	657	662
Na ₂ Si ₃ O ₇	646	652	651	653	698	668
Na ₂ SnO ₃	681	665	664	663	693	655
Na ₂ Ta ₄ O ₁₁	685	684	695	691	700	679
Na ₂ Ti ₂ O ₃ (SiO ₄)	685	677	649	647	668	658
Na ₂ TiOSi ₄ O ₁₀	657	661	644	644	668	654
Na ₂ TiSi ₅ O ₁₃	642	657	640	641	668	660
Na ₂ ZrSi ₄ O ₁₁	628	658	648	648	662	659
Na ₃ AlF ₆	636	628	607	597	631	621
Na ₃ Ca ₂ TaO ₆	691	696	676	679	699	681

Composition	XGB.r	RF.r	Lasso.r	R.r	KNN.r	SVM.r
Na ₃ Li ₃ Al ₂ F ₁₂	632	635	597	599	632	600
Na ₃ Li ₃ Sc ₂ F ₁₂	632	635	597	599	632	600
Na ₃ Li ₃ Ti ₂ F ₁₂	632	635	598	600	632	603
Na ₃ ScF ₆	636	628	607	597	631	614
Na ₃ ScSi ₂ O ₇	681	673	650	649	676	663
Na ₄ Sc ₂ Ge ₄ O ₁₃	680	668	665	662	682	666
Na ₄ Sc ₂ Si ₄ O ₁₃	678	668	655	653	680	665
Na ₄ Sn ₂ (SiO ₄) ₃	680	662	657	657	660	659
Na ₄ Sn ₃ O ₈	691	661	664	663	694	657
Na ₅ Ti ₆ O ₁₃	655	662	662	658	655	659
Na ₆ Li ₂ W ₂ O ₁₀	681	684	674	673	702	673
Na ₈ Si(Si ₆ O ₁₈)	669	654	647	649	673	665
Na ₈ SnSi ₆ O ₁₈	687	656	649	651	694	651
NaAlO ₂	684	667	663	663	699	680
NaBa ₄ Sb ₃ O ₁₂	703	697	691	693	685	698
NaCa ₂ Ta ₃ O ₁₀	699	700	694	695	692	689
NaCa ₄ Nb ₅ O ₁₇	683	686	613	617	654	639
NaCa ₅ TaO ₈	687	688	672	676	693	677
NaGaSi ₂ O ₆	640	662	658	657	671	660
NaLaTi ₂ O ₆	704	695	679	681	683	700
NaNb ₃ Te ₄ O ₁₆	638	661	668	663	683	673
NaNbO ₃	684	662	664	665	696	672
NaSbGeO ₅	648	665	668	667	699	677
NaSbO ₃	698	670	672	671	695	679
NaScGe ₂ O ₆	648	667	662	661	672	666
NaScO ₂	682	668	663	663	699	672
NaScSi ₂ O ₆	640	664	651	651	670	664
NaSr ₂ Nb ₅ O ₁₅	668	680	669	672	692	665
NaSr ₄ Sb ₃ O ₁₂	692	687	683	683	685	685
NaTaO ₃	712	695	691	688	701	686
NaTi ₂ Ga ₅ O ₁₂	673	688	666	668	667	679
NaTi ₈ O ₁₃	695	662	663	660	655	661
NaTiSi ₂ O ₆	641	662	654	653	662	659
NaYTiO ₄	694	689	676	680	683	680
Rb ₁₂ Nb ₃₃ O ₉₀	663	653	666	666	655	660
Rb _{2.6} Al ₂₂ O ₃₄	694	660	667	666	667	662
Rb ₂ Ge ₄ O ₉	658	653	665	663	659	660
Rb ₂ GeTeO ₆	677	663	687	683	681	689
Rb ₂ KScF ₆	634	637	627	629	632	618
Rb ₂ KTiF ₆	633	638	625	627	631	617
Rb ₂ NaAlF ₆	633	637	607	611	632	603
Rb ₂ NaTiF ₆	633	638	628	630	631	620
Rb ₂ SnSi ₃ O ₉	647	657	670	670	666	668
Rb ₂ TiSi ₃ O ₉	684	662	667	667	667	676
RbAl ₃ (P ₃ O ₁₀) ₂	659	675	660	663	669	663

