# Interpretable machine learning screening and analysis of pressure sensitivity and high-pressure emission line shifts in lanthanide and transition metal doped phosphors

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## Brief introduction to the mathematical principles of algorithms

### 1. Linear Regression

Linear Regression serves as the fundamental baseline for regression analysis, aiming to model the relationship between the scalar dependent variable and one or more explanatory variables. It estimates the regression coefficients by minimizing the residual sum of squares between the observed and predicted targets. The classical objective function is expressed as:

$$\min_{\beta} \| y - X\beta \|_2^2 \tag{1}$$

Where $y$ denotes the vector of observed values, $X$ represents the feature matrix, and $\beta$ is the vector of regression coefficients to be optimized.

### 2. Ridge Regression

Ridge Regression addresses the issue of multicollinearity often present in multiple linear regression by introducing an L2-norm regularization term. This method constrains the magnitude of the coefficients, thereby reducing model variance and preventing overfitting. The cost function is modified as follows:

$$J(\beta) = \sum_{i=1}^{n}(y_i - \sum_{j=0}^{p} x_{ij}\beta_j)^2 + \lambda \sum_{j=0}^{p} \beta_j^2 \tag{2}$$

Here, $\lambda$ is the complexity parameter (regularization strength) that controls the amount of shrinkage applied to the coefficients $\beta_j$.

### 3. Decision Tree Regression (DT)

Decision Tree Regression is a non-parametric method that models the value of a target variable by learning simple decision rules inferred from the data features. The tree grows by recursively partitioning the feature space into rectangular regions. The quality of a split is typically measured by the Mean Squared Error (MSE). For a node $m$ representing a region $R_m$ with $N_m$ observations, the MSE is calculated as:

$$\mathrm{MSE} = \frac{1}{N_m} \sum_{i \in R_m} (y_i - \bar{y}_m)^2 \tag{3}$$

Where $y_i$ is the actual value of the sample and $\bar{y}_m$ is the mean response value of the samples falling into region $R_m$.

### 4. Random Forest Regression (RF)

Random Forest is an ensemble learning method that operates by constructing a multitude of decision trees during training. It employs the bagging (bootstrap aggregating) technique to generate diverse training subsets. The final prediction is obtained by averaging the output of individual trees to improve predictive accuracy and control over-fitting. The aggregation formula is:

$$\hat{y} = \frac{1}{B} \sum_{b=1}^{B} f_b(x) \tag{4}$$

In this equation, $B$ represents the total number of trees in the forest, and $f_b(x)$ denotes the prediction output from the $b$-th decision tree for the input vector $x$.

### 5. Gradient Boosting Decision Tree (GBDT)

Gradient Boosting Decision Tree is an iterative algorithm that constructs an ensemble of weak prediction models, typically decision trees, in a stage-wise fashion. Unlike Random Forest, GBDT builds trees sequentially, where each new tree aims to correct the pseudo-residuals (negative gradient of the loss function) left by the preceding models. The update rule for the model at step $m$ is given by:

$$F_m(x) = F_{m-1}(x) + \nu \cdot h_m(x) \tag{5}$$

Here, $F_{m-1}(x)$ is the ensemble prediction from the previous stage, $h_m(x)$ is the weak learner fitted to the current residuals, and $\nu$ is the learning rate scaling the contribution of each tree.

### 6. XGBoost Regression

eXtreme Gradient Boosting (XGBoost) is a scalable and highly efficient implementation of gradient boosting. It distinguishes itself by utilizing a second-order Taylor expansion of the loss function to optimize the objective and incorporates a regularization term explicitly into the objective function to control model complexity. The objective function at iteration $t$ is:

$$L^{(t)} = \sum_{i=1}^{n} l\left(y_i, \hat{y}_i^{(t-1)} + f_t(x_i)\right) + \Omega(f_t) \tag{6}$$

Where $l$ is the differentiable convex loss function measuring the difference between the prediction $\hat{y}_i$ and the target $y_i$, and $\Omega(f_t)$ represents the regularization term penalizing the complexity of the tree structure.

