MSE 542 AUT 22

Term Paper - Vinsensius

Perovskites is a new material for solar cells that is able to generate more electricity from the sun cheaper than silicon based solar cells that are available in the market. However, perovskites solar cell (PSC) has problems that are preventing them from going into commercial use. Firstly, scalability and reproducibility is a challenge because deposition of high quality electron and hole transport layers (ETL and HTL) are important to achieve high power conversion efficiency(PCE). The challenge is choosing the deposition methods that are scalable. The next challenge is stability because PSC has stability problems when used outdoors. The last challenge is toxicity due to having some lead from creating perovskites. The research will be focused on the scalability which is predicting solar cell PCE based on manufacturing processes with probabilistic constraints.

Since there are many different parameters such as Temperature, plasma flow, spray speed and nozzle height that can affect the PCE of a solar cell, we can use data science to predict the PCE based on the manufacturing process. We can employ different optimization methods to get the optimal process that will be used to train the regression model. Furthermore, we will incorporate the material science constraint such as density functional theory into the model to help with optimization.

We can get the data from other researchers that researches solar cell manufacturing and collecting data. Assuming we will be able to gather data from other researchers on different manufacturing processes and their solar cells PCE, we can start analyzing the data. We first create the contour plot of different pairs of parameters and PCE be their color gradient. We then apply optimization on the contour. Based on the reference paper, we can apply different models, such as pure Bayesian optimization, Bayesian optimization with probabilistic constraint, Latin hypercube sampling, factorial sampling with progressive grid subdivision, and one-variable-at-a-time sampling(OVATS). We can then use the results from the optimization to train the regression model. The regression model is gradient boosting with decision trees. The regression model is used to show that the correlation between predicted PCE and experiment is linear monotonic.

However, if we cannot get data from other researchers, we will be manufacturing the solar cells in the lab based on different conditions.

For the timeline of the project, we will consider the timeline for when we are creating our own dataset from experiments. The plan is about 3-4 years. The first year would be learning different manufacturing processes for solar cells. The second year will be manufacturing the solar cells for datasets. The last 2 years will be studying the data set, learning different machine learning and optimization models so that it can be applied to the dataset and the interpretation of the results.

If we have the data set, we might be able to shorten the timeline to about 2 years, mainly focusing on developing the algorithm to be able to predict the PCE accurately. This has an impact on my career because I am interested in renewable energy and solar cells are part of it.

Therefore, the paper proposes the idea of using optimization of the manufacturing process of PSC which then can be used to develop models to predict the PCE of the solar cells.

Reference:

Perovskite solar cells: why they're the future of solar power - https://www.solarreviews.com/blog/are-perovskite-solar-cells-the-future-of-solar-power

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