Composition	XGB.r	RF.r	Lasso.r	R.r	KNN.r	SVM.r
RbAlTi ₃ O ₈	692	687	683	689	691	679
RbCa ₂ Nb ₃ O ₁₀	688	688	686	692	691	698
RbNb(SiO ₃)O ₂	658	658	662	658	683	658
RbNbGe ₃ O ₉	687	661	672	673	689	675
RbTaGe ₃ O ₉	691	670	680	679	689	669
Sr _{0.5} Al ₁₁ O ₁₇	669	660	664	663	667	658
Sr ₂ Al ₆ O ₁₁	671	661	670	666	655	662
Sr ₂ LaSbO ₆	707	692	700	702	693	704
Sr ₂ LuNbO ₆	696	694	705	707	691	709
Sr ₂ Sc _{0.5} Al _{1.5} O ₅	693	694	685	689	691	699
Sr ₂ ScGaO ₅	690	694	680	681	668	681
Sr ₂ ScSbO ₆	706	694	698	702	693	704
Sr ₂ SnO ₄	707	688	690	689	700	688
Sr ₂ Ta ₂ O ₇	684	681	673	667	660	653
Sr ₂ YSbO ₆	704	695	691	695	702	699
Sr ₃ MgTa ₂ O ₉	695	702	710	713	716	700
Sr ₃ NaNbO ₆	696	687	680	680	699	692
Sr ₃ NaSbO ₆	704	693	683	683	699	692
Sr ₃ NaTaO ₆	699	694	690	688	699	689
Sr ₃ Ta ₆ Si ₄ O ₂₆	666	677	687	685	695	669
Sr ₃ Zr ₂ O ₇	707	680	686	683	672	677
Sr ₄ Ti ₅ (Si ₂ O ₇) ₂ O ₈	663	667	675	670	678	671
Sr ₇ Na ₂ Al ₆ F ₃₄	627	635	602	604	629	590
Sr ₇ Zr(Si ₂ O ₇) ₃	633	648	638	646	631	634
SrAl ₈ Ti ₃ O ₁₉	669	672	676	670	659	648
SrGd ₂ Sc ₂ O ₇	702	700	707	711	701	701
SrLa ₂ Sc ₂ O ₇	700	697	696	698	702	704
SrLi ₂ Ti ₆ O ₁₄	664	666	666	660	661	657
SrNb ₂ O ₆	676	666	678	677	657	676
SrNb ₄ O ₆	713	694	695	694	697	699
SrNb ₈ O ₁₄	692	673	682	681	659	682
SrNbO ₃	712	693	689	689	696	695
SrSi ₂ O ₅	660	654	667	668	671	674
SrSnO ₃	718	694	695	694	700	693
SrZrO ₃	707	687	686	685	699	688
SrZrSi ₂ O ₇	641	662	669	668	667	672

Table S3. Feature set.

Feature number	Variable	Feature number	Variable
1	Fluoride/Oxide/Oxyfluoride (1/2/3)	14	Difference between oxidation state of Mn^{4+} and substitute element
2	Number of element type	15	Difference between ionic radii of Mn^{4+} and that of the substitute element (\AA)
3	Crystal system	16	Average electronegativity
4	Space group	17	Average ionization energy (kJ/mol)
5	Number of molecules in unit cell(Z)	18	Average electron affinity energy (kJ/mol)
6	Crystal volume (\AA^3)	19-24	lattice (\AA)
7	Crystal density (g/cm^3)	25-30	bond length (\AA)
8	Species of Octahedra	31-42	Edge length of octahedron (\AA)
9	Number of substitutable octahedrons	43-57	Bond angle
10	Number of irreplaceable octahedrons	58-62	Whether the element is an activator or not (takes 1/0)
11	Number of atoms in unit cell	63-67	Atomic number of elements
12	Ionic radii of substituted elements (\AA)	68-72	Oxidation state
13	Coordination number (CN)	73-77	Electronegativity

Feature number	Variable	Feature number	Variable
78-82	Ionization energy (<i>kJ/mol</i>)	98-102	Number of valence electrons present in highest sub-shell (0/1/2...)
83-87	Electron affinity energy (<i>kJ/mol</i>)	103-107	Total Valence Electrons
88-92	Number of valence electrons present in lowest sub-shell (1/2/3...)	108-112	The number of atoms per element
93-97	Number of valence electrons present in middle sub-shell (0/1/2...)		

Table S4. Synthesis conditions of samples.

