Machine Learning on Experimental Data for Optimizing Colloidal Quantum Dot Solar Cells

Ariana B. Hofelmann, Kevin Lee, Susanna M. Thon
Department of Electrical and Computer Engineering
Johns Hopkins University

Abstract

In this project, we used machine learning models to assist in the characterization process of PbS colloidal quantum dot (CQD) solar cells. We performed spatially-resolved optoelectronic measurements and used experimental data to train a neural network to automatically predict several materials parameters.

Introduction

Spatially-resolved optoelectronic property maps allow us to study how various kinds of macroscopic defects affect the performance of photovoltaic devices. While this type of scan allows us to exceed the limitations of single point measurements, the practice greatly increases the amount of data obtained and adds complexity to the physical setup. For a complete picture of the underlying performance of a device, we must perform multiple types of scans including photoluminescence, transient photovoltage, transient photocurrent, and current-voltage curves.

If it is possible to find correlations between the above-mentioned parameters and a single measurement type, then each photovoltaic device could be completely characterized by simply performing a single kind of scan. We propose the use of machine learning to achieve this goal.

Method

We characterized PbS CQD solar cells, Figure 1, using the apparatus shown in Figure 1. The device structure consists of a glass substrate, fluorine-doped tin oxide layer, zinc oxide layer, PbS CQD absorbing layer, PbS-EDT CQD hole transport layer, and gold top contact. Our scanning setup had a step size of $25\ \mu m$ and a scanning area of $2.05\ mm \times 2.05\ mm$, corresponding to a grid of 82 by 82 points.

The photoluminescence (PL) curves were fit using a Gaussian model, and the transient photovoltage and photocurrent curves were fit to the convolution of a Gaussian impulse and exponential decay curve.

We used experimental data to train the machine learning model abstracted in Figure 2. Using a single input vector (the current-voltage curve), we were able to produce an output vector containing the different materials parameters of interest. Two devices were used in the training process. The model was trained on one device, and then the model was used to predict the parameters for the other device.

