FABRICATION AND CHARACTERIZATION OF HYBRID POLYMER SOLAR CELL

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FABRICATION AND CHARACTERIZATION OF HYBRID POLYMER SOLAR CELL

Field of Study: Organic Electronics

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ABSTRACT

The easy fabrication method, tunable physical and chemical properties and cost-effective fabrication process, makes organic solar cells (OSC) very attractive in photovoltaic application. Nonetheless, the device performance is limited due to the low charge mobility of the organic semiconductors that results in a less efficient of charge transport to the respective electrodes. In order to address such problems, hybrid polymer solar cells based on bulk heterojunction (BHJ) structure, which composed of a combination of both organic and inorganic semiconductors are employed. However, the BHJ device performances are strongly dependent on good processing conditions, especially enhancement of photons absorption as well as the improvement of charge transport properties. Hence, the involved parameters and properties should be well optimized.

This dissertation describes the study of effects of blend composition and types of acceptor materials used on the optical, structural, morphological as well as the electrical properties of the three different hybrid BHJ systems. The hybrid materials consist of a blend of p-type conjugated polymer of poly(3-hexylthiophene) (P3HT) and n-type inorganic metal oxide nanoparticles, namely, zinc oxide (ZnO), titanium dioxide (TiO$_2$) and yttrium oxide (Y$_2$O$_3$). The optical, structural and morphological characterizations of the blend thin films using UV-Visible absorption spectroscopy, X-ray diffraction (XRD) spectroscopy, Atomic Force Microscopy (AFM) and Field-effect Scanning Electron Microscopy (FESEM) are discussed. Furthermore, the co-relation of the thin film property with the device performance is presented. The results show that the device performance has been improved by optimizing the blend composition. This is due to an enhancement in light absorption in broader wavelength regime and improved charge transport through the formation of interpenetrating bicontinuous pathway for the holes and electrons to reach the respective electrodes. These results are supported by the observation of the AFM and FESEM images of the increment in RMS roughness and formation of phase separation features in the blends. Besides, the well dispersion of inorganic nanoparticles over P3HT yields a larger interfacial area for charge carrier generation. Among the three hybrid systems investigated, P3HT:ZnO device performs the best with an optimal blend composition of 3% of ZnO nanoparticles in blend.

In order to further improve the device performances, ZnO sol-gel synthesis route has been utilized to produce a better mixing blend of P3HT and ZnO. Additionally, several approaches have been employed, namely modifying the sol content in blends, varying the annealing temperature, and inserting an additional ZnO buffer layer between the active layer and cathode. An optimal annealing treatment offers improved optical absorption properties and more uniform film surface morphology with eliminated redundant large pores and grain agglomerations. The role of the ZnO buffer layer in the blend system can be seen as an agent in facilitating the electron collection from the active layer to the cathode. The results indicate that the device efficiency has been improved by about 5 times for P3HT:ZnO sol gel device with optimized sol content (0.1ml sol), annealed at an optimized temperature of 100°C with additional ZnO buffer layer, compared to the P3HT:ZnO nanoparticles-based device.
ABSTRAK

Fabrikasi yang mudah, ciri-ciri fizikal dan kimia bolehlaras dan kos efektif proses fabrikasi, telah menyebabkan sel suria organik (OSC) amat menarik dalam bidang penggunaan fotovoltaik. Walau bagaimanapun, prestasi peranti menjadi terbatas disebabkan oleh kelincahan pembawa cas yang rendah bagi semikonduktor organik yang mengakibatkan angkutan cas ke elektrod menjadi kurang cekap. Dalam usaha untuk menangani masalah tersebut, sel suria polimer hibrid berasaskan struktur simpang-hetero pukal (BHJ) yang terdiri daripada kombinasi semikonduktor organik dan bukan organik telah digunapakai. Namun demikian, prestasi peranti amat bergantung kepada keadaan pemprosesan yang baik, terutamanya peningkatan serapan foton serta penambah-baikan sifat angkutan. Oleh yang demikian, parameter dan sifat yang terlibat perlu dioptimakan dengan sebaiknya.