	Temperature (°C)	Time (h)
$\text{Sr}_2\text{ScSbO}_6: 0.004\text{Mn}^{4+}$	1350	12
$\text{Ba}_2\text{YNbO}_6: \text{Mn}^{4+}$	1350	8
$\text{Ba}_2\text{YSbO}_6: 0.01\text{Mn}^{4+}$	1300	10
$\text{Sr}_2\text{LaSbO}_6: 0.008\text{Mn}^{4+}$	1300	6
$\text{Mg}_2\text{TiO}_4: 0.004\text{Mn}^{4+}$	1250	9
$\text{Sr}_2\text{LaSbO}_6: 0.003\text{Mn}^{4+}$	1300	6

Table S5 The parameters of the phosphor characterization that make the KNN.r algorithm perform optimally.

	O/F/O F	lat_para_ b	cryst_de ns	species_octahed ra	valence_ 1	num_atomic 2	valence_ 3	EA_3	valence_ 4	IE_4	EA_4	num_VEPM 4	AVG_E A
(NH ₄) ₂ NaIn F ₆	1	8.67	2.94	1	3	8	1	72.77	1	495.85	52.87	0	146.27
(NH ₄) ₂ SiF ₆	1	8.40	2.00	1	4	8	1	72.77	-1	1681.0 0	328.1 6	5	157.95
(NH ₄) ₂ SnF ₆	1	6.08	2.86	1	4	2	1	72.77	-1	1681.0 0	328.1 6	5	156.38
(NH ₄) ₂ TiF ₆	1	5.97	2.21	1	4	2	1	72.77	-1	1681.0 0	328.1 6	5	150.51
Ba ₂ CaWO ₆	2	8.39	6.69	1	6	8	2	2.37	-2	1313.9 0	140.9 8	4	95.49
Ba ₂ GdNbO ₆	2	8.50	6.72	1	5	4	3	0.00	-2	1313.9 0	140.9 8	4	96.22
Ba ₂ LaNbO ₆	2	6.06	6.41	1	5	4	3	45.35	-2	1313.9 0	140.9 8	4	100.75
Ba ₂ LaSbO ₆	2	6.08	6.54	1	5	2	3	45.35	-2	1313.9 0	140.9 8	4	102.01
Ba ₂ LuNbO ₆	2	8.36	7.25	1	5	8	3	32.81	-2	1313.9 0	140.9 8	4	99.50
Ba ₂ LuTaO ₆	2	8.38	8.21	1	5	8	3	32.81	-2	1313.9 0	140.9 8	4	93.77
Ba ₂ MgWO ₆	2	8.13	7.14	1	6	8	2	0.00	-2	1313.9 0	140.9 8	4	95.25
Ba ₂ MgWO ₆	2	8.13	7.14	1	6	8	2	0.00	-2	1313.9 0	140.9 8	4	95.25
Ba ₂ YNbO ₆	2	8.44	6.10	2	5	8	3	29.62	-2	1313.9 0	140.9 8	4	92.48
Ba ₂ YTaO ₆	2	8.45	7.07	1	5	8	3	29.62	-2	1313.9 0	140.9 8	4	93.45
BaGe ₄ O ₉	2	11.61	5.15	2	4	9	-2	140.9 8	0	0.00	0.00	0	21.56
BaGeF ₆	1	4.83	4.93	1	4	1	-1	328.1 6	0	0.00	0.00	0	262.73
BaLaMgNb O ₆	2	8.06	6.20	1	5	8	3	45.35	2	737.75	0.00	0	87.74
BaLaZnTaO 6	2	8.09	7.77	1	5	4	3	45.35	2	906.40	0.00	10	10.04
BaSn(PO ₄) ₂	2	5.25	4.37	1	4	2	5	72.04	-2	1313.9 0	140.9 8	4	116.10
BaSnF ₆	1	7.43	5.20	1	4	3	-1	328.1 6	0	0.00	0.00	0	275.27

