Title: Structure and thickness optimization of active layer in nanoscale organic solar cells

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Abstract: This paper presents the development of a two-dimensional model of multilayer bulk heterojunction organic nanoscale solar cells, consisting of the thickness of active layer and morphology of the device. The proposed model is utilized to optimize the device parameters in order to achieve the best performance using particle swarm optimization algorithm. The organic solar cells under research are from poly (3-hexylthiophene) and [6,6]-phenyl C61-butyric acid methyl ester type which are modelled to be investigated for performance enhancement. A three-dimensional fitness function is proposed involving domain size and active layer thickness as variables. The best results out of 20 runs of optimization show that the optimized value for domain size is 17 nm, while the short-circuit current vs. voltage characteristic shows a very good agreement with the experimental results obtained by previous researchers.