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Synergistic passivation of ZnO electron transport layer using 2D self-assembled monolayer and ZnO nanoparticles to improve stability of non-fullerene organic solar cells

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Organic solar cells (OSCs) have emerged as a promising next generation source of green energy due to some desirable properties such as low-cost fabrication, mechanical flexibility, and tunable opto-electronic properties [1]. Despite achieving power conversion efficiencies around 20%, the limited long-term stability of the multi-layer OSCs remains a major challenge for the full commercialization [2]. Herein, we have investigated the role of Zinc Oxide (ZnO) electron transporting layer (ETLs) and their modification strategies to improve device performance and stability. ZnO films were prepared using sol-gel method and further modified with 2D self-assembled monolayers (SAM) and ZnO nanoparticle (ZnONP) as a bi-layer to suppress the ZnO ETL interfacial defect states and improve interface contacts at the ETL and photo-active layer. Devices were characterized using current-voltage measurements, Raman spectroscopy, intensity modulated photo-current and photo-voltage (IMPS and IMVS), and impedance spectroscopy. Stability tests were measured after one-week of dark storage without encapsulation. Optical and electrical characterization techniques revealed that the synergistic effect of ZnO nanoparticles and SAM surface passivation effectively reduced carrier recombination, resulting in a 14% increase in efficiency compared to the pristine ZnO ETL-based OSC device. More importantly, devices with modified ZnO ETLs retained over 80% of their initial efficiency whereas the pristine ZnO ETLs based device were degraded significantly. These results highlight the critical role of interface engineering in stabilizing OSCs and provide a practical pathway toward their large-scale application.

Keywords: Organic solar cells, electron transporting layer, Sol-gel ZnO, Surface passivation, impedance spectroscopy, IMPS/IMVS

References

1. Li, S., Li, Z., Wan, X., & Chen, Y. Recent progress in flexible organic solar cells *eScience* 2023, 3, 100085.
2. Ding, P., Yang, D., Yang, S., & Ge, Z. (2024). Stability of organic solar cells: toward commercial applications. *Chemical Society Reviews*, 53(5), 2350-2387.

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