

Analyzing Perovskites through Confocal Photoluminescence Mapping

Introduction

Perovskites are compounds characterized by the chemical structure ABX₃, where A refers to a large cation, B refers to a smaller metallic cation, and X refers to an anion. While they appear to be ideal for the production of solar cells thanks to their high efficiency compared to other similar materials and their relatively cheap cost to manufacture, several issues such as their poor stability limit their commercial applications. In particular, mixed halide perovskites (an incredibly versatile subset of perovskites thanks to their tunable optoelectronic properties) are difficult to use because of a process that occurs upon photoexcitation known as halide segregation (Figure 1). During this process, the various kinds of halides present within the perovskite separate, forming regions with smaller band gaps and decreasing the overall efficiency of the material.



Figure 1. As the halides segregate, a region with a higher valence band edge is formed. When excited electrons move from the conduction band back down to the valence band, less energy is obtained as the band gap is narrower. Figure adapted from Motti et al., Proceedings HOPV21 conference.

To allow us to better understand the process of halide segregation, we examined the light emitted by various perovskites upon exposure to photons using a technique known as confocal microscopy (Figure 2). Using a confocal microscope, we constantly exposed a sample to light while detecting any light it emits in return, noting its wavelength and the time at which it was emitted. We collected data in this manner for three perovskites (MAPbI₃, MAPbI₁₅Br₁₅, and MAPbBr₃), hoping to eventually use software such as MATLAB to more precisely examine intensity for each sample as it relates to time, wavelength, and space.



Figure 2. A basic schematic drawing for a standard confocal microscope, similar to the one used at Wesleyan. Figure adapted from Wang et al., Engineering, 1, 315, (2015).

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Data Collection

Since the results of confocal microscopy must account for any area of the sample that emits light, the wavelength of any light being emitted, and the time at which any light was emitted, the data from confocal microscopy takes the form of an imageset. Each image represents the same small section of the sample (determined by the placement of the focal point), and each image is associated with a specific wavelength and time value. Brighter pixels correspond to greater intensities of light being emitted.

Series003_t10_la0 4_RAW_ch00	Series003_t10_la0 5_RAW_ch00	Series003_t10_la0 6_RAW_ch00	Series003_t10_la0 7_RAW_ch00	Se
Series003_t11_la0 4_RAW_ch00	Series003_t11_la0 5_RAW_ch00	Series003_t11_la0 6_RAW_ch00	Series003_t11_la0 7_RAW_ch00	Se
Series003_t12_la0 4_RAW_ch00	Series003_t12_la0 5_RAW_ch00	Series003_t12_la0 6_RAW_ch00	Series003_t12_la0 7_RAW_ch00	Se
Series003_t13_la0 4_RAW_ch00	Series003_t13_la0 5_RAW_ch00	Series003_t13_la0 6_RAW_ch00	Series003_t13_la0 7_RAW_ch00	Se

Figure 3. Part of an imageset created as a result of confocal microscopy. This particular data was the result of our analysis of $MAPbI_{15}Br_{15}$.

From there, in order to enable analysis of intensity as a function of time and wavelength, we converted each image to a matrix of its pixel values (0 corresponding to black and 255 corresponding to white) and took the average of those values for each image, creating a table of average pixel values (corresponding to average intensity) that we could produce graphs from. Additionally, in order to account for different subregions within the observed region that could potentially act differently, we used the newly obtained average pixel value for each image along with the standard deviation of pixel values for each image to automatically produce two subregions for each imageset, with one subregion containing abnormally bright pixels and one subregion containing abnormally dark pixels. This allowed us to perform intensity analysis for each subregion by slightly modifying our average function to only include pixels from a given subregion for each image.



Figure 4. Intensity vs Time and Intensity vs Wavelength graphs for MAPbI₃. Subregions established did not produce qualitatively different graphs.







understanding of the process of halide segregation.