### 7. LightGBM Regression

Light Gradient Boosting Machine (LightGBM) is a distributed gradient boosting framework that uses tree-based learning algorithms. It is designed for efficiency and faster training speed, employing a histogram-based algorithm to bucket continuous feature values. A key feature is the leaf-wise (best-first) tree growth strategy with max depth limitation, which tends to achieve lower loss than level-wise growth. The split gain for a leaf is calculated based on gradients:

$$\text{Gain} = \frac{1}{2}\left[\frac{G_L^2}{H_L + \lambda} + \frac{G_R^2}{H_R + \lambda} + \frac{(G_L + G_R)^2}{H_L + H_R + \lambda}\right] - \gamma \tag{7}$$

In this formula, $G_L$ and $G_R$ are the sums of the first-order gradients of the samples in the left and right child nodes, $H_L$ and $H_R$ are the sums of the second-order gradients (Hessians), and $\gamma$ is the regularization parameter for leaf formulation.

### 8. CatBoost Regression

CatBoost is an advanced gradient boosting library that handles categorical features automatically using an algorithm called Ordered Target Statistics. To prevent prediction shift—a common issue in boosting—it utilizes an ordered boosting scheme. The algorithm minimizes the expected loss function defined as:

$$L(\theta) = E_{(x,y)\sim P}[L(y,F(x))] \tag{8}$$

Where $L$ is the loss function (e.g., squared error for regression), and $F(x)$ is the predictive model. CatBoost builds symmetric (oblivious) trees where the same split feature and condition are used across the entire level of the tree, which facilitates efficient execution and reduces the risk of overfitting.

**Table S1.**

The optimal hyperparameters of the machine learning models determined by Genetic Algorithm.

| Model | Hyperparameter | Optimal Value |
|---|---|---|
| Linear Regression | Fit Intercept | TRUE |
| Decision Tree | Fit Intercept | TRUE |
| Ridge Regression | Alpha | 0.743 |
| Random Forest | Number of Estimators | 97 |
| | Max Depth | 10 |
| | Min. Samples Leaf | 1 |
| CatBoost | Iterations | 166 |
| | Learning Rate | 0.197 |
| | Depth | 6 |
| | L2 Leaf Reg | 7.687 |
| | Random Strength | 6.777 |
| XGBoost | Learning Rate | 0.15 |
| | Max Depth | 37 |
| | Min. Child Weight | 6 |
| | Gamma | 0.008 |
| LightGBM | Learning Rate | 0.274 |
| | Max Depth | 10 |
| | Number of Leaves | 88 |
| | Min. Child Samples | 8 |
| | Subsample | 0.595 |
| | Colsample By Tree | 0.619 |
| | Reg Alpha (L1) | 1.535 |

| | | |
|---|---|---|
| | Reg Lambda (L2) | 0.293 |
| GBDT | Learning Rate | 0.141 |
| | Max Depth | 21 |
| | Min. Samples Split | 17 |
| | Min. Samples Leaf | 1 |
| | Max Features | 0.313 |

**Table S2.** Dataset for predicting pressure-induced emission shifts and sensitivity in lanthanide and transition metal doped phosphors.

