Design and Optimization of Thin Film Organic Solar Cells for Enhanced Light Trapping

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Optical performance of thin film solar cell can be improved using light trapping techniques, such as anti-reflective coatings, surface gratings, and metallic (plasmonic) particles. These techniques reduce reflection, create multiple scattering, and induce near field effects to trap light inside absorbing semiconductor. A rigorous design of thin film solar cells with enhanced light trapping structures requires precise characterization of the dependencies of electromagnetic distribution to geometry parameters. Optical properties of structures at sub-wavelength scales are measured by numerically solving first principle electromagnetic equations, e.g., by means of finite difference time domain (FDTD) method. These methods are time-consuming, and therefore limit the possibility of exhaustive design optimization. However, surrogate models can be trained and used to accurately predict the optical properties of thin film solar cells to optimize their structures. The objective function of the optimization problem can be the number of photons absorbed in the semiconductor, the relative enhancement in the optical performance when light trapping techniques are employed (enhancement factor), and the ratio of the number of electrons contributing to the photocurrent to the number of incident photons (quantum efficiency). There are a wide range of possible surrogate models, such as Neural Networks, Gaussian Process, and Support Vector Machines. These models are trained and cross validated in order to obtain the smallest in-sample and out-sample errors. The optimization procedure can be coupled by training, by utilizing adaptive sampling, or can be done once an accurate and reliable surrogate model is achieved. The surrogate-based modeling also provides investigation of individual contributions of each input by means of sensitivity analysis to predict the fabrication errors. In the present study, the input space involves the geometry vector of the solar cell and radiation wavelength and incident angle. A neural-network-based optimization method is used to optimize a plasmonic organic solar cell, and the solutions found by surrogate-based optimization demonstrate enhancement factors greater than 200 % for the optical absorptivity compared to a bare structure. The constructed surrogate model is also used to model the solar cell under different source light irradiance spectra and incident angle conditions. This procedure is found more than 3 times faster than direct optimization.