Disertasi ini menerangkan kesan komposisi campuran dan jenis bahan penerima yang digunakan terhadap ciri-ciri optik, struktur, morfologi serta sifat elektrik bagi tiga sistem hybrid BHJ berbeza. Bahan hybrid terdiri daripada campuran bahan jenis-p polimer berkonjugat (3-hexylthiophene) (P3HT) dan bahan jenis-n nanopartikel oksida logam bukan organik, iaitu zink oksida (ZnO), titanium dioksida (TiO₂) dan yttrium oksida (Y₂O₃). Pencirian optik, struktur dan morfologi dibincangkan bagi filem nipis campuran yang menggunakan spektroskopi serapan ultraungu-cahaya-nampak (UV-Vis), spektroskopi belauan sinar-X (XRD), mikroskop daya atom (AFM) dan mikroskop electron daya imbasan (FESEM). Malahan, hubung-kait antara sifat filem nipis dengan prestasi peranti juga dibentangkan. Dapatkan kajian menunjukkan bahawa prestasi peranti telah ditingkatkan dengan mengoptimumkan komposisi campuran. Ini disebabkan oleh peningkatan dalam penyerapan cahaya di rantau gelombang yang lebih luas dan meningkatnya angkutan cas melalui pembentukan laluan dwi-berterusan saling-menyusup untuk pergerakan lohong dan electron sampai ke elektrod. Hasil ini disokong oleh pemahatan terhadap imej AFM and FESEM yang mana terdapat peningkatan dalam nilai kekasaran RMS dan pembentukan pemisahan fasa dalam filem campuran. Selain itu, penyerakan nanopartikel bukan organik yang seragam dalam P3HT menghasilkan kawasan sempadan antara-fasa yang lebih luas untuk menjana pembawa cas. Antara tiga jenis sistem hybrid yang dikaji, peranti P3HT:ZnO memberikan prestasi terbaik dengan 3% nanopartikel ZnO di dalam komposisi campuran optimum.

Selanjutnya, sintesis sol-jel ZnO telah dijalankan bagi menghasilkan suatu campuran P3HT and ZnO yang lebih baik. Tambahan pula, beberapa pendekatan telah diambil, iaitu dengan mengubah isi kandungan sol dalam campuran, mempelbagaikan suhu pemanasan, dan memasukkan satu lapisan penampan ZnO di antara lapisan aktif dan katod. Rawatan pemanasan yang optimum menawarkan ciri-ciri penyerapan optik yang lebih baik dan permukaan morfologi filem yang lebih seragam dengan menghapuskan liang dan gumpalan besar. Peranan lapisan penampan ZnO dalam sistem campuran tersebut boleh dilihat sebagai suatu ejen yang memudahkan kutipan elektron dari lapisan aktif ke katod. Dapatkan kajian ini menunjukkan bahawa prestasi bagi peranti berasaskan P3HT:sol-jel ZnO yang disediakan pada komposisi campuran (0.1 ml sol) dan suhu pemanasan optimum pada 100°C dan mengandungi satu lapisan penampan ZnO, telah meningkat sebanyak 5 kali ganda berbanding dengan peranti berasaskan P3HT:nanopartikel ZnO.
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LIST OF SYMBOLS

> Less than
< More than
π Pi
σ Sigma
T Transmittance
A Absorbance
I₀ Light intensities
E Energy
λ Wavelength
d Interatomic spacing distance
θ Diffraction angle
Eₐ Energy gap
Δr Bond length alternation
I_SC Short-circuit current
V_OC Open circuit voltage
P_max Maximum power
P_out Output power
V_max Voltage at maximum power
I_max Current at maximum power
P_in Input power
FF Fill factor
η Power conversion efficiency
α Absorption coefficient
t Film thickness
B Full width at half maximum
t_c Crystallite size
C Scherrer constant
ε Strain
Λₑ Exciton diffusion length
Dₑ Exciton diffusion coefficient
τₑ Exciton lifetime
Rₐ Mean surface roughness
V_on Turn-on voltage
J_sc Short-circuit current density
R_sh Shunt resistance
R_s Series resistance
D/A Donor/Acceptor
J-V Current density-voltage
δ Dislocation density
T_a Annealing temperature
## Lists of Abbreviations