| Name | Valence | a(Å) | b(Å) | c(Å) | V(Å$^3$) | Coord. No. | Ionic Radius(Å) | Centroid (nm) | Phonon Energy(cm$^{-1}$) | Sensitivity (nm/GPa) | Ref. |
|---|---|---|---|---|---|---|---|---|---|---|---|
| $Ca_2Gd_8Si_6O_{26}:Ce^{3+}$ | 3 | 9.74 | 9.74 | 5.74 | 531.752 | 7 | 1.07 | 395 | 554 | 3 | [1] |
| $Ca_2Gd_8Si_6O_{26}:Ce^{3+}$ | 3 | 9.74 | 9.74 | 5.74 | 531.752 | 9 | 1.196 | 395 | 554 | 3 | [1] |
| $Y_6Ba_4(SiO_4)_6F:Ce^{3+}$ | 3 | 9.8894 | 9.8894 | 7.3584 | 623.24 | 9 | 1.196 | 465 | 600 | 0.63 | [2] |
| $Y_6Ba_4(SiO_4)_6F:Ce^{3+}$ | 3 | 9.8894 | 9.8894 | 7.3584 | 623.24 | 7 | 1.07 | 465 | 600 | 0.63 | [2] |
| $Y_2SiO_5:Pr^{3+}$ | 3 | 12.5 | 6.73 | 10.42 | 839.5 | 7 | 1.066 | 320 | 550 | 1.04 | [3] |
| $Y_2Ge_{0.1}Si_{0.9}O_5:Pr^{3+}$ | 3 | 12.55 | 6.75 | 10.46 | 865 | 7 | 1.066 | 320 | 570 | 1.28 | [3] |
| $Y_2Ge_{0.25}Si_{0.75}O_5:Pr^{3+}$ | 3 | 12.6 | 6.78 | 10.5 | 885 | 7 | 1.066 | 320 | 600 | 0.69 | [3] |
| $Ca_9NaZn(PO_4)_7:Eu^{2+}$ | 2 | 10.3478 | 10.3478 | 37.0491 | 3435.64 | 8 | 1.25 | 495 | 720 | 5.21 | [4] |
| $BaCN_2::Eu^{2+}$ | 2 | 6.0249 | 6.0249 | 7.1924 | 262.6 | 4 | 1.17 | 660 | 600 | 19 | [5] |
| $BaLi_2Al_2Si_2N_6::Eu^{2+}$ | 2 | 7.85 | 7.85 | 9.898 | 613.4 | 8 | 1.39 | 532 | 650 | 1.58 | [6] |
| $SrB_4O_7:Sm^{2+}$ | 2 | 4.431 | 10.707 | 4.237 | 200.81 | 9 | 1.41 | 685 | 700 | 0.29 | [7] |
| $NaBiF_4:Er^{3+}$ | 3 | 6.144 | 6.144 | 3.721 | 119.8 | 9 | 1.06 | 1500 | 350 | 0.8 | [8] |
| $YVO_4:Er^{3+}$ | 3 | 7.1224 | 7.1224 | 6.2913 | 319.15 | 8 | 0.985 | 1605 | 900 | 1.77 | [9] |
| $YVO_4:Er^{3+}$ | 3 | 7.1224 | 7.1224 | 6.2913 | 319.15 | 8 | 0.985 | 1596 | 900 | 1.282 | [9] |
| $Zn_2GeO_4:Mn^{2+}$ | 2 | 14.0719 | 14.0719 | 9.7212 | 1606.23 | 6 | 0.66 | 536 | 600 | 21.3 | [10] |
| $ZnS/CaZnOS:Mn^{2+}$ | 2 | 3.757 | 3.757 | 11.401 | 139.42 | 6 | 0.83 | 618.57 | 365 | 6.2 | [11] |
| $Na_3CsMg_7(PO_4)_6:Eu^{2+}$ | 2 | 12.7263 | 10.6969 | 15.5196 | 1945.43 | 6 | 1.17 | 451 | 700 | 2.13 | [12] |
| $Na_3CsMg_7(PO_4)_6:Eu^{2+}$ | 2 | 12.7263 | 10.6969 | 15.5196 | 1945.43 | 7 | 1.2 | 451 | 700 | 2.13 | [12] |
| $Li_4SrCa(SiO_4)_2:Eu^{2+}$ | 2 | 4.983 | 9.93 | 14.057 | 696.671 | 6 | 1.17 | 584 | 845 | 5.19 | [13] |

