Using a genetic algorithm to explore compositional space of perovskite

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1. Introduction

Combining AI and materials science has already led to the discovery of many unique and novel materials. Metal halide perovskites (MHP) with their large compositional space and tuneable properties [1] have emerged as the perfect material class to use AI to discover unique combinations with exceptional properties for a variety of applications [2]. However, their very tunability makes it challenging to synthesize in a stable form and measure their properties. In this work we use different genetic algorithms combined with optical pulses to synthesize and characterize novel materials.

Light stimuli can be used to change the local composition of a material by changing the potential energy landscape, enabling ion migration and new local compositions. This process also modifies the local defect density and structure, leading to the alteration of material properties such as photoluminescence quantum yield (PLQY). In situ tracking of these properties can tell us the light sequence that drives a material into a state of improved PLQY and subsequently improved optoelectronic properties. The challenge is that the sequence of light pulses, which leverages the interplay between process timescales and guides it to the desired state, is unknown a-priori.

2. Methods

We use a genetic algorithm [2] to find the optimal light cycle maximizing the PLQY. Each cycle is defined by a series of steps, characterized by the pulse peak energy and the time of exposure. Our experiment shows that the optimal cycle is highly nonlinear regarding the average energy injected into the system, highlighting the role of traps and their interplay with slow lattice reorganization. This can be taken advantage of by

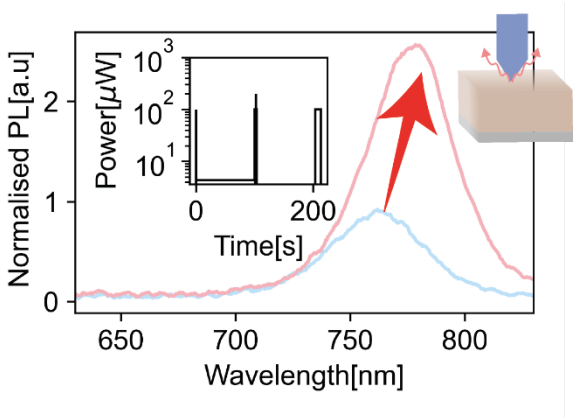

Figure 1: Using an optimized pulse of light shown in the inset we can enhance the photoluminescence (PL) and the optoelectronic properties of our material

varying the composition and frequency to alter different physical and chemical processes revealing long-lasting effects on photoluminescence. We can improve the PLQY of freshly made samples by a factor of 4 with the ideal light pulse sequence, but also fully recover and even improve upon the performance of degraded samples that were left in air for several months (40X increase in PLQY).

Our approach paves the way for a general framework to quickly enhance MHP thin film optoelectronic performance and can be used to explore the compositional space of MHP.

References

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