Three Machine-Learning Models to Accelerate the Discovery of Inorganic Phosphors

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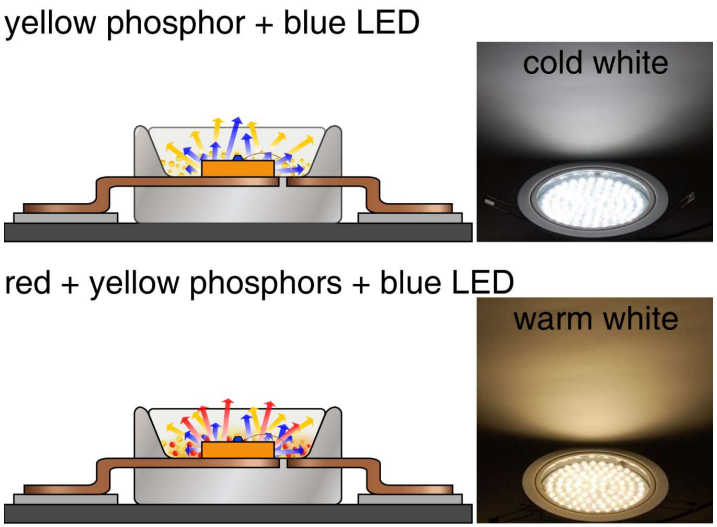
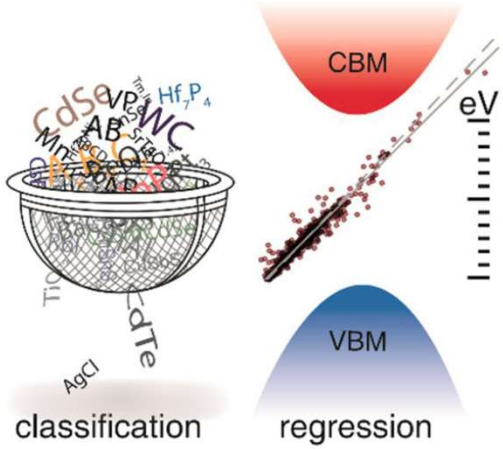
Solid State Lighting (SSL) Advantages
High efficiency
Small, compact size
Long device lifetimes
Chemically stable
Environmentally benign composition



Conventional SSL devices produce white light by using one or three inorganic phosphors to down-convert the blue or near-UV-photons produced by a light emitting diode (LED).

The combination of the partial down-conversion and the LED emission is a broad spectrum which appears as white light.

Band Gap Energy Predictor

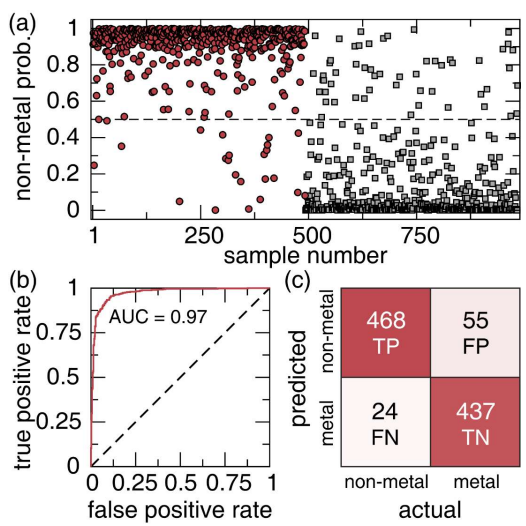


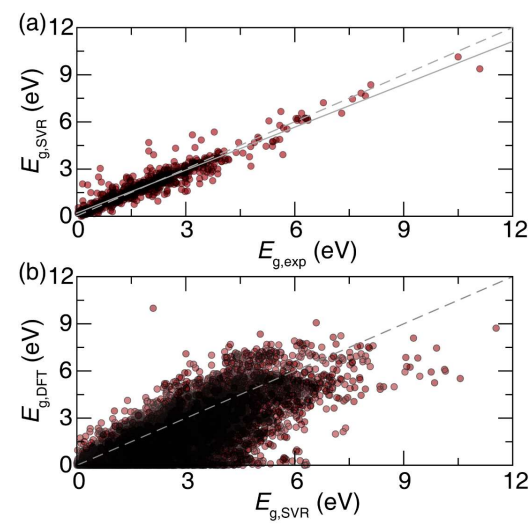
Training set of the classification model is composed of 2458 experimentally measured non-zero band gap values and 2458 DFT calculated zero band gap values.

Training set of the regression model is only composed of 2458 experimentally measured non-zero band gap values.

Statistics shows that both classification and regression model has good predicting power.

The comparison between the model predicted band gap values and DFT calculated ones indicates that the model prediction is closer to experimentally measured values than DFT calculation.





