Development of Optimal Microstructure Morphology in Organic Solar Cell Active Layer through Genetic Algorithm

Ardayfio, Caine (School: University High School of Indiana)

The morphology of the active layer in organic solar cells is critical to performance. By studying the photovoltaic properties of organic solar cell's microstructure, it is possible to increase the solar cells efficiency. A graph-based surrogate model was created to approximate the efficiency, measured as short circuit current, in the solar cell. Through the use of probabilistic graph-based optimization, a class of microstructures were optimized with an efficiency surpassing that of more conventional morphologies. These optimized solar cells surpass the efficiency of more conventional photovoltaic devices as they better facilitate charge transport, generation, and reaction rate. We design a device with a 40.29% increase in short circuit current, the metric for efficiency, from solar cells with the currently believed optimal morphology. The designed morphologies feature two dendritic clusters of the donor material poly(3-hexylthiophene-2,5-diyl) (P3HT) and the acceptor material phenyl-C61-Butyric-Acid-Methyl Ester (PCBM). The algorithmically designed microstructure's increase in performance contrasts with more conventional structures featuring interdigitated or bilayer strands of P3HT and PCBM. The change of microstructure morphology through graph-based evolution obtains an organic solar cell with an efficiency significantly greater than conventional organic solar cells, proves the validity of graph-based surrogate models for the simulation of materials science models, and advances the vision of an inexpensive and efficient form of sustainable energy.