Electronic Supplementary Information

Interpretable Machine Learning-Assisted Screening of Perovskite Oxides

Jie Zhao*[a], Xiaoyan Wang*[b], Haobo Li[c], Xiaoyong Xu*[c]

[a] College of Chemical Engineering, Nanjing Tech University, Nanjing, Jiangsu 211816, China

[b] School of Computer Science, Nanjing Audit University, Nanjing, Jiangsu 211815, China

[c] School of Chemical Engineering, The University of Adelaide, Adelaide, SA 5005, Australia

Corresponding Authors:

j.zhao1@njtech.edu.cn, xywang@nau.edu.cn, xiaoyong.xu@adelaide.edu.au

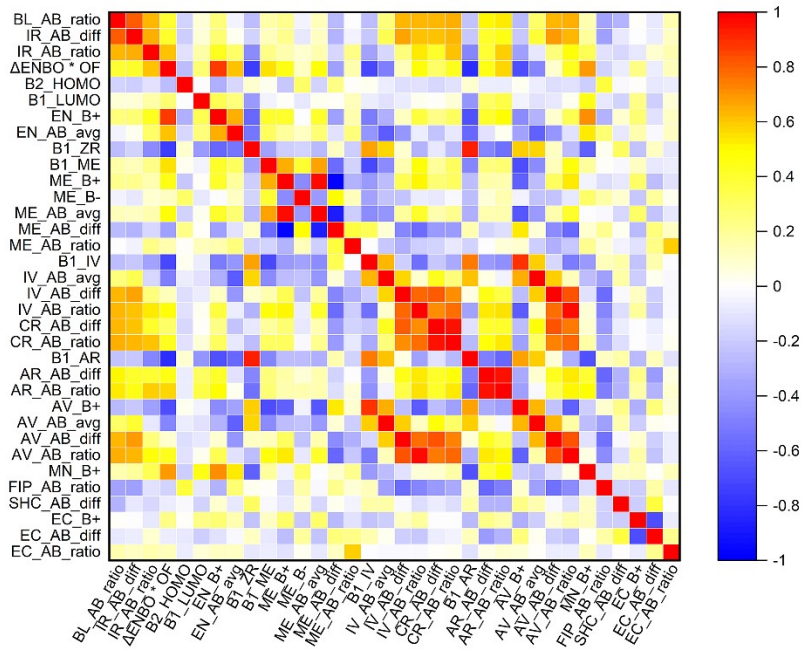

Fig. S1 Pairwise Pearson correlation coefficient heatmap of the 34 features screened from the 291 features.