	O/F/O F	lat_para b	cryst_de ns	species_octahe dra	valence_ 1	num_atomic 2	valence_ 3	EA_3	valence_ 4	IE_4	EA_4	num_VEP M_4	AVG_E A
BaTiF ₆	1	7.37	4.37	1	4	0	-1	328.1 6	0	0.00	0.00	0	40.60
BaTiOF ₄	3	13.76	4.69	1	4	4	-2	140.9 8	-1	1681.0 0	328.1 6	5	210.74
BaZn ₁₋₀₆ Al ₉₋₉₄ O ₁₇	2	5.61	4.02	2	3	2	2	0.00	-2	1313.9 0	140.9 8	4	95.67
Ca ₁₄ Al ₁₀ Zn ₆ O ₃₅	2	14.87	3.60	1	3	24	2	0.00	-2	1313.9 0	140.9 8	4	86.55
Ca ₁₄ Zn ₆ Ga ₁₀ O ₃₅	2	15.08	4.28	1	3	56	2	0.00	-2	1313.9 0	140.9 8	4	82.81
Ca ₂ AlNbO ₆	2	5.42	4.43	2	3	4	5	88.38	-2	1313.9 0	140.9 8	4	98.08
Ca ₂ InSbO ₆	2	5.69	5.51	2	5	4	3	28.95	-2	1313.9 0	140.9 8	4	98.05
Ca ₂ LaSbO ₆	2	5.88	5.32	1	5	4	3	45.35	-2	1313.9 0	140.9 8	4	99.69
Ca ₂ LaTaO ₆	2	5.89	6.04	1	5	4	3	45.35	-2	1313.9 0	140.9 8	4	92.70
Ca ₂ MgWO ₆	2	5.55	5.49	1	6	4	2	0.00	-2	1313.9 0	140.9 8	4	92.94
Ca ₂ MgWO ₆	2	5.55	5.49	1	6	4	2	0.00	-2	1313.9 0	140.9 8	4	92.94
Ca ₂ ScSbO ₆	2	5.62	4.68	1	5	4	3	18.14	-2	1313.9 0	140.9 8	4	96.97
Ca ₂ WO ₂ F ₄	3	6.28	5.39	1	6	2	-2	140.9 8	-1	1681.0 0	328.1 6	5	186.45
CaMg ₂ Al ₁₆ O ₂₇	2	5.59	3.73	7	3	2	2	0.00	-2	1313.9 0	140.9 8	4	97.33
CaMg ₂ Al ₁₆ O ₂₇	2	5.59	3.73	7	3	2	2	0.00	-2	1313.9 0	140.9 8	4	98.56
Cs ₂ GeF ₆	1	8.99	4.14	1	4	8	-1	328.1 6	0	0.00	0.00	0	242.10
Cs ₂ HfF ₆	1	6.39	5.24	1	4	2	-1	328.1 6	0	0.00	0.00	0	229.04
Cs ₂ KCrF ₆	1	9.00	4.28	1	3	8	1	48.39	-1	1681.0 0	328.1 6	5	217.26
Cs ₂ NaAl ₃ F ₁₂	1	7.31	3.82	1	3	2	1	52.87	-1	1681.0 0	328.1 6	5	233.73
Cs ₂ SiF ₆	1	8.92	3.86	1	4	8	-1	328.1 6	0	0.00	0.00	0	243.78

