DEVELOPMENT AND STUDY OF ORGANIC/INORGANIC HYBRID SOLAR CELLS

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Development and Study of Organic/Inorganic Hybrid Solar Cells
有機/無機雜化太陽能電池的開發與研究

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ABSTRACT OF DISSERTATION

Both the increasing demand for energy and the environmental crisis lead to development of clean and renewable energy sources. Among a variety of new energy sources exploited in the past decades, solar energy is believed to be the ultimate solution to satisfy the energy demand and the environmental challenge. Solar energy can be converted to electricity using photovoltaic effect induced in electronic devices, known as solar cells. Since the first practical photovoltaic cell invented in 1954, significant progress has been made in the development of solar cells, but the cost for electricity produced by solar cells is still 2 to 3-times higher than that obtained from the conventional fuel resources. Therefore major breakthrough in technology of solar cells is still needed to meet the fundamental cost requirement. As a result several new technologies, devices and materials have been introduced and used to develop efficient and cost effective solar cells. Among them, organic/inorganic hybrid solar cells (HSCs) are devices that may meet the demands of high power conversion efficiency (PCE), low cost and environmental compatibility. The organic/inorganic hybrid system combines the merits of both organic and inorganic components showing great potential to fabricate low cost and highly efficient solar cells.

In consistence with recent development, this work focuses on development and study of hybrid organic/inorganic devices. In particular, attention is given to
investigations of organic/inorganic HSCs with the architecture combining conjugated p-type polymer, poly (3-hexylthiophene) (P3HT), and inorganic ZnO/Sb$_2$S$_3$ to form heterojunctions. Herein, the ZnO/Sb$_2$S$_3$/P3HT heterojunction solar cell is studied systematically via device design, modeling, and optimization. Both the planar and the bulk ZnO/Sb$_2$S$_3$/P3HT heterojunctions are used to construct the solar cells. The effects of thickness, annealing, and recombination for individual layer are investigated using the planar solar cells, while the effects of light trapping and the enlarged interfacial area on device performance are investigated with assistance of bulk heterojunction architectures.

Firstly, numerical simulation employing the computer code Analysis of Microelectronic and Photovoltaic Structures (AMPS) is performed to explore fundamental mechanism and principle of planar ZnO/Sb$_2$S$_3$/P3HT heterojunction solar cells. The device performance dependent on some parameters, such as the thickness and carrier mobility of Sb$_2$S$_3$ (or P3HT) films, is studied by AMPS modeling. It is demonstrated that the performance significantly depends on the layer (Sb$_2$S$_3$ or P3HT) thickness, mobility, and the possible recombination presented; while the performance is hardly affected by the electron mobility (0.01~100 cm$^2$/Vs) and thickness variations (60~400 nm) of ZnO film, which is mainly due to the large electron diffusion length in ZnO. The simulated results provide us a qualitative understanding of the performance
solar cells based on ZnO/Sb₂S₃/P3HT heterojunctions, which in turn guides us to fabricate the solar cells with higher performances.

With the insights based on numerical simulations, the HSCs with planar ZnO/Sb₂S₃/P3HT heterojunctions are fabricated and studied. The study shows that the device performance is significantly affected by the thermal annealing and the thickness of individual Sb₂S₃ or P3HT layers. The electronic structure of the Sb₂S₃ film is also investigated by ultraviolet photoelectron spectroscopy (UPS), which enables us to study energy alignment in the designed hybrid heterojunction solar cells. X-ray photoelectron spectroscopic (XPS) study further demonstrates that the surface of Sb₂S₃ layer is partially oxidized, and oxide layer is about 0.5 nm thick. This thin layer oxide film (Sb₂O₃) is in fact a passivation layer between the Sb₂S₃ and P3HT, which in turn reduces the carrier recombination and improves the device performance. The obtained analytical data qualitatively agree with the prediction based on the numerical simulation.

In addition, ZnO nanowire arrays have been incorporated into the ZnO/Sb₂S₃/P3HT heterojunction solar cells (bulk heterojunction). Optical measurements demonstrate that the absorbance of Sb₂S₃ is increased by ~5% in the wavelength ranging from 450 to 650 nm due to the light trapping effect induced by scattering process in ZnO nanowire arrays. The solar cells with ZnO nanowire arrays
show PCE of 2.9%, which is higher by 20% than that of the control device assembled without the ZnO nanowire arrays. AMPS modeling further evidences that the improved performance mainly arises from both the increased absorbance and the reduced bulk recombination in Sb$_2$S$_3$ layer.

Compared to the inorganic materials, organic materials exhibit much lower carrier mobility, which significantly limits the performance of organic/inorganic HSCs. Improving the carrier transport properties of organic materials is thus of great importance for high performance of HSCs. The electrical properties of P3HT blended with square planar nickel complexes are also study here. Novel square planar nickel complexes with molecular alignment has been synthesized and introduced into the P3HT matrix. The study indicates that a variation in the cations-anions interaction of the prepared complex affects both the molecular packing and physical properties. An enhanced carrier transport is observed in the blends due to the additional charge carriers from the electronic states of nickel complexes. In the context of observed phenomena, a physical model is proposed to explain the enhancement of the charge transport property. The blends of P3HT and nickel complex with enhanced carrier transport may find their applications in polymer based HSCs.
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