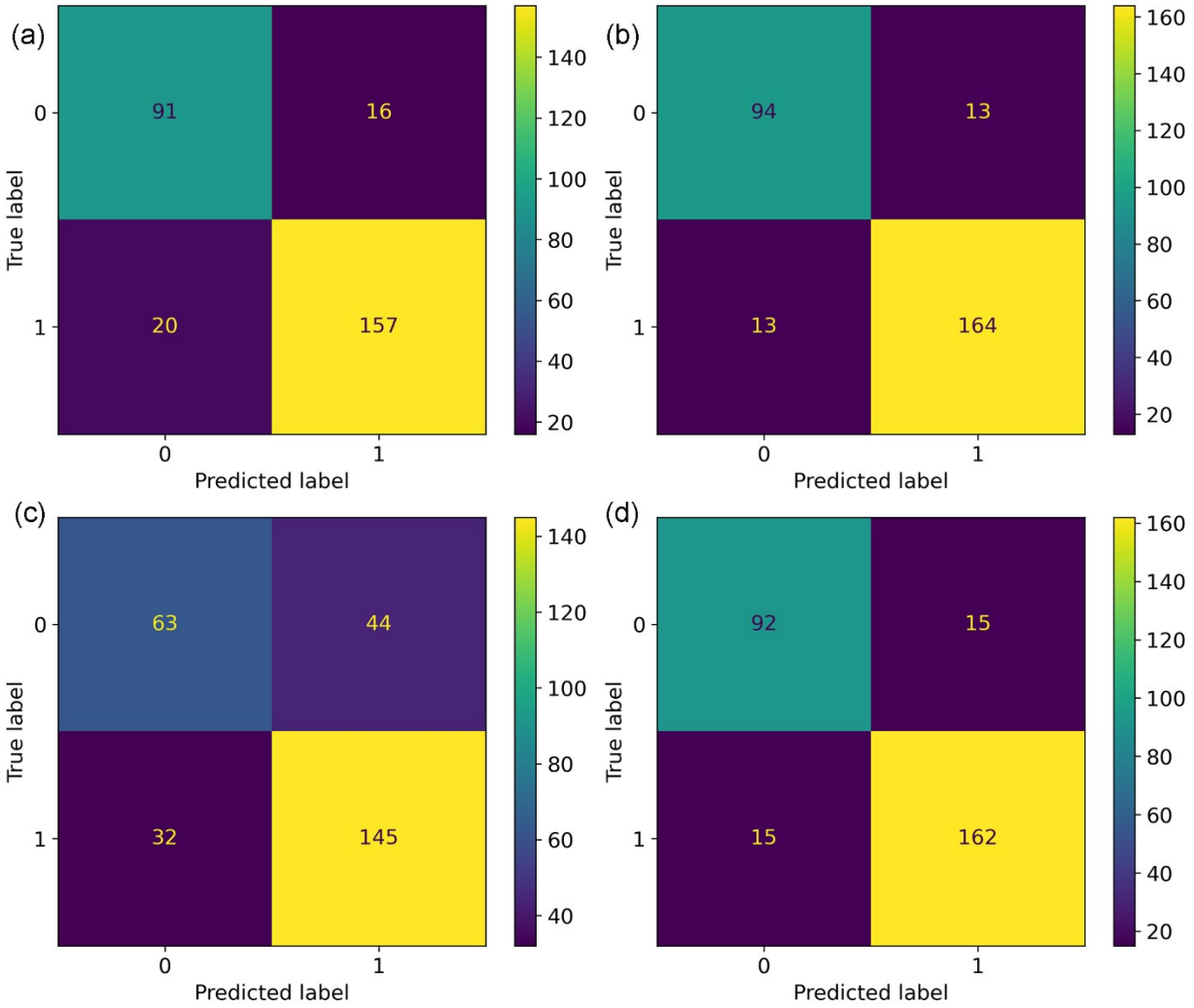

Fig. S2 Confusion matrices of the (a) ABC-23, (b) GBC-23, (c) LRC-23, and (d) RFC-23 models.