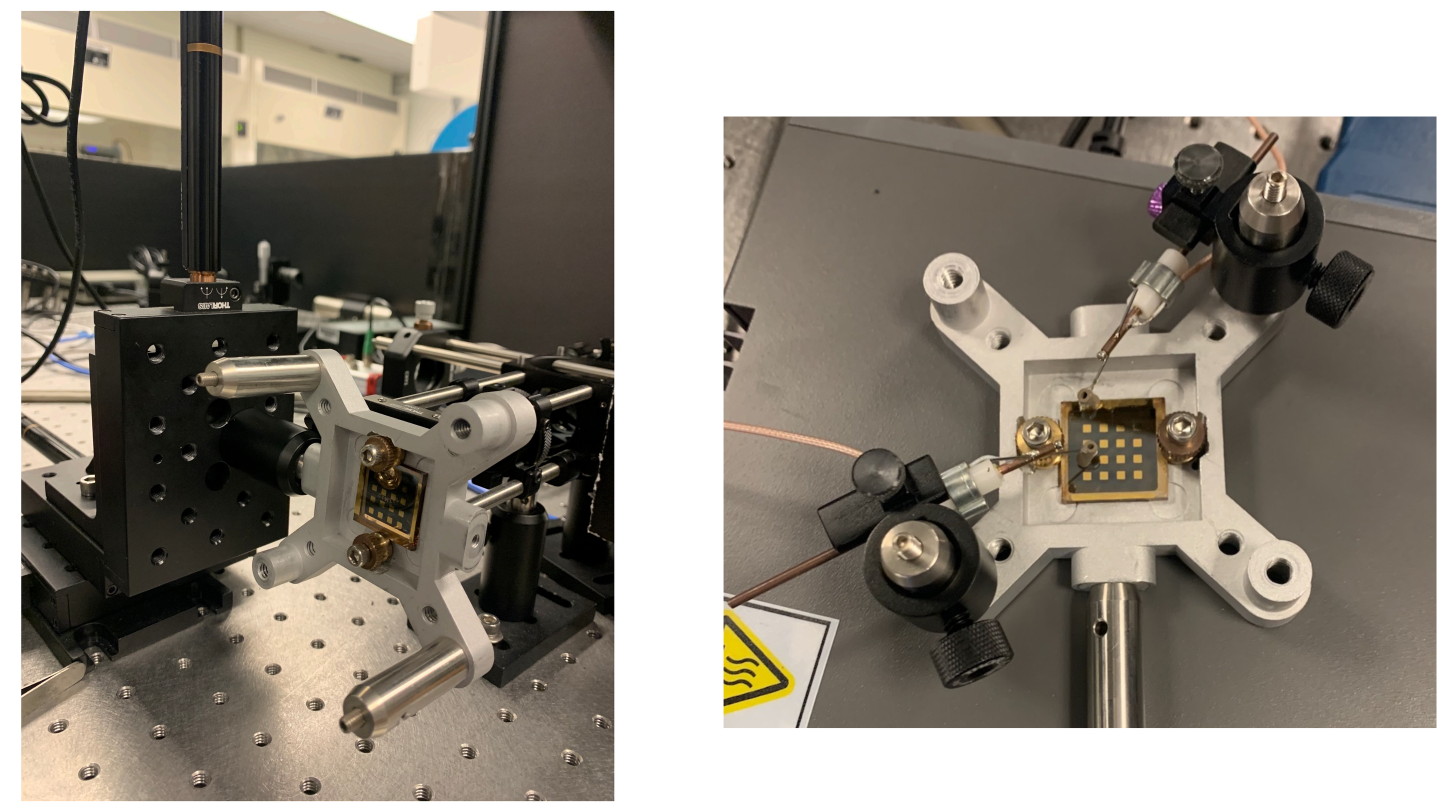

Figure 1. Scanning set up (left) and closer look at the PbS CQD solar cell in the holder with probes attached (right).

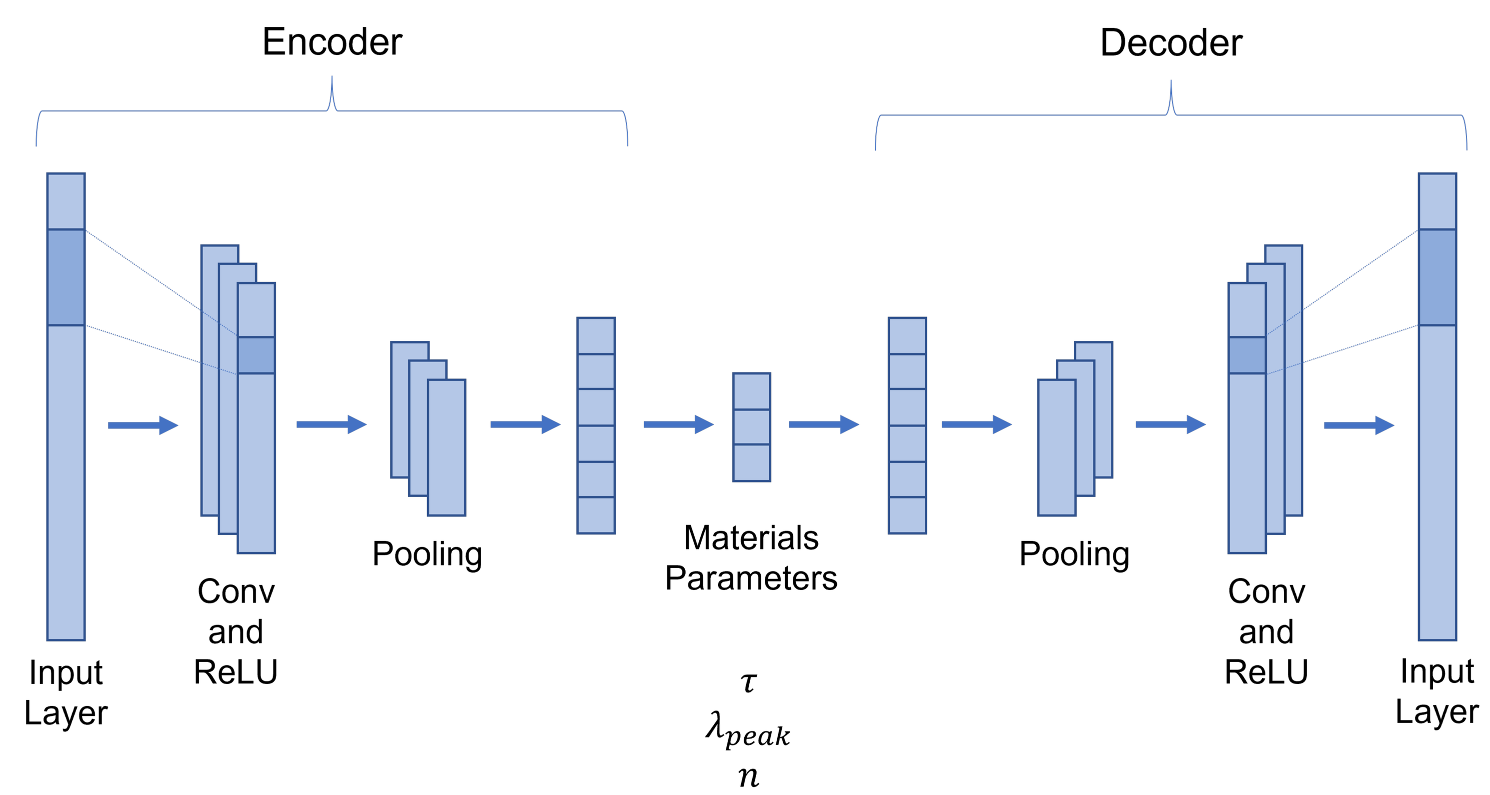

Figure 2. A schematic of the neural network architecture used for materials parameter extraction. Additional convolution and pooling layers may be added.