	O/F/O F	lat_para_ b	cryst_de ns	species_octahe dra	valence_ 1	num_atomic 2	valence_ 3	EA_3	valence_ 4	IE_4	EA_4	num_VEPM 4	AVG_E A
Cs ₂ ZrF ₆	1	6.41	4.39	1	4	2	-1	328.1 6	0	0.00	0.00	0	233.45
CsMoO ₂ F ₃	3	6.46	4.22	1	6	4	-2	140.9 8	-1	1681.0 0	328.1 6	5	197.73
Gd ₂ ZnTiO ₆	2	5.66	7.47	1	4	4	2	0.00	-2	1313.9 0	140.9 8	4	85.35
Gd ₂ ZnTiO ₆	2	5.66	7.47	1	4	4	2	0.00	-2	1313.9 0	140.9 8	4	85.35
K ₂ BaGe ₈ O ₁₈	2	11.73	4.70	4	4	12	2	13.95	-2	1313.9 0	140.9 8	4	124.13
K ₂ GeF ₆	1	5.63	3.44	1	4	2	-1	328.1 6	0	0.00	0.00	0	242.74
K ₂ LiAlF ₆	1	7.84	3.11	1	3	8	1	59.63	-1	1681.0 0	328.1 6	5	216.71
K ₂ NaInF ₆	1	8.56	3.49	1	3	8	1	52.87	-1	1681.0 0	328.1 6	5	214.75
K ₂ SiF ₆	1	8.13	2.72	1	4	8	-1	328.1 6	0	0.00	0.00	0	244.42
K ₂ TiF ₆	1	5.72	3.03	1	4	2	-1	328.1 6	0	0.00	0.00	0	230.37
K ₃ AlF ₆	1	18.84	2.85	5	3	23	-1	328.1 6	0	0.00	0.00	0	219.08
KGaP ₂ O ₇	2	9.87	3.30	1	3	4	5	72.04	-2	1313.9 0	140.9 8	4	110.98
KNaSiF ₆	1	5.50	2.70	1	4	4	1	52.87	-1	1681.0 0	328.1 6	5	244.92
KZnF ₃	1	4.07	4.02	1	2	1	-1	328.1 6	0	0.00	0.00	0	206.57
La(MgTiO ₆) 0.5	2	3.96	5.96	1	4	1	2	0.00	-2	1313.9 0	140.9 8	4	79.32
La ₂ ZnTiO ₆	2	5.60	6.53	2	4	4	2	0.00	-2	1313.9 0	140.9 8	4	94.42
La ₃ GaGe ₅ O ₁₆	2	8.09	6.00	1	4	6	3	41.49	-2	1313.9 0	140.9 8	4	121.12
LaAlO ₃	2	5.36	6.52	1	3	2	-2	140.9 8	0	0.00	0.00	0	102.01
LaScO ₃	2	5.79	5.78	1	3	4	-2	140.9 8	0	0.00	0.00	0	97.29
LaSrZnNbO 6	2	8.00	6.24	1	5	4	2	4.63	2	906.40	0.00	10	15.37
LaSrZnSbO ₆	2	5.66	6.61	1	5	2	2	0.00	-2	1313.9 0	140.9 8	4	28.72

	O/F/O F	lat_para b	cryst_de ns	species_octahe dra	valence 1	num_atomic 2	valence 3	EA_3	valence 4	IE_4	EA_4	num_VEPM 4	AVG_E A
LaTiSbO ₆	2	5.21	5.54	1	5	1	4	7.62	-2	1313.9 0	140.9 8	4	111.09
Li ₂ MgZrO ₄	2	4.21	3.96	1	4	4	2	0.00	-2	1313.9 0	140.9 8	4	90.54
Li ₂ SnO ₃	2	9.18	6.00	2	4	16	-2	140.9 8	0	0.00	0.00	0	108.25
Li ₂ ZnTi ₃ O ₈	2	8.37	3.97	1	4	8	2	0.00	-2	1313.9 0	140.9 8	4	90.71
Li ₃ Mg ₂ NbO ₆	2	8.56	3.84	1	5	24	2	0.00	-2	1313.9 0	140.9 8	4	92.76
Li ₅ La ₃ Nb ₂ O ₁₂	2	12.80	5.26	2	5	40	3	45.35	-2	1313.9 0	140.9 8	4	104.67
Li ₅ La ₃ Ta ₂ O ₁₂	2	12.81	6.36	1	5	40	3	45.35	-2	1313.9 0	140.9 8	4	99.46
Li ₆ SrLa ₂ Sb ₂ O ₁₂	2	12.89	5.22	1	5	48	2	4.63	3	538.09	45.35	1	102.03
LiLa ₂ SbO ₆	2	5.72	6.51	1	5	2	3	45.35	-2	1313.9 0	140.9 8	4	109.71
LiSrAlF ₆	1	5.07	3.45	1	3	2	0	549.4 7	0	3.98	1681. 0	2	47.73
Mg ₇ Ga ₂ GeO ₁₂	2	25.45	4.30	1	3	14	4	118.9 4	-2	1313.9 0	140.9 8	4	86.08
Na _{1.57} Zn _{0.57} Al _{10.43} O ₁₇	2	5.62	3.43	2	3	5	2	0.00	-2	1313.9 0	140.9 8	4	98.30
Na ₂ GeF ₆	1	9.06	3.19	2	4	6	-1	328.1 6	0	0.00	0.00	0	243.74
Na ₂ MgAl ₁₀ O ₁₇	2	5.61	3.30	2	3	6	2	0.00	-2	1313.9 0	140.9 8	4	97.38
Na ₂ NbF ₅ O	3	5.51	3.25	1	5	8	-1	328.1 6	-2	1313.9 0	140.9 8	4	219.54
Na ₂ SiF ₆	1	8.86	2.74	2	4	6	-1	328.1 6	0	0.00	0.00	0	245.42
Na ₃ AlF ₆	1	5.60	2.97	1	3	6	-1	328.1 6	0	0.00	0.00	0	216.93
Na ₃ Li ₃ Al ₂ F ₁₂	1	12.12	2.77	1	3	24	1	59.63	-1	1681.0 0	328.1 6	5	217.27
Na ₃ Li ₃ Sc ₂ F ₁₂	1	12.61	2.70	1	3	24	1	59.63	-1	1681.0 0	328.1 6	5	215.58
Na ₃ Li ₃ Sc ₂ F ₁₂	1	12.61	2.70	1	3	24	1	59.63	-1	1681.0 0	328.1 6	5	215.58