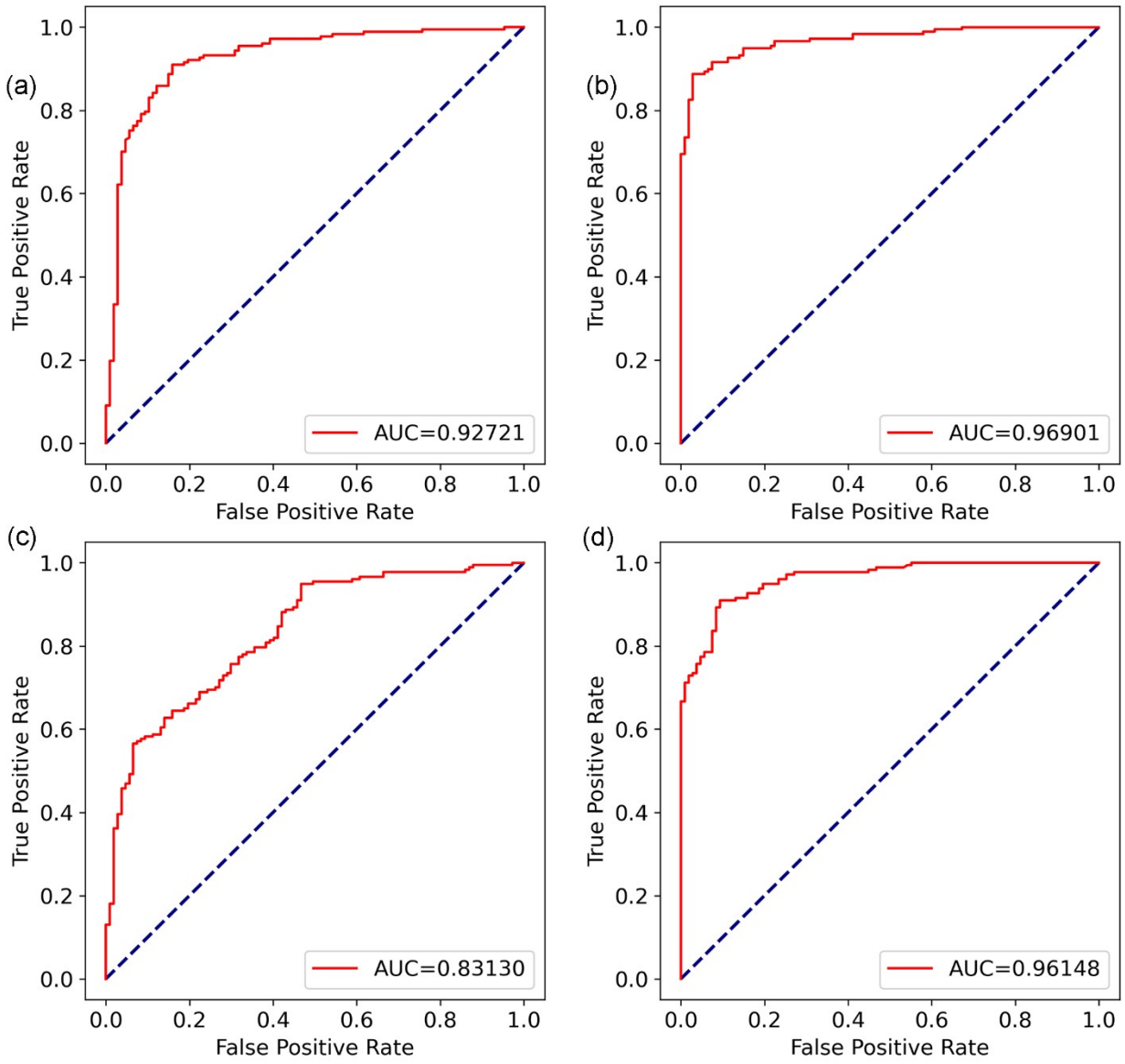

Fig. S3 ROC curves of the (a) ABC-23, (b) GBC-23, (c) LRC-23, and (d) RFC-23 models.

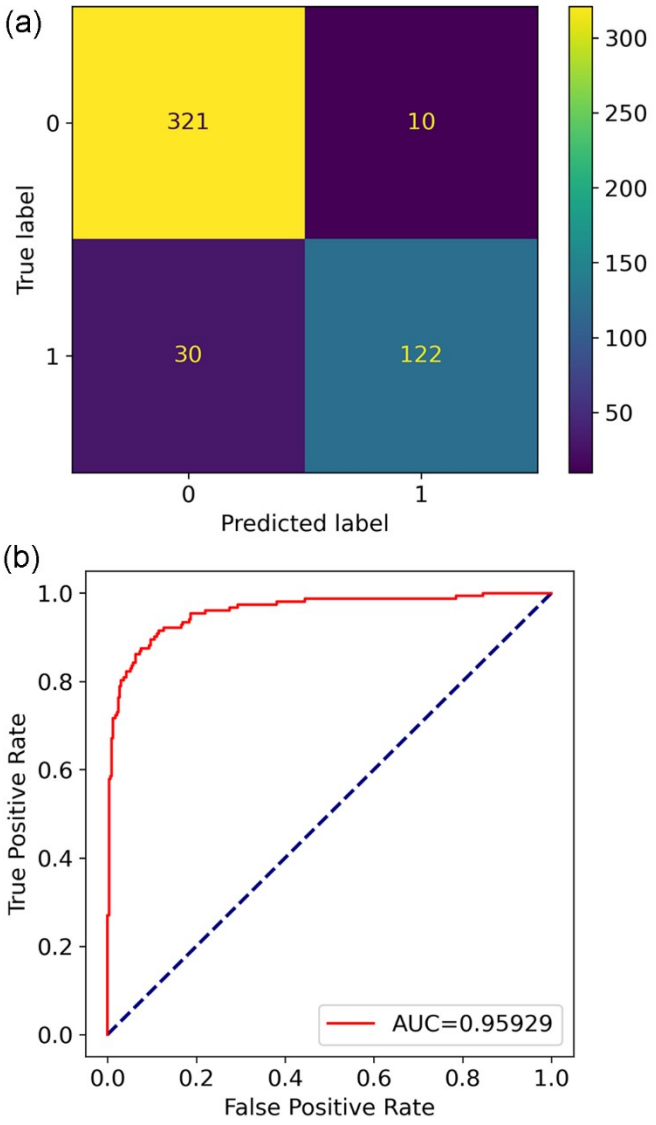

Fig. S4 The (a) confusion matrix and (b) ROC curve of the XGBC-ref model.

