Electro-photonic optimization of organic solar cells

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Micropatterned organic solar cells have been shown to exhibit enhanced light absorption, and therefore, light-trapping strategies are frequently suggested for improving organic photovoltaic cell efficiency. The patterning may also have an adverse affect on the charge carrier collection, however, as local variations in the electric field strength may increase recombination losses.

We investigate this tradeoff between light absorption enhancement and charge carrier collection deterioration by numerical simulation and optimization with a three-dimensional model of light absorption and charge carrier transport in micro-patterned materials. Rigorous coupled wave analysis is used to simulate the multiple scattering and absorption of light in a layered solar cell device. The non-linearly coupled steady-state electric field and charge transport equations are solved iteratively by a sequence of linear partial differential equations (PDEs). Each linear PDE is discretized by an exponential upwind finite difference scheme, and the preconditioned conjugate gradient method is applied to the resulting algebraic system. The electro-photonic solver is coupled with the simulated annealing optimization algorithm to investigate the effect of micro-patterning upon performance of organic bulk heterojunction solar cells and to find optimal patterns.

Starting from the baseline configuration of a cell formed from flat layers of optimal thickness, the shape optimization algorithm leads to improvements of up to 15 % in energy conversion efficiency by patterning both the front and back electrodes with a periodic ridge shape, with conformally coated layers in-between. In the case where only the (metal) back electrode is patterened our results suggest that an inverted device architecture has a better chance to outperform an optimized flat device than a conventional device architecture, provided that the hole mobility in the photoactive material is smaller than the electron mobility.