	O/F/O F	lat_para_ b	cryst_de ns	species_octahed ra	valence_ 1	num_atomic 2	valence_ 3	EA_3	valence_ 4	IE_4	EA_4	num_VEPM 4	AVG_E A
NaHF ₂	1	3.48	2.15	1	1	3	-1	328.1 6	0	0.00	0.00	0	195.49
NaKSnF ₆	1	6.00	3.40	1	4	4	1	48.39	-1	1681.0 0	328.1 6	5	56.31
NaKSnF ₆	1	6.00	3.40	1	4	4	1	48.39	-1	1681.0 0	328.1 6	5	241.95
NaLaMgTe O ₆	2	5.53	5.60	1	6	2	3	45.35	2	737.75	0.00	0	113.43
NaLaMgW O ₆	2	7.82	6.42	1	6	4	3	45.35	2	737.75	0.00	0	102.29
Rb ₂ HfF ₆	1	6.14	4.90	1	4	2	-1	328.1 6	0	0.00	0.00	0	229.34
Rb ₂ KGaF ₆	1	8.81	3.83	1	3	8	1	48.39	-1	1681.0 0	328.1 6	5	215.26
Rb ₂ NaAlF ₆	1	8.31	3.88	1	3	8	1	52.87	-1	1681.0 0	328.1 6	5	215.74
Rb ₂ SiF ₆	1	8.45	3.45	1	4	8	-1	328.1 6	0	0.00	0.00	0	244.09
Rb ₂ ZrF ₆	1	6.16	3.94	1	4	2	-1	328.1 6	0	0.00	0.00	0	233.76
Rb ₃ Nb ₃ OF ₁₈	3	15.53	3.76	2	5	20	-2	140.9 8	-1	1681.0 0	328.1 6	5	242.50
Sr ₂ CaWO ₆	2	5.77	5.94	2	6	4	2	2.37	-2	1313.9 0	140.9 8	4	93.63
Sr ₂ InSbO ₆	2	5.73	6.34	1	5	4	3	28.95	-2	1313.9 0	140.9 8	4	98.50
Sr ₂ MgAl ₂₂ O 36	2	5.58	3.77	4	3	2	2	0.00	-2	1313.9 0	140.9 8	4	101.35
Sr ₂ MgWO ₆	2	7.95	6.33	1	6	8	2	0.00	-2	1313.9 0	140.9 8	4	93.39
Sr ₂ MgWO ₆	2	7.95	6.33	1	6	8	2	0.00	-2	1313.9 0	140.9 8	4	93.39
Sr ₂ YTaO ₆	2	5.86	6.40	1	5	4	3	29.62	-2	1313.9 0	140.9 8	4	94.77
Sr ₂ ZnMoO ₆	2	7.95	5.71	1	6	8	2	0.00	-2	1313.9 0	140.9 8	4	92.73
Sr ₂ ZnWO ₆	2	7.93	6.94	1	6	8	2	0.00	-2	1313.9 0	140.9 8	4	93.39
Sr ₃ Al ₁₀ SiO ₂₀	2	11.18	3.71	2	3	6	4	134.0 7	-2	1313.9 0	140.9 8	4	99.56