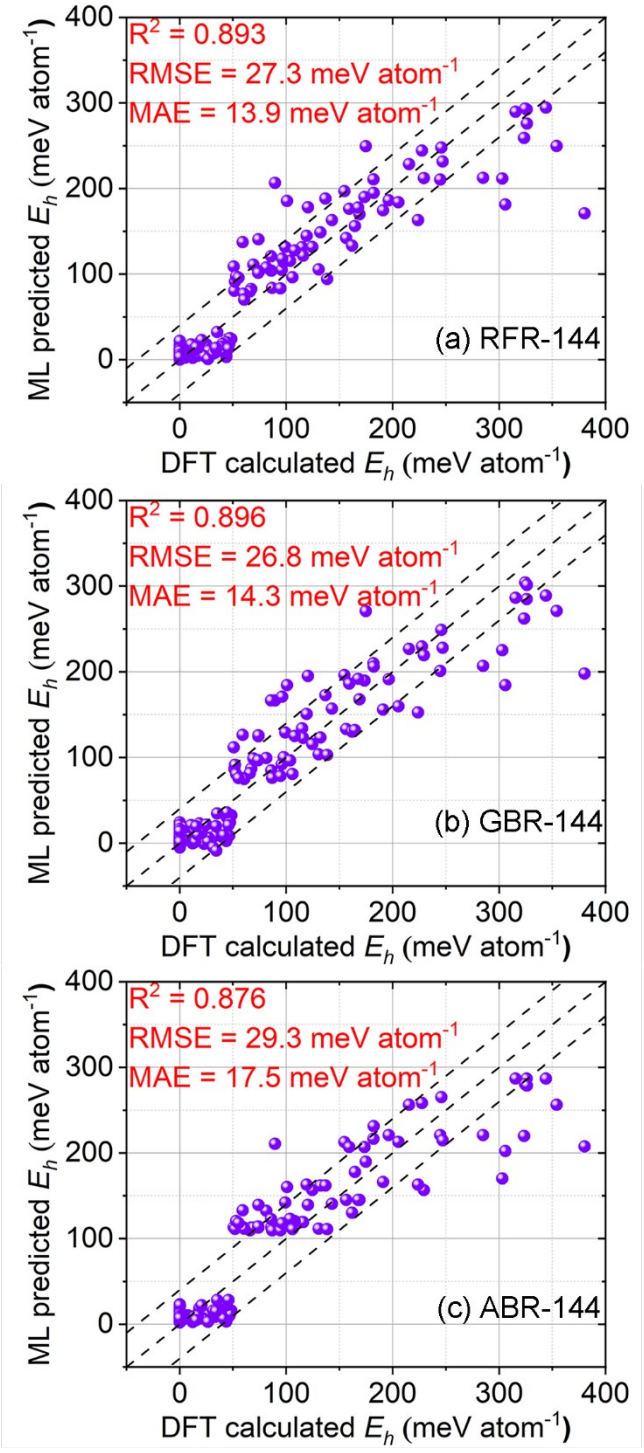

Fig. S5 Performance of the RFR-144, GBR-144, and ABR-144 regression models.

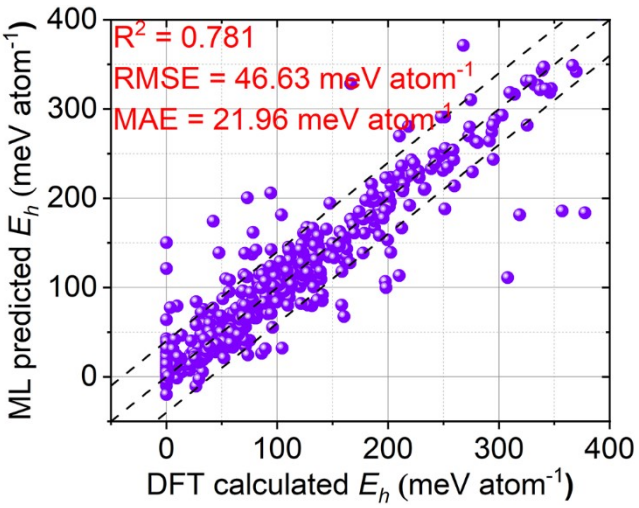

Fig. S6 Performance of the XGBR-ref model that was trained on the dataset of ref 22.

Table S1 The 23 optimal features and the 11 removed features during feature selection for classification model training.

23 optimal features	*BL_AB_ratio*, *IR_AB_ratio*, *B2_HOMO*, *B1_LUMO*, *EN_B+*, *EN_AB_avg*, *B1_ZR*, *B1_ME*, *ME_B-*, *ME_AB_avg*, *ME_AB_ratio*, *IV_AB_avg*, *IV_AB_diff*, *IV_AB_ratio*, *CR_AB_diff*, *AR_AB_diff*, *AV_B+*, *MN_B+*, *FIP_AB_ratio*, *SHC_AB_diff*, *EC_B+*, *EC_AB_diff*, *EC_AB_ratio*
11 removed features	*IR_AB_diff*, ΔEN_{BO}**OF*, *ME_B*$^+$, *ME_AB_diff*, *B1_IV*, *CR_AB_ratio*, *B1_AR*, *AR_AB_ratio*, *AV_AB_avg*, *AV_AB_diff*, *AV_AB_ratio*

Table S2 Hyperparameters for various machine learning models.