<table>
<thead>
<tr>
<th>Abbreviation</th>
<th>Description</th>
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<tbody>
<tr>
<td>BHJ</td>
<td>Bulk heterojunction</td>
</tr>
<tr>
<td>1-D</td>
<td>One dimensional</td>
</tr>
<tr>
<td>AFM</td>
<td>Atomic force microscopy</td>
</tr>
<tr>
<td>Ag</td>
<td>Silver</td>
</tr>
<tr>
<td>Al</td>
<td>Aluminum</td>
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<tr>
<td>AM 1.5</td>
<td>Air mass 1.5</td>
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<tr>
<td>Au</td>
<td>Gold</td>
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<tr>
<td>BL</td>
<td>Buffer layer</td>
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<tr>
<td>C₆₀</td>
<td>Buckminsterfullerene</td>
</tr>
<tr>
<td>Ca</td>
<td>Calcium</td>
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<tr>
<td>CB</td>
<td>Conduction band</td>
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<tr>
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<td>Cadmium selenide</td>
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<tr>
<td>CHCl₃</td>
<td>Chloroform</td>
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<tr>
<td>Cu</td>
<td>Copper</td>
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<tr>
<td>DEA</td>
<td>Diethanolamine</td>
</tr>
<tr>
<td>EDX</td>
<td>X-ray spectroscopy</td>
</tr>
<tr>
<td>FESEM</td>
<td>Field-effect scanning electron microscopy</td>
</tr>
<tr>
<td>FWHM</td>
<td>Full width at half maximum</td>
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<td>HCl</td>
<td>Hydrochloric acid</td>
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<td>HE</td>
<td>High energy</td>
</tr>
<tr>
<td>HOMO</td>
<td>Highest occupied molecular orbital</td>
</tr>
<tr>
<td>ITO</td>
<td>Indium tin oxide</td>
</tr>
<tr>
<td>JCPDS</td>
<td>Joint committee on powder diffraction standards</td>
</tr>
<tr>
<td>LE</td>
<td>Low energy</td>
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<tr>
<td>LUMO</td>
<td>Lowest unoccupied molecular orbital</td>
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<tr>
<td>MEH-PPV</td>
<td>Poly[2-methoxy-5-(2′-ethylhexyloxy)-p-phenylene vinylene]</td>
</tr>
<tr>
<td>MgPh</td>
<td>Magnesium phthalocyanine</td>
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<tr>
<td>NPs</td>
<td>Nanoparticles</td>
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<tr>
<td>OSCs</td>
<td>Organic solar cells</td>
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<tr>
<td>P3HT</td>
<td>Poly(3-hexylthiophene)</td>
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<tr>
<td>PbS</td>
<td>Plumbum sulfide</td>
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<tr>
<td>PCBDM.</td>
<td>[6,6]-phenyl-C₆₁-butyric acid methyl ester</td>
</tr>
<tr>
<td>PCE</td>
<td>Power conversion efficiency</td>
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<tr>
<td>PEDOT:PSS</td>
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<tr>
<td>PPP</td>
<td>Poly-para-phenylene</td>
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<td>PT</td>
<td>Poly(thiophene)</td>
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<td>PV</td>
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<td>RMS</td>
<td>Root-mean-square</td>
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<tr>
<td>rpm</td>
<td>Rotations per minute</td>
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<tr>
<td>SMU</td>
<td>Source measuring unit</td>
</tr>
<tr>
<td>STC</td>
<td>Standard test condition</td>
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<td>TiO₂</td>
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<td>UV-VIS-NIR</td>
<td>Ultraviolet-visible-near-infrared</td>
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<td>VB</td>
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