Zhuo, Y., Mansouri Tehrani, A., and Brgoch, J., J. Phys. Chem. Lett., 9, 1668 (2018).

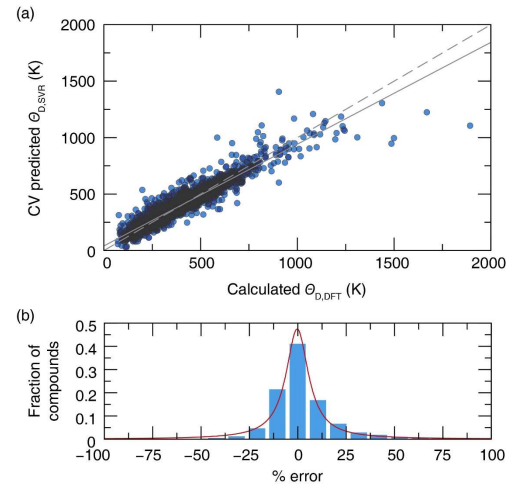
Screening highly efficient phosphors through a sorting diagram

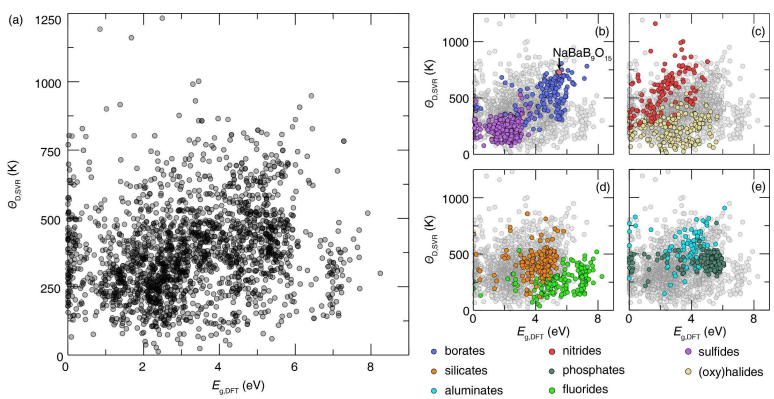
High Debye temperature (Θ_D) and wide bandgap indicate highly efficient phosphor.

The machine-learning model was constructed based on a Support Vector Machine regression (SVR) analysis.

Training set is composed of 2610 Θ_D.

RMSECV = 60.0 K (within 4% of the ranges covered for each Θ_D)





A sorting diagram helps to optimize Θ_D and E_g.

Compounds can be visualized by its compositional categories.

$NaBaB_9O_{15}$ shows outstanding predicted Θ_D (729K) and DFT calculated E_g (5.5 eV).

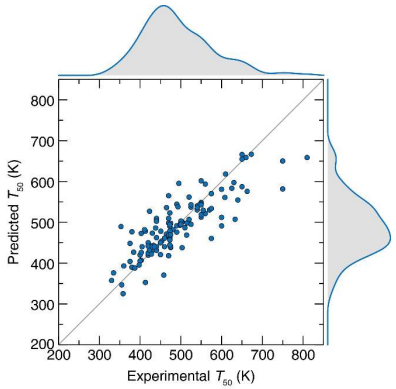
Experiment validation shows $NaBaB_9O_{15}:Eu^{2+}$ has a high efficiency (>90%).

Zhuo, Y., Mansouri Tehrani, A., Oliynyk, A.O., Duke, A.C., and Brgoch, J., Nat. Commun., 9, 4377 (2018).

Machine Learning Thermal Quenching Temperature (T50)

T_{50} is the temperature when the emission intensity is half of the room temperature value.

A machine-learning regression algorithm is developed based on 134 experimentally measured temperature-dependent Eu^{3+} emission data points



The validation results demonstrate reasonable prediction power.

The histograms show the training and validation sets contain a good spread of data.

The T_{50} was predicted for over 1000 potential phosphors.

Selective compounds for experimental validation.

composition	space group	pred. T_{50} (K)	exp. T_{50} (K)	% diff.
$Sr_2ScO_3F:Eu^{3+}$	*I*4/*mmm*	479	450	6
$Cs_2MgSi_5O_{12}:Eu^{3+}$	*Ia*3*d*	553	540	2
$Ba_2P_2O_7:Eu^{3+}$	*P*62*m*	575	475	21
$BaLiB_9O_{15}:Eu^{3+}$	*R*3*c*	643	650	–1
$Y_3Al_5O_{12}:Eu^{3+}$	*Ia*3*d*	681	760	–10

Zhuo, Y., Hariyani, S., Armijo, E., Abolade Lawson, Z., and Brgoch, J., ACS Appl. Mater. Interfaces, 12, 5244 (2019).