Model	Hyperparameter	Model	Hyperparameter
ABC-23	'learning_rate': 0.5, 'n_estimators': 250	ABR-144	'learning_rate': 0.2 'n_estimators': 100
GBC-23	'max_depth': 6, 'n_estimators': 250	GBR-144	'max_depth': 5 'n_estimators': 150
LRC-23	'C': 100, 'penalty': 'l2'	RFR-144	'max_depth': 13 'n_estimators': 200
RFC-23	'max_depth': 13, 'n_estimators': 100	XGBR-144	'max_depth': 6 'n_estimators': 100
XGBC-23	'max_depth': 13, 'n_estimators': 100		

Table S3 Comparison of the E_h values predicted by the XGBR-144 model and calculated by density functional theory that are not included in the input dataset.

Formula	**E_h-DFT (meV atom^{-1})**	**E_h-predicted (meV atom^{-1})**	**Formula**	**E_h-DFT (meV atom^{-1})**	**E_h-predicted (meV atom^{-1})**
Ba_2CaOsO_6 [1]	0	9	$BaPdO_3$	29	1
Ba_2CeZrO_6 [2]	24	19	$CaFeO_3$ [3]	52	0
Ba_2CePtO_6	0	0	$EuHfO_3$ [4]	0	6
Ba_2CeHfO_6	23	18	$EuNbO_3$ [5]	24	6
Ba_2DyNbO_6	0	2	$EuVO_3$ [6]	43	0
Ba_2ErNbO_6 [7]	0	8	$PrCuO_3$ [8, 9]	25	7
Ba_2EuReO_6 [10]	0	5	$SrFeO_3$ [11]	0	0
Ba_2HoMoO_6	0	0	$YbTaO_3$ [12]	26	0
Ba_2HoNbO_6 [13]	0	0	$BaTaO_3$ [14]	32	6
Ba_2LuMoO_6 [15]	0	7	$KReO_3$ [16]	37	14
Ba_2LuNbO_6 [17]	0	0	$NaReO_3$ [16]	42	11
Ba_2LuRuO_6 [18]	0	18	$SrNiO_3$ [19]	46	0
Ba_2LuSbO_6 [20]	0	1	Ba_2BiLaO_6 [21]	28	30
Ba_2LuTaO_6 [22]	0	0	Ba_2BiDyO_6 [21]	3	36
Ba_2NbVO_6 [23]	0	5	Ba_2BiCeO_6 [21]	48	38
Ba_2NbFeO_6	0	0	Ba_2BiSmO_6 [21]	8	35
Ba_2NbInO_6	0	3	Ba_2BiGdO_6 [21]	6	26
Ba_2SmMnO_6	45	26	Ba_2BiTbO_6	11	37
Ba_2TaTlO_6	0	22	Ba_2BiLuO_6	2	32

Ba_2TmNbO_6	0	25	Ba_2BiYO_6	3	36
Ba_2TmRuO_6	0	33	Eu_2CrSbO_6	39	7
Ba_2TmMoO_6	0	30	Eu_2CrSnO_6	47	12
Ba_2ZrSnO_6	0	20	Eu_2FeWO_6	29	3
Ba_2ZrTiO_6	5	19	Eu_2HfTiO_6	17	6
Ba_2LaFeO_6	42	0	Eu_2HfSnO_6	22	5
$BaSrMo_2O_6$	47	1	Eu_2HfFeO_6	44	17
$BaSrCoWO_6$ [24]	15	0	Eu_2LuTaO_6	22	6
$Sr2HfSnO_6$	19	18	Eu_2MgWO_6	0	6
$Sr2HfTiO_6$	22	12	Eu_2MnWO_6	0	0
$Sr2HfFeO_6$	42	5	Eu_2NbFeO_6	37	1
$Sr2HfCrO_6$	33	6	Eu_2NiWO_6	34	3
$Sr2HfZrO_6$	44	15	Eu_2TaAlO_6	0	10
Sr_2NiRuO_6 [25]	0	2	Eu_2TiNbO_6	8	6
Sr_2VWO_6 [26]	13	0	Eu_2TmTaO_6	36	17
Sr_2FeCoO_6 [27]	20	0	Eu_2VWO_6	33	0
Sr_2FeHfO_6 [28]	42	5	Eu_2ZnWO_6	0	4

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