Constructing a Bulk Heterojunction Generator Algorithm for Organic Photovoltaic

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Abstract
The purpose of this research project is to create an organic P3HT:PCBM bulk heterojunction photovoltaic via a Java script algorithm that can be adjusted by the user to find an optimized photovoltaic. An algorithm made in Java along with Sentaurus Device Editor created the bulk heterojunction, P3HT:PCBM region, for the organic photovoltaic through P-type and N-type cell assignment randomization. A layer of aluminum is laid on top of the P3HT:PCBM region and a layer of PEDOT, ITO, and glass are below the P3HT:PCBM region. The Java algorithm produced a P3HT:PCBM bulk heterojunction that can be altered by the researcher. With this Java script algorithm, researchers can create any kind of organic/inorganic bulk heterojunction, model the photovoltaic in Sentaurus Device Simulator, and measure the power conversion efficiency. From the testing, researchers can go back to the Java script and adjust any variables that hinder performance in the power conversion efficiency test. Researchers can utilize this Java script algorithm to find the most power conversion efficient organic bulk heterojunction semiconductor configuration.

Introduction

- Innovation in the principal components of photovoltaic cells is a limitless endeavor.
- Utilization of organic materials within photovoltaic cells allow for the organic photovoltaic (OPV) to be a thin, flexible, and transparent film.
- The OPV’s ability to flex and use of thin layering allows it to be placed on almost any surface, which is very beneficial when the goal of these OPV cells is to collect sunlight.
- Despite OPVs being a more accessible and more cost effective option, they do lack efficiency in power conversion.
- Finding an efficient configuration in an OPV cell’s semiconductor through the bulk heterojunction technique is the target of this research project.

Methods

- The program Sentaurus Work Bench was used alongside a Java script algorithm to generate unique OPV bulk heterojunctions (P3HT:PCBM).
- The bulk heterojunction was made up of a grid system that could be any dimension; through the grid system each cell was randomly assigned to be either a P-type (P3HT) region or a N-type (PCBM) region.
- The respective doping substance was used for the P-type regions and N-type regions.
- The algorithm to create this system was a “nested for loop” that produced and randomly assigned the P-type regions and N-type regions.
- To implement the actual doping, a “for loop” was used alongside a counter variable for each P-type and N-type regions to produce the correct number of doping profiles.
- A layer of aluminum is laid on top of the P3HT:PCBM region and a layer of PEDOT, ITO, and glass are below the P3HT:PCBM region.
- A single layer of mesh was used to cover the entire bulk heterojunction.
- Through Sentaurus Device Editor, an OPV bulk heterojunction was generated via the command function.

Results

The Java script algorithm successfully created a bulk heterojunction composed of 40x40 square regions. The bulk heterojunction was correctly implemented into a P3HT:PCBM semiconductor, as well as proper assignment of the appropriate doping concentration to the respective region.

Discussion

With the Java script algorithm produced from this research project, the generated bulk heterojunction can be used for more accurate photovoltaic modeling instead of the conventional “effective medium” method. Other organic semiconductors researcher can utilize the myriad of variables and adjustable functions to create a more efficient energy conversion organic semiconductor. From further Sentaurus Device simulations of the semiconductor, researchers can use the Java script algorithm and take what they have learned about the semiconductor’s energy conversion efficiency and adjust any variables, such as: the material used for the P-type and N-type regions, doping concentration level, or phase separation morphology. From the combination of process simulation, Java script/ Sentaurus Device Editor and device simulation the photovoltaic performance can be properly optimized.

A more efficient bulk heterojunction organic semiconductor will hopefully be the product of the Java script algorithm. From these more efficient organic semiconductors, reliable and cost effective organic photovoltaic will be made and implemented in our cities, schools, homes, and everyday life. Efficient organic photovoltaic cannot only produce a supplemental quantity of clean energy, it can also be placed on almost any surface as it is flexible, light, and easy to install. The world will be closer to fully transitioning to clean energy sources.

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