

Supplementary

Integrating NSGA-II and TOPSIS for Stacking Model Optimization in Pursuit of Halide Double Perovskite Screening

Guiqin Liang^{1,2,*} and Jian Zhang^{3,4,*}

1 College of Information and Communication, Guilin University of Electronic Technology, Guilin 541004, China

2 College of Physics and Electronic Information Engineering, Guilin University of Technology, Guilin 541004, China

3 College of Materials Science and Engineering, Guilin University of Electronic Technology, Guilin 541004, China

4 Guangxi Key Laboratory of Information Materials, Guangxi Collaborative Innovation Center of Structure and Property for New Energy and Materials, Guilin 541004, China

* Corresponding authors:

E-mail addresses: 2014054@glut.edu.com (G.L.), jianzhang@guet.edu.cn (J.Z.)

ORCID: 0000-0003-1289-2416 (G.L.)

Table S1 The specific information of the base models of the stacking models and its corresponding performance on the test set with 40 runs of 5-fold cross-validation for E_g prediction.

No.	Num_Base_Models	Base_Models	Meta_Model	MSE	RMSE	MAE	R2
1	3	CatBR, Bag, LGBR	LR	0.0362	0.1869	0.1110	0.9424
2	4	Ada, BR, Bag, XGBR	LR	0.0432	0.2048	0.1285	0.9309
3	5	Ada, ETR, CatBR, Bag, RFR	LR	0.0358	0.1861	0.1106	0.9429
4	6	RFR, LGBR, Bag, XGBR, ETR, DTR	LR	0.0435	0.2053	0.1297	0.9304
5	7	BR, CatBR, DTR, XGBR, ETR, LR, Ada	LR	0.0356	0.1853	0.1098	0.9433
6	8	Ada, ETR, LR, BR, Bag, LGBR, DTR, RFR	LR	0.0542	0.2297	0.1536	0.9131
7	9	ETR, RFR, LR, Bag, XGBR, BR, Ada, DTR, LGBR	LR	0.0433	0.2048	0.1291	0.9307
8	10	ETR, Ada, RFR, LGBR, DTR, CatBR, XGBR, LR, BR, Bag	LR	0.0361	0.1867	0.1106	0.9425
9	11	GBR, ETR, Ada, RFR, LGBR, DTR, CatBR, XGBR, LR, BR, Bag	LR	0.0359	0.1862	0.1101	0.9426

Table S2 The specific information of the base models of the stacking models and its corresponding performance on the test set with 40 runs of 5-fold cross-validation for H_f prediction.

No.	Num_Base_ Models	Base_Models	Meta_Model	MSE	RMSE	MAE	R2
1	3	CatBR, Bag, LGBR	LR	0.00016	0.01178	0.00650	0.99716
2	4	Ada, BR, Bag, XGBR	LR	0.00017	0.01257	0.00765	0.99680
3	5	Ada, ETR, CatBR, Bag, RFR	LR	0.000136	0.010891	0.006088	0.997500
4	6	RFR, LGBR, Bag, XGBR, ETR, DTR	LR	0.00017	0.01224	0.00736	0.99693
5	7	BR, CatBR, DTR, XGBR, ETR, LR, Ada	LR	0.00015	0.01179	0.00615	0.99717
6	8	Ada, ETR, LR, BR, Bag, LGBR, DTR, RFR	LR	0.00017	0.01250	0.00754	0.99683
7	9	ETR, RFR, LR, Bag, XGBR, BR, Ada, DTR, LGBR	LR	0.00015	0.01166	0.00710	0.99718
8	10	ETR, Ada, RFR, LGBR, DTR, CatBR, XGBR, LR, BR, Bag	LR	0.00015	0.01147	0.00615	0.99729
9	11	GBR, ETR, Ada, RFR, LGBR, DTR, CatBR, XGBR, LR, BR, Bag	LR	0.00015	0.01166	0.00710	0.99718