Results

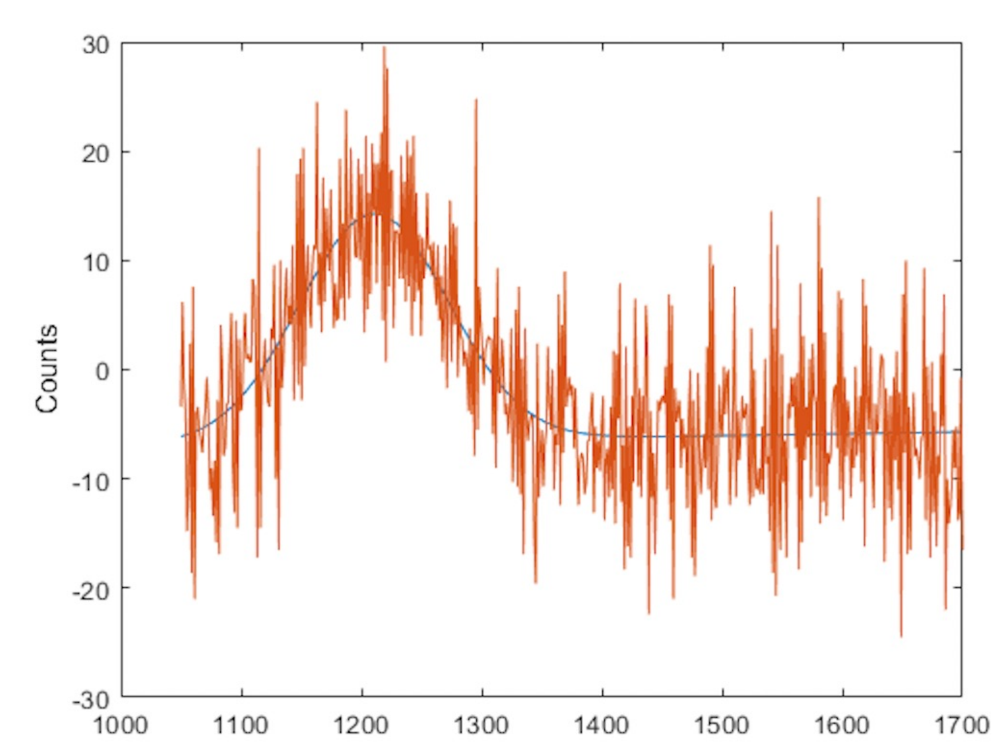

Figure 2. Photoluminescence (red) for a single point in the scan fit to a Gaussian curve (blue).

