

algorithm	hyperparameter	investigated values	selected value	
			without alloy_name	with alloy_name
RFR	n_estimators	[10, 50, 100]	100	100
	max_depth	[3, 5, 10]	10	10
	min_samples_split	[2, 3, 5]	3	3
	min_samples_leaf	[1, 2, 4]	1	1
MLP	hidden_layer_sizes	[(10,), (10, 10), (25,)]	(10, 10)	(10)
	alpha	[0.01, 0.1, 1.0, 3.0]	0.1	0.01
	activation	['relu', 'tanh']	tanh	tanh
XGBoost	n_estimators	[100, 300]	300	300
	max_depth	[2, 3, 4]	2	2
	learning_rate	[0.01, 0.05]	0.05	0.05
	subsample	[0.8, 1.0]	0.8	0.8
	colsample_bytree	[0.8, 1.0]	1.0	1.0
	reg_lambda	[0.1, 1, 5, 10]	0.1	0.1
	gamma	[0, 0.1, 0.3]	0.3	0.3
	min_child_weight	[2, 3, 5]	2	2

Further information on the individual hyperparameters and their effects can be found in the scikit-learn documentation (https://scikit-learn.org/stable/user_guide.html).