Key factors governing the external quantum efficiency of TADF OLEDs: evidence from machine learning

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Abstract

Thermal activated delayed fluorescence (TADF) materials enable the organic light emitting devices (OLEDs) exhibiting high external quantum efficiency (EQE), as they can fully utilize singlets and triplets. Despite of the high level of the theoretical limit in EQE of TADF OLEDs, the reported values of EQE in the literature vary a lot. Hence, it is critical to quantify the effects of the factors on device EQE based on data-driven approaches. Herein, we use the machine learning (ML) algorithms to map the relation between the material/device structural factors and the EQE. We established the dataset from a variety of experimental reports. Four algorithms are employed, among which the neural network performs best in predicting the EQE. The root mean square error is 1.96% and 3.39% for train and test sets, respectively. Based on the correlation and the feature importance studies, key factors governing the device EQE are screened out. These results provide an essential guidance for material screen and experimental device optimization of TADF OLEDs.

Keywords: Thermal activated delayed fluorescence; external quantum efficiency; machine learning; organic light emitting devices; photoluminescence quantum yield