Results

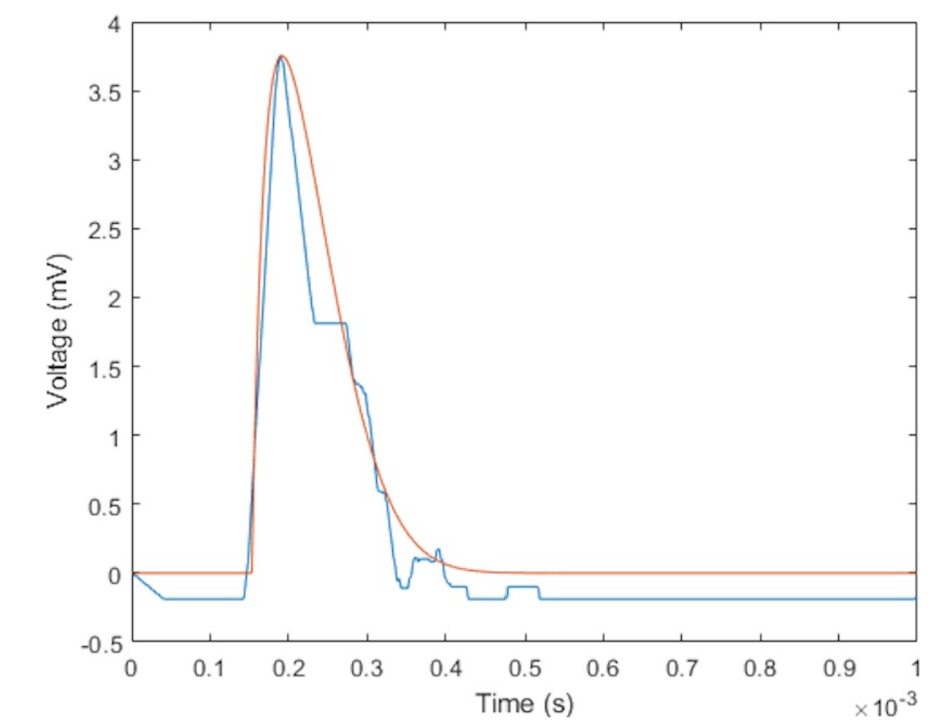

Figure 3. Transient photovoltage (blue) for a single point in the scan fit to a Gaussian-exponential decay convolution.

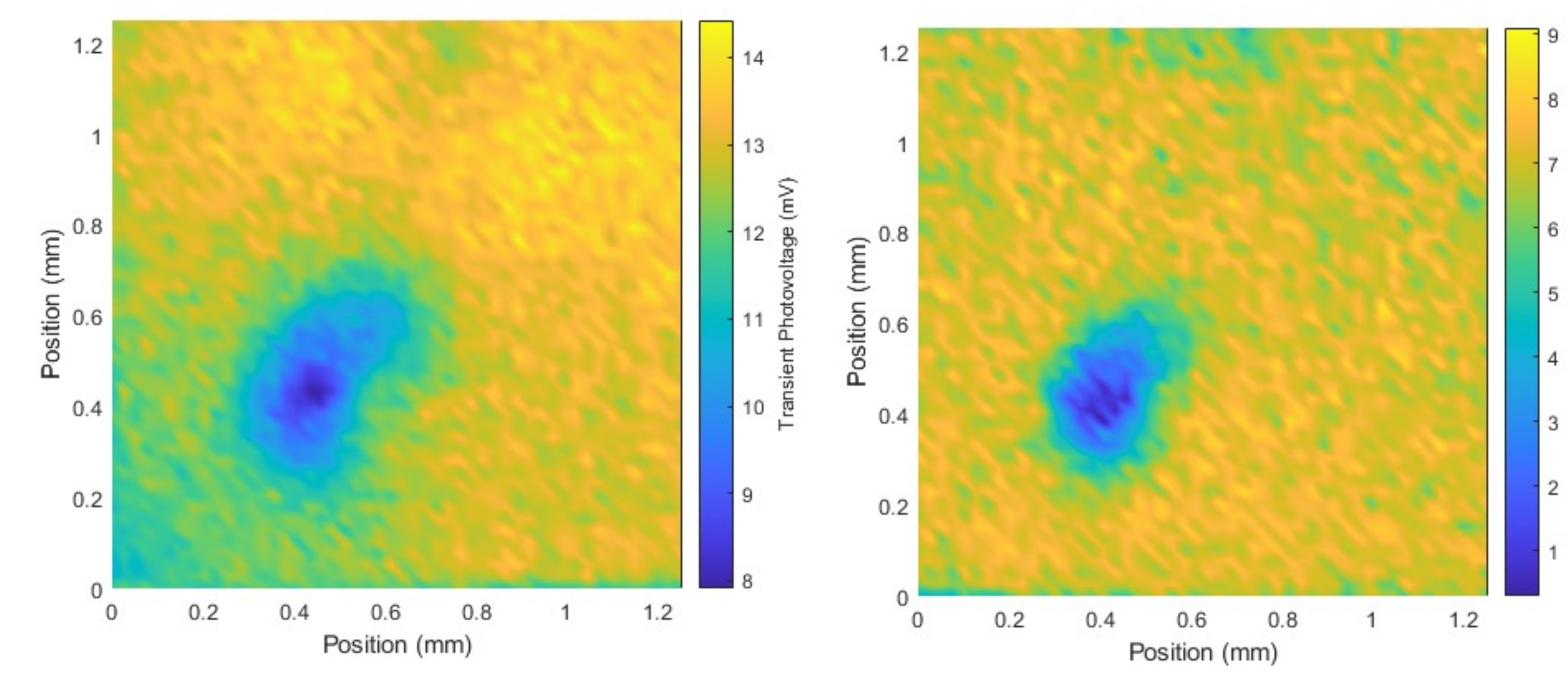

Figure 4. The measured transient photovoltage map (left) and predicted map generated by the neural network (right).

Conclusions

Our preliminary work demonstrated that machine learning models can be used to expedite the characterization process of photovoltaic devices. The neural network was able to accurately predict various complex materials parameters solely using current-voltage curves. In the future, we plan to use the decoder of our model to generate datasets from noise, and we would also like to expand our current setup to include additional types of measurements.

Acknowledgements

This research was funded by the National Science Foundation (DMR1807342).