Computational molecular design of the lanthanide luminescence materials from the database of emission and quenching pathways

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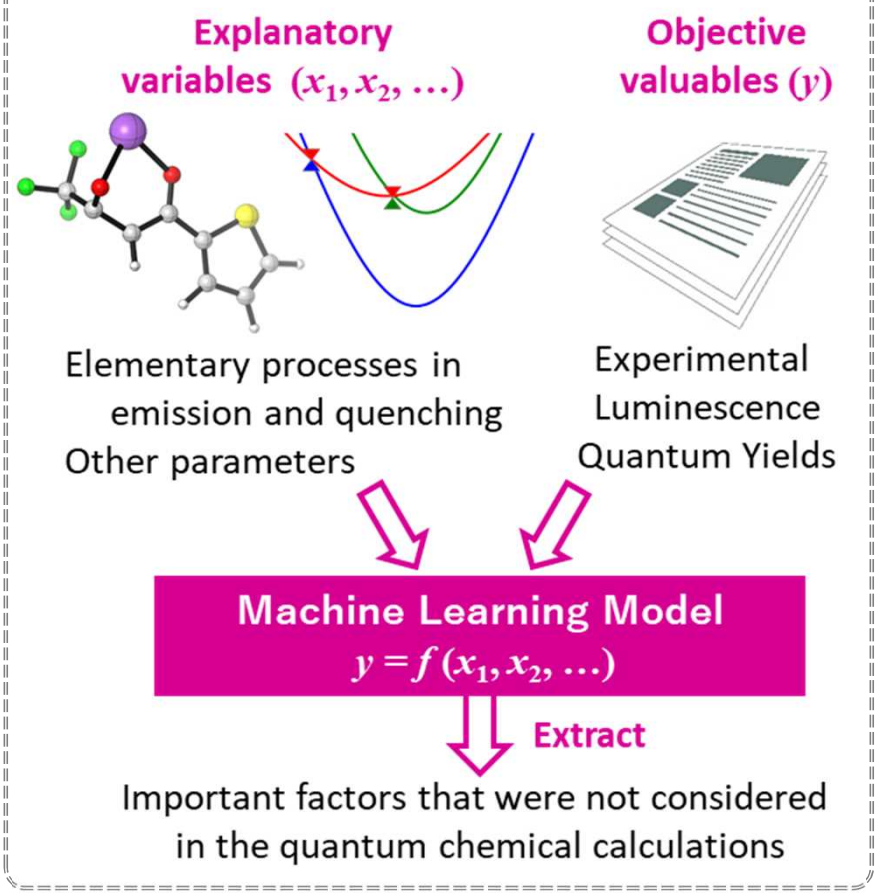
Brief overview

Lanthanide (Ln) luminescence originating from 4f–4f transitions (especially green and red emissions from Tb^{3+} and Eu^{3+}, respectively) has found application in various optical materials. The emission wavelengths of Ln complexes are independent of the surroundings, whilst the emission intensities depend heavily on the surroundings. Therefore, an appropriate ligand design is indispensable. To build the ligand design strategy, I focused on the emission and quenching pathways (i.e. critical points on and between the potential energy surfaces (PESs) of the ground and excited states), which could control the emission intensity. The local minima and crossing points on and between the PESs of various model complexes have been gathered and the ligand design strategy was build based on this database.

Achievement

Based on the database, it was found that the most stable crossing point was induced by a local vibration of one of the moieties and there was a ranking for such moieties. The ligands for strong emissive Ln complexes could be designed by changing the moiety with a higher rank to another moiety with a lower rank. This strategy was successfully applied to Tb^{3+} systems, whilst several inconsistencies between the theoretical and experimental results were found for Eu^{3+} systems. To overcome this problem, the machine learning (ML) model predicting the experimental quantum yield of Eu^{3+} complexes were built based on the database of emission and quenching pathways and the data of experimental conditions. This ML model succeeded in extracting the important factors to predict the emission intensity.



Reference/Link

https://www.jst.go.jp/kisoken/presto/en/research_area/ongoing/areah27-4.html

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