	O/F/O F	lat_para_ b	cryst_de ns	species_octahe dra	valence_ 1	num_atomic 2	valence_ 3	EA_ 3	valence_ 4	IE_4	EA_ 4	num_VEPM 4	AVG_E A
Sr ₃ Al ₁₀ SiO ₂₀	2	11.18	3.71	2	3	6	4	134.0 7	-2	1313.9 0	140.9 8	4	99.56
Sr ₃ LiSbO ₆	2	9.77	5.25	1	5	18	1	59.63	-2	1313.9 0	140.9 8	4	92.76
Sr ₃ LiTaO ₆	2	9.81	5.83	1	5	18	1	59.63	-2	1313.9 0	140.9 8	4	86.41
Sr ₃ NaSbO ₆	2	9.76	5.25	1	5	18	1	52.87	-2	1313.9 0	140.9 8	4	92.14
Sr ₄ Al ₁₄ O ₂₅	2	8.49	3.65	3	3	8	-2	140.9 8	0	0.00	0.00	0	95.99
SrAl ₁₂ O ₁₉	2	5.57	4.20	3	3	2	-2	140.9 8	0	0.00	0.00	0	99.51
SrGd ₂ Al ₂ O ₇	2	3.71	6.94	1	3	2	3	0.00	-2	1313.9 0	140.9 8	4	89.58
SrGe ₄ O ₉	2	11.34	4.91	2	4	3	-2	140.9 8	0	0.00	0.00	0	124.94
SrLa ₂ Sc ₂ O ₇	2	5.74	5.53	1	3	4	3	45.35	-2	1313.9 0	140.9 8	4	93.21
SrLaAlO ₄	2	3.76	5.91	1	3	2	3	45.35	-2	1313.9 0	140.9 8	4	89.78
SrLaGaO ₄	2	3.84	6.39	1	3	2	3	45.35	-2	1313.9 0	140.9 8	4	93.63
SrLaScO ₄	2	5.75	5.39	1	3	4	3	45.35	-2	1313.9 0	140.9 8	4	90.29
SrMgAl ₁₀ O ₁₇	2	5.63	3.54	2	3	2	2	0.00	-2	1313.9 0	140.9 8	4	97.20
Y ₃ Al ₅ O ₁₂	2	12.01	4.55	1	3	24	-2	140.9 8	0	0.00	0.00	0	99.47
YCa ₃ (AlO) ₃ (B O ₃) ₄	2	10.39	3.58	1	3	7	2	2.37	3	800.64	26.99	1	82.08

Table S6. Hyper-parameter.

XGB.r	n_estimators=66 learning_rate=0.09 Booster =" gbtree"
RF.r	n_estimators=145 max_depth=7 max_features=4 min_sample_leaf=1 min_samples_split=4 random_state=31
Lasso.r	Alpha=0.625370743
R.r	Alpha=3
KNN.r	n_neighbors=3 Algorithm=" ball_tree" Weights=" distance"
SVM.r	C=159.074647 Epsilon=1.2138 Gamma=0.01 Kernel=" rbf"

Table S7. Predicted emission wavelength (nm) and the experimental (exp.) emission wavelength (nm).

	exp(nm)	XGB.r	%diff.	Lasso.r	%diff.	R.r	%diff.
Ba ₂ LaNbO ₆	677	666	-1.62	696	+2.81	696	+2.81
Ba ₂ YNbO ₆	695	685	-1.44	672	-3.31	674	-3.02
Sr ₂ LaSbO ₆	694	671	-3.31	664	-4.32	666	-4.03
Mg ₂ TiO ₄	657	695	+5.78	683	+3.96	684	+4.11
Ba ₂ YSbO ₆	697	706	+1.29	707	+1.43	710	+1.87
Sr ₂ ScSbO ₆	703	706	+0.43	698	-0.71	702	-0.14
Ca ₂ LaSbO ₆	687	714	+3.93	689	+0.29	689	+0.29
CaYAlO ₄	713	709	-0.56	685	-3.93	686	-3.79
K ₂ NaGaF ₆	630	639	+1.43	636	+0.95	635	+0.79
La ₂ MgGeO ₆	710	711	+0.14	703	-0.99	704	-0.85
Li ₂ MgTi ₃ O ₈	680	682	+0.29	677	-0.44	679	-0.15
Na ₂ WO ₂ F ₄	620	667	+7.58	634	+2.26	630	+1.61
Rb ₂ MoO ₂ F ₄	632	674	+6.65	637	+0.79	633	+0.16
BaSiF ₆	632	641	+1.42	609	-3.64	607	-3.96
K ₃ SiF ₇	633	640	+1.11	612	-3.32	609	-3.79
Ba ₂ GdSbO ₆	687	681	-0.87	710	+3.35	711	+3.49
Sr ₃ NaSbO ₆	695	712	+2.45	699	+0.58	698	+0.43
SrLaSc ₂ O ₇	704	708	+0.57	692	-1.70	692	-1.70
KNaWO ₂ F ₄	625	638	+2.08	655	+4.8	663	+6.08

