Data-driven analysis of Eu(III) complexes photoluminescence spectra using machine leaning

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Rare-earth elements possess a unique characteristic in which their 4f electrons are well-shielded from the external environment by the 5d and 6s orbitals. Utilising this feature, extensive research has been conducted on their photoluminescent properties [1]. In particular, Europium (Eu) complexes, which exhibit red luminescence, are vital materials in optical fields such as lasers and sensors. Whilst it is possible to theoretically calculate photoluminescence spectra based on a complex's structure, predicting the structure from photoluminescence spectra remains extremely challenging. Achieving this would represent a breakthrough in the design and development of highly luminescent Eu complexes. Therefore, the objective of this study is to predict complex structures from photoluminescence spectra using machine learning to identify the geometric features required for high photoluminescence efficiency.

The machine learning system developed in this study comprises three stages. Specifically, the first stage predicts the complex structure from the ligand field matrix; the second stage predicts the 4f–4f ligand field matrix from energy levels split by spin–orbit interaction; and the third stage predicts the 4f–5d ligand field matrix from photoluminescence spectra.This study focused solely on 8-coordinate complexes, as they are the most frequently reported, and utilised a point-charge model consisting of an Eu ion and eight ligands. The dataset for machine learning was derived from theoretical results obtained using ligand field and multiplet calculations. For the energy difference between the 4f and 5d orbitals, a value of 0.6621 eV was adopted, as it exhibits the best fit with experimental data. In the first stage, a two-tower model employing three single-layer neural networks was used to predict the complex structure from the ligand field matrix. Specifically, a total of nine structural parameters—comprising R_1–R_8 (the distances between the Eu ion and the ligands) and ϕ (the rotation angle between the upper and lower sets of four ligands)—were predicted from 84 ligand field

As a result, high predictive accuracy was achieved for all parameters (R_1–R_8 and ϕ), with coefficients of determination (R^2) exceeding 0.97. Furthermore, the prediction errors were maintained below 1.6% for all parameters. By advancing to the second and third stages to enable the prediction of complex structures from emission spectra, further discussion regarding highly luminescent Eu complexes will become possible.

References

[1] A.J. Freeman and et al, Phys. Rev. 127 2058-2075 (1962)