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|---|---|---|---|---|---|---|---|---|---|---|---|
| $Lu_2Mg_2Al_2Si_2O_{12}:Mn^{2+}$ | 2 | 11.872 | 11.872 | 11.872 | 1673.51 | 6 | 0.83 | 597.61 | 750 | 3.53 | [14] |
| $NaY_9(SiO_4)_6O_2:Mn^{2+}$ | 2 | 9.33375 | 9.33375 | 6.74936 | 509.2204 | 9 | 1.045 | 617.2 | 775 | 7 | [15] |
| $NaY_9(SiO_4)_6O_2:Mn^{2+}$ | 2 | 9.33375 | 9.33375 | 6.74936 | 509.2204 | 7 | 0.9 | 617.2 | 775 | 7 | [15] |
| $K_2HfSi_2O_7:Eu^{2+}$ | 2 | 9.6122 | 14.2105 | 5.5633 | 676.89 | 7 | 1.46 | 450 | 675 | 3.25 | [16] |
| $Mg_2Gd_8(SiO_4)_6O_2:Ce^{3+}$ | 3 | 9.38763 | 9.38763 | 6.78468 | 517.855 | 9 | 1.196 | 515 | 2200 | 1.84 | [17] |
| $La_6Sr_4(SiO_4)_6F_2:Ce^{3+}$ | 3 | 9.75 | 9.75 | 7.27 | 598.7 | 7 | 1.07 | 573 | 520 | 2 | [18] |
| $Cs_2TeCl_6$ | 3 | 10.4688 | 10.4688 | 10.4688 | 1147.335 | 6 | 0.605 | 596.3 | 225 | 3.54 | [19] |
| $La_3Mg_2SbO_9:Mn^{4+}$ | 4 | 7.9565 | 5.652 | 18.6237 | 757.4 | 6 | 0.53 | 691 | 825 | 1.2 | [20] |
| $Ca_8Zn(SiO_4)_4Cl_2:Eu^{2+}$ | 2 | 15.118 | 15.118 | 15.118 | 3454.95 | 8 | 1.25 | 500.2 | 675 | 4.18 | [21] |
| $Ca_4Y_3Si_7O_{15}N_5:Eu^{2+}$ | 2 | 10.028 | 10.028 | 10.033 | 873.834 | 6 | 1.17 | 507 | 725 | 1.13 | [22] |
| $Ca_4Y_3Si_7O_{15}N_5:Eu^{2+}$ | 2 | 10.028 | 10.028 | 10.033 | 873.834 | 8 | 1.25 | 507 | 725 | 1.13 | [22] |
| $Sr_2LuNbO_6:Mn^{4+}$ | 4 | 5.7845 | 5.8139 | 8.2033 | 275.88 | 6 | 0.53 | 686.6 | 865 | 0.82 | [23] |
| $Ba_3Lu(BO_3)_3:Cr^{3+}$ | 3 | 9.3814 | 9.3814 | 17.4305 | 1328.56 | 6 | 1.01 | 485 | 2200 | 3.51 | [24] |
| $Ba_3Lu(BO_3)_3:Cr^{3+}$ | 3 | 9.3814 | 9.3814 | 17.4305 | 1328.56 | 9 | 1.2 | 485 | 2200 | 3.51 | [24] |
| $Sr_2[MgAl_5N_7]:Eu^{2+}$ | 2 | 10.4917 | 10.422 | 3.2573 | 356.17 | 8 | 1.25 | 650 | 675 | 5.07 | [25] |
| $Zn_3Ga_2GeO_8:Mn^{4+}$ | 4 | 8.25 | 8.25 | 8.25 | 561.5 | 6 | 0.53 | 695.6 | 725 | 0.844 | [26] |
| $Sr_4Al_{14}O_{25}:Mn^{4+}$ | 4 | 24.7803 | 8.4797 | 4.8873 | 1026.9659 | 6 | 0.535 | 653 | 880 | 1.35 | [27] |
| $YPO_4:Er^{3+}$ | 3 | 6.8791 | 6.8791 | 6.0147 | 285.7 | 8 | 0.985 | 1589 | 1100 | 0.539 | [28] |
| $Ca_2Gd_8(SiO_4)_6O_2:Mn^{2+}$ | 2 | 9.4042 | 9.4042 | 6.8651 | 525.801 | 7 | 0.83 | 592.2 | 554 | 7.25 | [29] |
| $Cs_2PtCl_6$ | 3 | 10.2131 | 10.2131 | 10.2131 | 1065.301 | 6 | 0.625 | 675 | 335 | 7.19 | [30] |
| $SrF_2:Er^{3+}$ | 3 | 5.79 | 5.79 | 5.79 | 194.1 | 8 | 0.98 | 520 | 296 | 0.74 | [31] |
| $YF_3:Er^{3+}$ | 3 | 6.36 | 6.89 | 4.32 | 189.7 | 8 | 0.98 | 545 | 350 | 0.1855 | [32] |
| $SrB_2O_4:Sm^{2+}$ | 2 | 7.12 | 8.43 | 5.41 | 323.5 | 8 | 1.41 | 685.5 | 725 | 0.244 | [33] |

