

Supplementary Information for

A compositional feature-driven prediction model for the emission wavelength of Eu²⁺-doped whitlockite-type phosphors coupled with a material design framework

Zhichao Zhang ^{a,c}, Jun Zhou ^b, Jinhui Wang ^c, Guotao Chu ^c, Xuerui You ^c, Chunping Liang ^c, Jifan Hu ^{a,*}

^a *College of Materials Science and Engineering, Taiyuan University of Science and Technology, Taiyuan 030024, China*

^b *Department of Physics, Beijing Technology and Business University, Beijing 100048, China*

^c *Department of Energy Chemistry and Materials Engineering, ShanXi Institute of Energy, Jinzhong 030600, China*

Table S1 | Hyperparameter settings for machine learning models

model	hyperparameter	value
SVR	C	50
	degree	3
	gamma	0.2
	epsilon	0.05
DTR	max_depth	7
	random_state	47
	random_state	47
Xgboosting	n_estimators	30
	max_depth	8
	learning_rate	0.1
	iterations	160
Catboosting	learning_rate	0.12
	depth	8
	random_seed	42
GBR	n_estimators	200
	random_state	53
	learning_rate	0.09
	n_estimators	100
	max_samples	0.8
Stacking	random_state	47
	C	10
	degree	2
	gamma	0.001
	epsilon	0.01
Adaboosting	n_estimators	170
	learning_rate	0.09
	random_state	14
Bagging	max_depth	19

	random_state	41
	n_estimators	100
	max_samples	0.9
	n_estimators	120
RFR	max_depth	18
	random_state	54
