High-throughput laser synthesis and active learning for optimization of luminescent materials

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Luminescent materials have applications in various fields such as anti-counterfeiting, signage, energy harvesting, or quantum computing [1]. A common strategy to obtain such materials is to dope an inorganic matrix with light emitting rare-earth elements. Usually, the synthesis of such materials requires high temperatures to ensure good crystallinity leading to good optical properties, hence requiring a long reaction time. This experimental constraint coupled with a vast phase space to explore (synthesis conditions, composition of the matrix, nature and number of the doping agents…) makes the optimization of their properties long and tedious. The use of artificial intelligence to accelerate this optimization would be of great interest but the long synthesis times are a serious brake to establish an exploitable database.

To face these limitations, we propose to develop an original high-throughput synthesis methodology based on laser irradiation [2, 3], allowing a rapid screening of the compositions and the synthesis parameters (Figure 1). Experimentally, this methodology is a two-step method consisting of the deposition of a reactive substrate, followed by its ultra-fast crystallisation induced by laser irradiation. The structural characterizations and the properties are automated and directly measured on the substrate without shaping step. Thanks to this approach, a few hundred of materials can be synthesized and characterized per week. In a second stage, all the data generated by this approach can be used to take advantage of machine learning tools to accelerate the optimization of the luminescent properties. First, the luminescence and the crystallographic structure of the phosphors are predicted as a function of the synthesis parameters. Second, Bayesian optimization is used to predict the future experiment to obtain the material with the desired luminescence properties.

In this project, a proof of concept of the proposed strategy is demonstrated on the $La_{1-x}PO_4:Eu_x$ luminophore [4]. The laser synthesis, starting from solid precursors, is performed by playing on different parameters such as the laser frequency, power, speed, diameter and the doping concentration. All samples are then characterized by X-ray diffraction and luminescence spectroscopy. Finally, the synthesis parameters to maximize the luminescence intensity are predicted by Bayesian optimization and the optimized luminophore synthesized.

References

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Figures

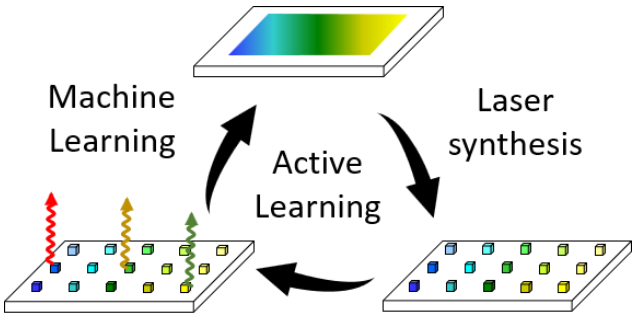

Figure 1. Accelerated optimization of luminescent materials by coupling high-throughput laser synthesis and machine learning