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|---|---|---|---|---|---|---|---|---|---|---|
| $Li_2Mg_3TiO_6:Cr^{3+}$ | 3 | 8.35 | 8.35 | 8.35 | 582.9 | 6 | 0.615 | 850 | 730 | 9.03 | [34] |
| $MgO:Cr^{3+}$ | 3 | 4.2192 | 4.2192 | 4.2192 | 74.0 | 6 | 0.615 | 720 | 760 | 0.504 | [35] |
| $Li_3Sc_2(PO_4)_3:Cr^{3+}$ | 3 | 10.48 | 6.72 | 13.46 | 958.5 | 6 | 0.615 | 980 | 1020 | 23.9 | [36] |
| $CaAl_{12}O_{19}:Cr^{3+}$ | 3 | 5.56 | 5.56 | 21.9 | 586.6 | 6 | 0.615 | 686 | 618 | 0.18 | [37] |
| $Ca_{0.8}Sr_{0.2}MgSi_2O_6:Cr^{3+}$ | 3 | 9.747 | 8.94 | 5.251 | 440.48 | 6 | 0.615 | 780 | 1010 | 6.8 | [38] |
| $K_2Ge_4O_9:Mn^{4+}$ | 4 | 11.84 | 11.84 | 9.79 | 1197.5 | 6 | 0.53 | 650 | 515 | 0.59 | [39] |
| $SrGdAlO_4:Mn^{4+}$ | 4 | 3.663 | 3.663 | 11.998 | 158.7 | 6 | 0.53 | 715.66 | 740 | 0.79 | [40] |
| $Ca_5(BO_3)_3F:Bi^{3+}$ | 3 | 8.12 | 12.45 | 6.58 | 658 | 6 | 1.03 | 457 | 923 | 4.76 | [41] |
| $SrFCl:Sm^{2+}$ | 2 | 5.96 | 5.96 | 2.98 | 107.5 | 9 | 1.27 | 690 | 500 | 1.10 | [42] |
| $BaFCl:Sm^{2+}$ | 2 | 6.2 | 6.2 | 3.1 | 119.1 | 9 | 1.27 | 688 | 500 | 1.05 | [42] |
| $Cs_2WCl_6:W^{4+}$ | 4 | 10.23 | 10.23 | 10.23 | 1070 | 6 | 0.66 | 973 | 261.2 | 7.9 | [43] |
| ZnAl2O4: $Mn^{2+}$ | 2 | 9.61 | 9.61 | 9.61 | 528.95 | 6 | 0.83 | 519.1 | 150 | 2.12 | [44] |
| ALN:$Eu^{2+}$ | 2 | 3.116 | 3.116 | 4.987 | 41.93 | 6 | 1.09 | 528 | 150 | 5.9 | [45] |
| CeF3: $Tb^{3+}$ | 3 | 7.1 | 7.1 | 7.26 | 314 | 6 | 0.919 | 543 | 50 | 1.1 | [46] |
| MgGeO3: $Mn^{2+}$ | 2 | 18.7112 | 8.7566 | 5.2595 | 861.75 | 6 | 0.89 | 680 | 445 | 5.43 | [47] |
| $Gd(Zn,Mg)B_5O_{10}:Mn^{2+}$ | 2 | 8.616 | 7.593 | 12.376 | 612.01 | 6 | 0.66 | 634.1 | 496 | 5.54 | [48] |
| ZnS: $Mn^{2+}$ | 2 | 3.822 | 3.822 | 6.258 | 79.18 | 4 | 0.66 | 586 | 430 | 9.9 | [49] |
| $CsPbBr_3:Pb^{2+}$ | 2 | 5.87 | 5.87 | 5.87 | 202 | 6 | 1.19 | 523.95 | 120 | 9.6 | [50] |
| $Sr_2MgSi_2O_7:Eu^{2+}$ | 2 | 7.84 | 7.84 | 5.03 | 309 | 8 | 1.25 | 485 | 800 | 8.11 | [51] |
| $Cs_2NaBiCl_6:Mn^{2+}$ | 2 | 10.78 | 10.78 | 10.78 | 1252 | 6 | 0.83 | 590 | 300 | 8.5 | [52] |
| SrZnOS: $Mn^{2+}$ | 2 | 3.8 | 3.8 | 6.27 | 78.5 | 4 | 0.66 | 608 | 300 | 5 | [53] |
| $Lu_3Al_5O_{12}:Tb^{3+}$ | 3 | 11.917 | 11.917 | 11.917 | 1692.7 | 8 | 1.04 | 667 | 750 | 0.85 | [54] |
| $Lu_3Al_5O_{12}:Eu^{3+}$ | 3 | 11.919 | 11.919 | 11.919 | 1693.6 | 8 | 1.066 | 667 | 750 | 0.86 | [54] |

