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

Abstract: One of society’s grand challenges is to reduce energy usage in ways that are cost-effective, sustainable, and environmentally benign. Replacing incandescent and compact fluorescent light bulbs with energy-efficient, solid-state white lights is one of the easiest and most promising solutions. Typically, phosphors must be nonmetals and band gap is the physical property to indicate whether a compound is metal or non-metal. Therefore, a machine-learning model capable of predicting the band gap of inorganic compounds was first developed based on only compositions. Metals and non-metals are classified followed by the specific band gap values predicted for non-metals with an accuracy surpassing DFT (PBE-level) calculations comparing to the experimental values. Another machine-learning model was then developed for rapid predicting the Debye temperature ($\Theta_D$) as $\Theta_D$ is a good descriptor for structural rigidity. A rigid, highly ordered phosphor structure tends to have a high quantum efficiency. Screening compounds of high $\Theta_D$ led to the identification of an efficient phosphor, NaBaB9O15:Eu2+, with a quantum efficiency of 95%. A third model combined machine learning with materials chemistry based on 134 reported temperature-dependent emission data, which can rapidly predict the thermal quenching temperature of more than 1,000 Eu3+ substituted phosphors. Selective compounds from the predictions were experimentally studied. Sr2ScO3F, Cs2MgSi5O12, Ba2P2O7, LiBaB9O15, and Y3Al5O12 all exhibit good thermal stability, suggesting the success of our methodology.