Table S8. Three nearest neighbors of different phosphors in the training set and their

	%diff	Neighbor	Dist.	Neighbor	Dist.	Neighbor	Dist.
CaYAlO ₄	-3.73	(NH ₄) ₂ TiF ₆	1.32	BaSnF ₆	1.36	Rb ₂ NaAlF ₆	1.37
La ₂ MgGeO ₆	-2.19	Na ₃ Li ₃ Sc ₂ F ₁₂	1.99	Rb ₂ HfF ₆	2.01	K ₂ BaGe ₈ O ₁₈	2.15
Sr ₂ ScSbO ₆	-1.91	La ₂ ZnTiO ₆	1.4	NaLaMgTeO ₆	1.43	Na ₃ Li ₃ Sc ₂ F ₁₂	1.46
K ₃ SiF ₇	-1.62	Na ₂ MgAl ₁₀ O ₁₇	2.38	BaGeF ₆	2.43	Ba ₂ GdNbO ₆	2.56
Ba ₂ YNbO ₆	-1.01	Na ₃ Li ₃ Sc ₂ F ₁₂	1.52	Rb ₂ HfF ₆	1.52	K ₂ LiAlF ₆	1.78
BaSiF ₆	-0.68	Na ₂ MgAl ₁₀ O ₁₇	2.44	LaTiSbO ₆	2.47	BaGeF ₆	2.5
Ba ₂ YSbO ₆	-0.36	Na ₃ Li ₃ Sc ₂ F ₁₂	0.63	Rb ₂ HfF ₆	1.63	K ₂ BaGe ₈ O ₁₈	1.8
SrLa ₂ Sc ₂ O ₇	-0.24	Ba ₂ CaWO ₆	0.93	BaSnF ₆	0.93	KNaSiF ₆	1.19
Sr ₂ LaSbO ₆	-0.19	NaLaMgTeO ₆	1.38	BaLaMgNbO ₆	1.4	Na _{1.57} Zn _{0.57} Al _{10.43} O ₁₇	1.41
Rb ₂ MoO ₂ F ₄	0	CsMoO ₂ F ₃	1.61	LaTiSbO ₆	2.47	BaGeF ₆	2.5
Li ₂ MgTi ₃ O ₈	+0.24	Ba ₂ LaSbO ₆	1.42	LaScO ₃	1.59	Ba ₂ MgWO ₆	1.72
Ca ₂ LaSbO ₆	+0.3	La ₂ ZnTiO ₆	0.8	LaScO ₃	0.94	NaLaMgTeO ₆	0.97
K ₂ NaGaF ₆	+0.37	Rb ₂ ZrF ₆	1.53	Cs ₂ HfF ₆	1.54	Na ₃ AlF ₆	1.55
Sr ₃ NaSbO ₆	+0.47	Rb ₂ HfF ₆	0.81	Na ₃ Li ₃ Sc ₂ F ₁₂	0.82	Li ₂ MgZrO ₄	1.58
Ba ₂ GdSbO ₆	+1.06	K ₂ BaGe ₈ O ₁₈	1.77	Ba ₂ LuNbO ₆	1.78	Na ₃ Li ₃ Sc ₂ F ₁₂	1.91
Mg ₂ TiO ₄	+1.92	Cs ₂ NaAl ₃ F ₁₂	2.46	Ca ₂ MgWO ₆	2.53	CaMg ₂ Al ₁₆ O ₂₇	2.62
Na ₂ WO ₂ F ₄	+1.95	CsMoO ₂ F ₃	2.04	Ca ₂ InSbO ₆	3.03	Li ₅ La ₃ Nb ₂ O ₁₂	4.34
Ba ₂ LaNbO ₆	+3.88	BaSnF ₆	1.02	Ba ₂ CaWO ₆	1.07	KNaSiF ₆	1.09
KNaWO ₂ F ₄	+6.46	Ba ₂ MgWO ₆	2.55	Rb ₂ NaAlF ₆	2.59	BaTiF ₆	2.59

Euclidean distances.