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|---|---|---|---|---|---|---|---|---|---|---|---|
| $K_3GaF_6:Cr^{3+}$ | 3 | 8 | 8 | 11.3 | 724 | 6 | 0.615 | 758 | 400 | 0.42 | [55] |
| $LiCaY_5(BO_3)_6:Ce^{3+}$ | 3 | 7.0164 | 7.0164 | 25.4399 | 1085 | 6 | 1.01 | 434 | 350 | 2.05 | [56] |
| $LiTaO_3:Tb^{3+}$ | 3 | 5.154 | 5.154 | 13.781 | 316.8 | 6 | 0.923 | 496 | 300 | 2.12 | [57] |
| $CaYMgNbO_6:Mn^{4+}$ | 4 | 5.49 | 5.49 | 7.89 | 246.87 | 6 | 0.53 | 690 | 690 | 1.01 | [58] |
| $Sr_8MgSc(PO_4)_7:Eu^{2+}$ | 2 | 17.98 | 17.98 | 18.35 | 2561.77 | 8 | 1.25 | 516 | 516 | 2.03 | [59] |

**Table S3.** The dataset of four unseen material systems used for evaluating the generalization capability of the proposed machine learning framework.

| **Name** | **Valence** | **a(Å)** | **b(Å)** | **c(Å)** | **V(Å$^3$)** | **Coord. No.** | **Ionic Radius(Å)** | **Centroid (nm)** | **Phonon Energy(cm$^{-1}$)** | **Sensitivity (nm/GPa)** | **Ref.** |
|---|---|---|---|---|---|---|---|---|---|---|---|
| $Sr_8Si_4O_{12}Cl_8:Eu^{2+}$ | 2 | 11.201 | 11.201 | 9.584 | 1202.39 | 8 | 1.25 | 500 | 633 | 9.69 | [60] |
| $LiScGeO_4:Cr^{3+}$ | 3 | 10.6738 | 5.9913 | 4.9689 | 317.761 | 6 | 0.615 | 1100 | 790 | 23.63 | [61] |
| $Gd_2ZnTiO_6:Mn^{4+}$ | 4 | 5.3844 | 5.6872 | 7.7075 | 236.018 | 6 | 0.53 | 705 | 825 | 1.11 | [62] |
| $NaMgBO_3:Ce^{3+}$ | 3 | 5.0131 | 8.8007 | 5.5283 | 243 | 8 | 1.143 | 469.3 | 993.3 | 2.94 | [63] |

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