

## Abstract

As the demand for secure, clean and sustainable energy increases, extensive research attention has been directed to photovoltaics (PVs) owing to its inexhaustibility, abundance and wide availability. Despite the great efforts devoted, for large scale implementation, price reduction of solar cells is still the main issue to enable the solar cells to be fully cost-competitive with traditional energy sources. On one hand, organic PVs have provided a low cost solution. On the other hand, semiconductor nanowire (NW) arrays open a new pathway to greatly reduce material consumption while maintaining or even improving device performance. To further lower the cost and improve energy conversion efficiency, hybrid solar cells (HSCs) based on III-V and organic materials have emerged as promising candidates to combine the advantages of inorganic materials and the low cost and flexibility provided by organic materials. In this work, at the first stage, an effective and efficient design is provided to guide the geometrical dimensions and topology for NW arrays to achieve maximal light harvesting regardless of the material, single or multiple diameters of NWs. Compared with time-consuming simulations, the proposed method maintains a low tolerance of below 2.2%. Next, an opto-electrical model is built to fully evaluate the performance of the HSCs elaborating the photo-generated excitons dissociation, transportation and collection within the hybrid active layer. Validation with published experimental results has proved the effectiveness of our theoretical work. Thirdly, highly efficient core-shell inorganic-inorganic HSCs are designed and experimentally fabricated combining nanospheres lithography, dry etching and PV fabrication techniques. Hexagonal closely packed polystyrene nanospheres of various diameters are achieved at centimeter scale. Plasma etching is accompanied to tune the diameter and inter-sphere spacing among adjacent nanospheres. Using these nanospheres as etching masks, ordered NWs arrays are obtained by optimizing various etching parameters including the flow rates of chlorine, boron trichloride, trifluoromethane, and the radio frequency power etc.. Inorganic core/organic shells are optimized serving as hybrid active layer. Finally HSCs are fabricated to fully unravel the role of inorganic NWs effect on the performance of device.