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Full Length Article

Enhanced performance of p-i-n perovskite solar cell via defect passivation of nickel oxide/perovskite interface with self-assembled monolayer

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ABSTRACT

The thin film of nickel oxide (NiO_x) nanoparticles was successfully applied as the hole transporting layer (HTL) in inverted (p-i-n) perovskite solar cells (PSCs), but inevitable surface defects and hydroxyl groups present on the NiO_x surface are limiting of performance and stability improvements. For overcome these problems, we introduce 3-(Triethoxysilyl)propylamine (TSPA), self-assembly molecule, as an interfacial modifier between NiO_x and perovskite film to attenuate the surface defect and prevent deterioration caused by direct contact of the hydroxyl groups and the perovskite. Self-assembled monolayer is formed by hydrogen-bond between amino group of TSPA and hydroxyl group on the surface of the NiO_x, which passivate surface and reduce defect density. In addition, a positive dipole was formed by the TSPA monolayer, which resulted in deeper work function at the NiO_x interface and improved energy level alignment in PSCs, improving charge extraction-transportation capabilities and reducing recombination of charge carriers at the interface. In consequence, PSCs based on NiO_x with TSPA monolayer have boosted PCE by up to 20.21% and showed long-term stability over 60 days under ambient air and varying humidity condition. This approach is expected to be further advanced as one of the methods for the development of high-performance PSCs.

1. Introduction

In past decades, due to the outstanding optoelectronic properties like as long carrier diffusion duration, superior carrier mobility, and extreme light absorption coefficient, solution-processable organometal halide-based perovskite has been considered to be an encouraging candidate for future photovoltaic applications [1–4]. The power conversion efficiency (PCE) of perovskite solar cells (PSCs) reached up to 25.5% quickly, which is close to previous generations of solar cells [5]. Furthermore, PSCs can offer a variety of application possibilities and options resulting from the solution process. In particular, the low-temperature and solution processable p-i-n PSCs are believed to enable convenient fabrication of flexible thin film and large-area solar cells [6,7].

However, despite these advantages, achieving high efficiency in PSCs is still hampered by losses in incomplete interfaces [8–11]. For this reason, many researchers focused their effort to improve interfacial properties and reduce interfacial loss. A variety of p-type semiconductors including organic and inorganic materials have been applied as a hole transporting layer (HTL) for resolving this problem. For instant, organic p-type semiconductors that is poly (N,N′-bis-4-butylphenyl-N,N′ bisphenyl) benzidine (Poly-TPD), poly [bis (4-phenyl) (2,4,6-trimethylphenyl) amine (PTAA), and poly(3,4-ethylenedioxythiophene)-poly (styrenesulfonate) (PEDOT:PSS) were introduced into PSCs and showed efficiency over 18% [12–15]. Wang tried to reduce the defect state of the interface by introducing functional organic molecules between HTL and perovskite as interface modifiers, and as a result improved efficiency by improving interface charging transportation [16]. On the other hand, inorganic HTLs capable of solution processing have been studied in consideration of the large expense and/or poor stability of the organic material that can interfere with the practical application [8,17,18]. PSCs with inorganic semiconductive HTLs like as NiO_x, CuSCN, and CuI have been stated to have better stability than organic semiconductor materials [19–21]. In addition, when inorganic semiconductive MoO_3 was introduced into the interface between the organic HTL and perovskite, it was reported that the efficiency was improved by reducing charge recombination and at the same time the stability of the device is greatly improved [22].

Among such inorganic semiconductor materials, especially, NiO_x is considered as a promising HTL; the wide bandgap (3.6–4.0 eV) and deep

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